

Dinuclear zinc(II) complexes of symmetric Schiff-base ligands with extended quinoline sidearms

Dipesh Prema, Alexander V. Wiznycia, Benjamin M. T. Scott, Jessica Hilborn, John Desper and Christopher J. Levy*

Supplemental Material: NMR, UV-Vis, and ECD spectra.

Note: compound are identified by the number given at the top of each page, not necessarily by numbers assigned in figures.

^1H and ^{13}C Spectra of **1** in CDCl_3

STANDARD ^1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-64

UNITYplus-400 "bones"

Relax. delay 2.000 sec

Pulse 9.5 degrees

Acq. time 3.700 sec

Width 8000.0 Hz

32 repetitions

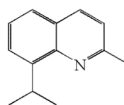
OBSERVE ^1H , 399.8248996 MHz

DATA PROCESSING

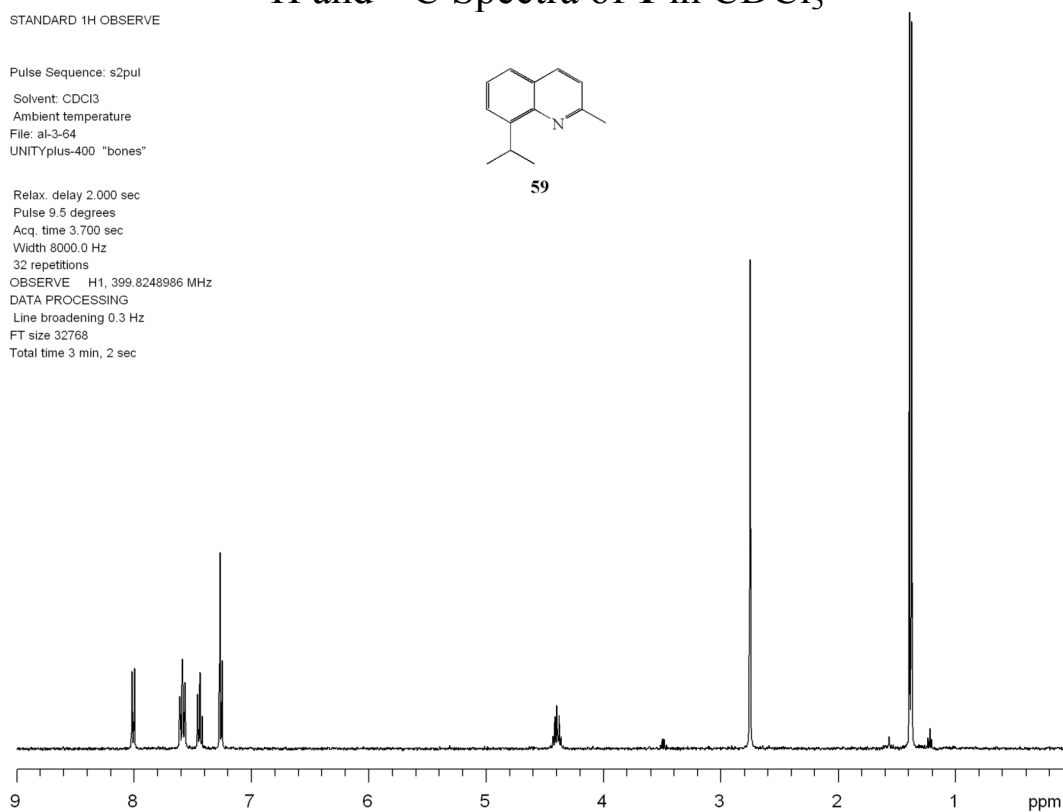
Line broadening 0.3 Hz

FT size 32768

Total time 3 min, 2 sec



59



^{13}C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-64

UNITYplus-400 "bones"

Relax. delay 2.000 sec

Pulse 90.0 degrees

Acq. time 1.199 sec

Width 25000.0 Hz

14208 repetitions

OBSERVE ^{13}C , 100.5294741 MHz

DECOUPLE ^1H , 399.8008479 MHz

Power 45 dB

continuously on

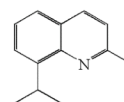
WALTZ-16 modulated

DATA PROCESSING

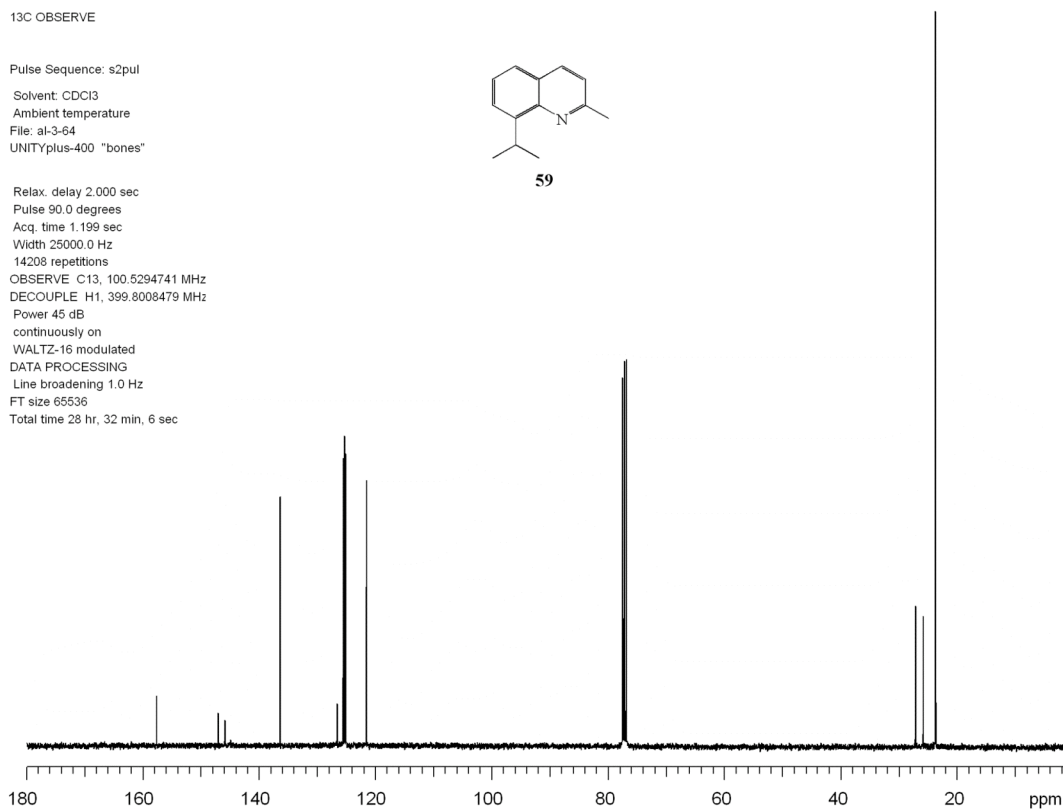
Line broadening 1.0 Hz

FT size 65536

Total time 28 hr, 32 min, 6 sec



59



^1H and ^{13}C Spectra of **2** in CDCl_3

STANDARD ^1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-75

UNITYplus-400 "bones"

Relax. delay 1.000 sec

Pulse 27.3 degrees

Acq. time 3.701 sec

Width 5000.0 Hz

32 repetitions

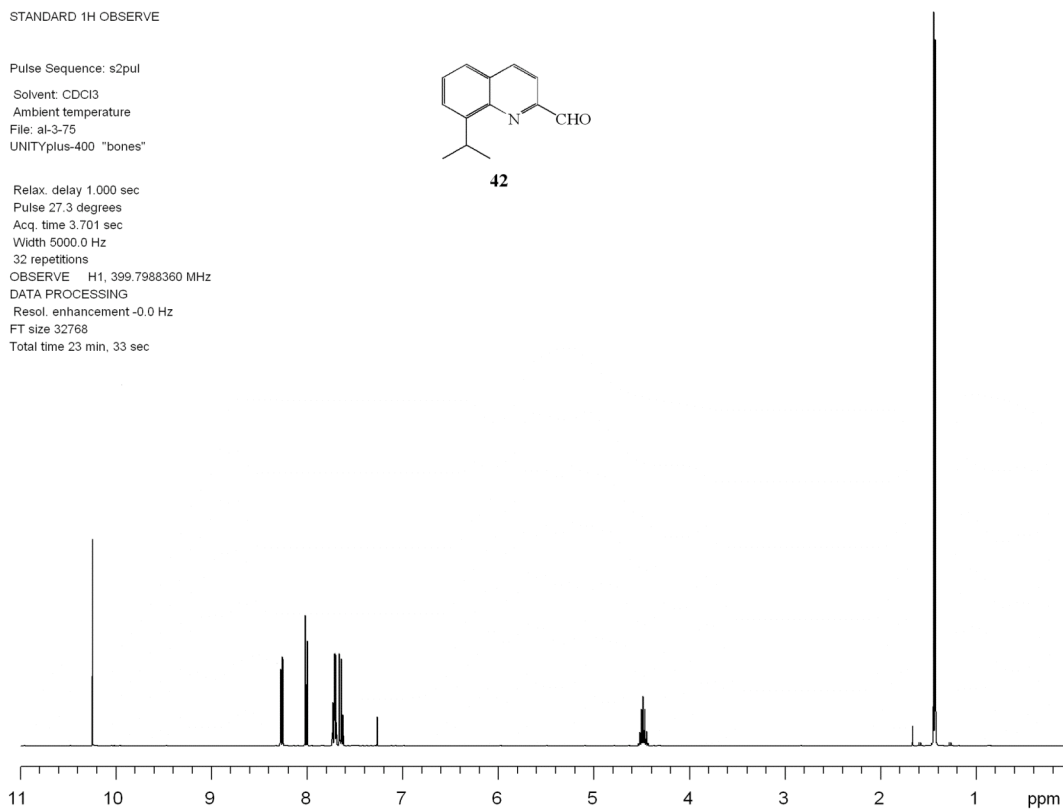
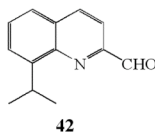
OBSERVE ^1H , 399.798360 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

FT size 32768

Total time 23 min, 33 sec



^{13}C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-75

UNITYplus-400 "bones"

Relax. delay 2.000 sec

Pulse 90.0 degrees

Acq. time 1.199 sec

Width 25000.0 Hz

13008 repetitions

OBSERVE ^{13}C , 100.5294764 MHz

DECOUPLE ^1H , 399.8008479 MHz

Power 45 dB

continuously on

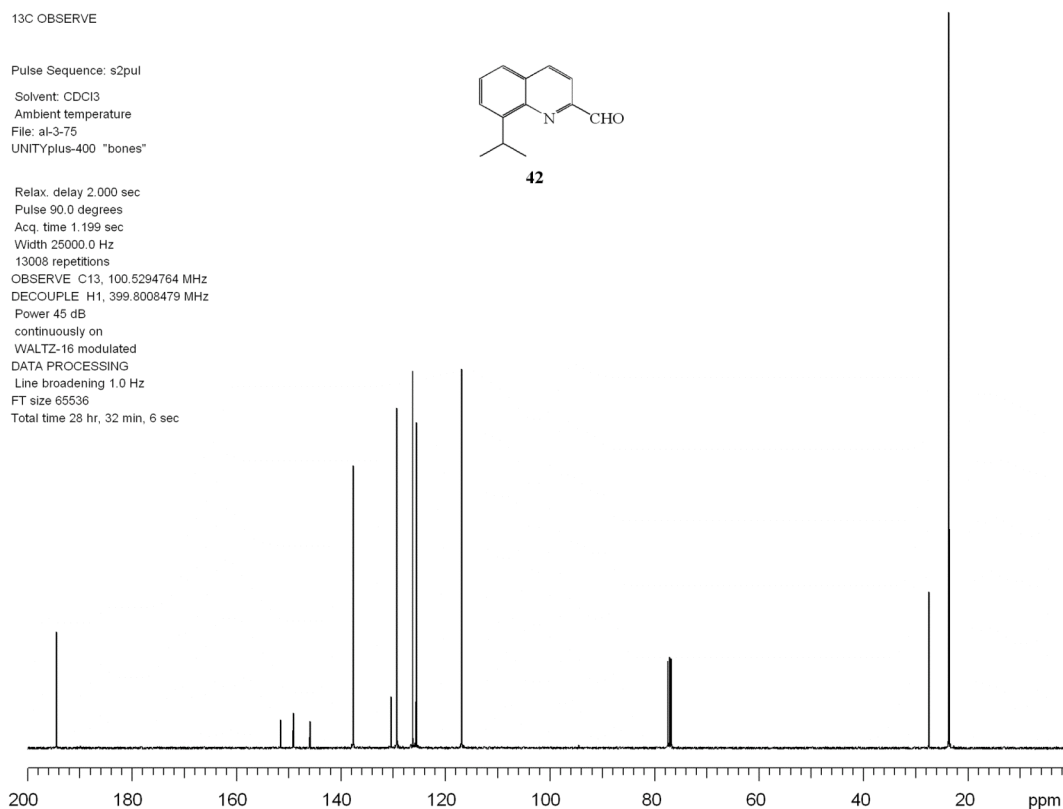
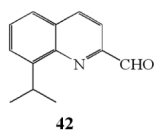
WALTZ-16 modulated

DATA PROCESSING

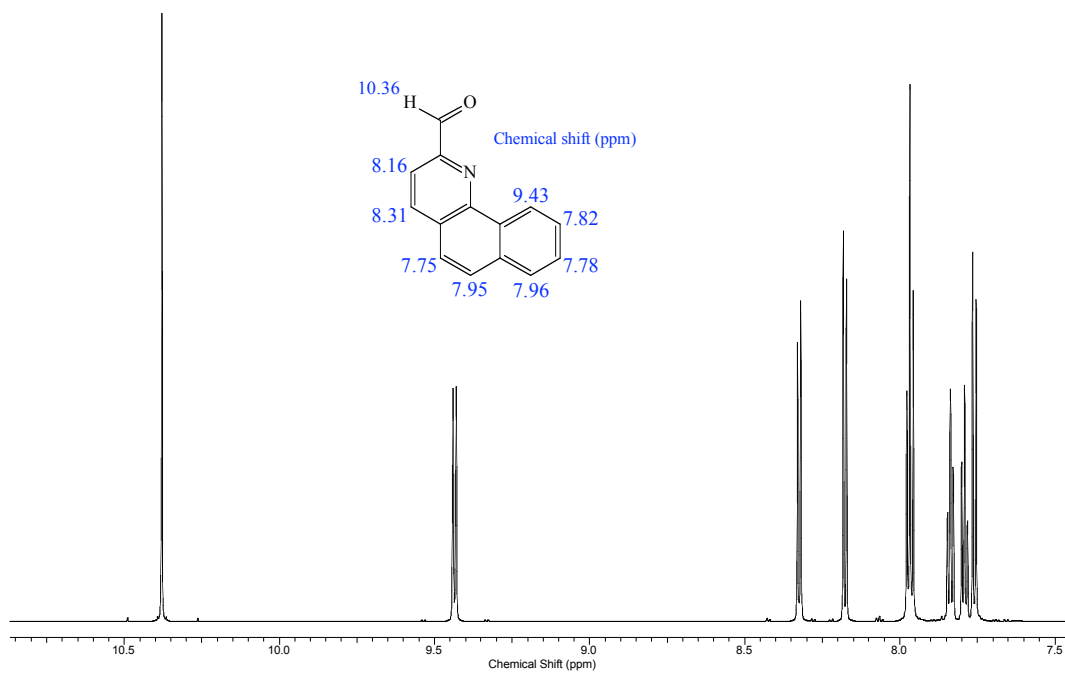
Line broadening 1.0 Hz

FT size 65536

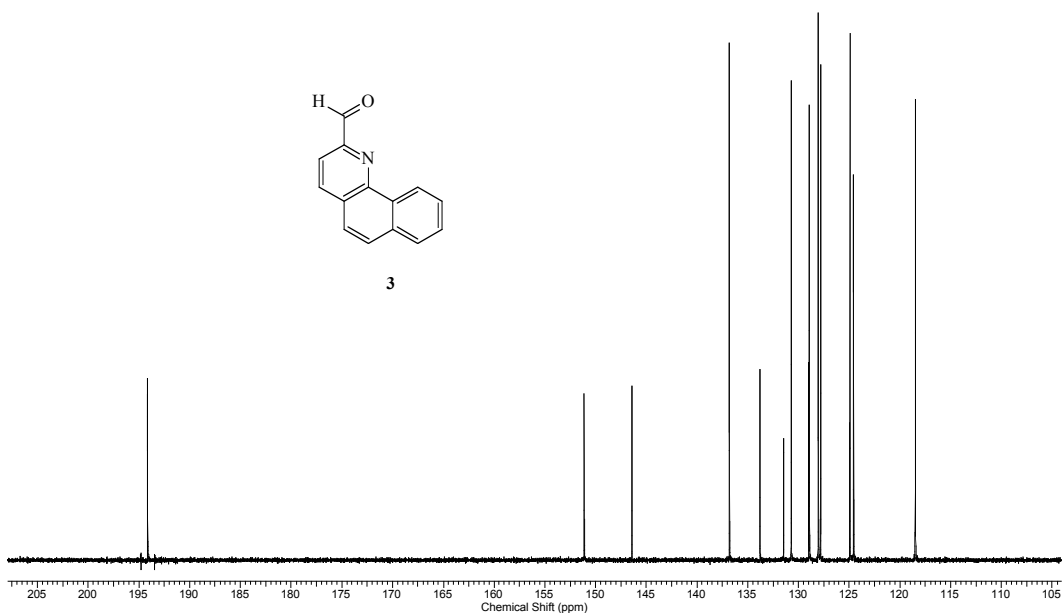
Total time 28 hr, 32 min, 6 sec



^1H and ^{13}C Spectra of **4** in CDCl_3



Acquisition Time (sec)	0.6802	Date	24 Nov 2006 18:37:52	Date Stamp	24 Nov 2006 18:37:52
File Name		Number of Transients	1032	Origin	spect
Nucleus	^{13}C	Points Count	32768	Pulse Sequence	zgpg30
Owner	nmisu	Solvent	CHLOROFORM-d	Receiver Gain	32768.00
SW(cyclical) (Hz)	48076.92	Temperature (degree C)	25.000	Spectrum Offset (Hz)	20121.3398
Sweep Width (Hz)	48075.45				



^1H Spectrum of (*R,R*)-**5** in CDCl_3

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-188

UNITYplus-400 "bones"

Relax. delay 1.000 sec

Pulse 27.3 degrees

Acq. time 3.701 sec

Width 6000.6 Hz

40 repetitions

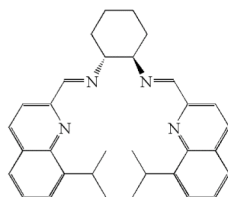
OBSERVE H1, 399.798363 MHz

DATA PROCESSING

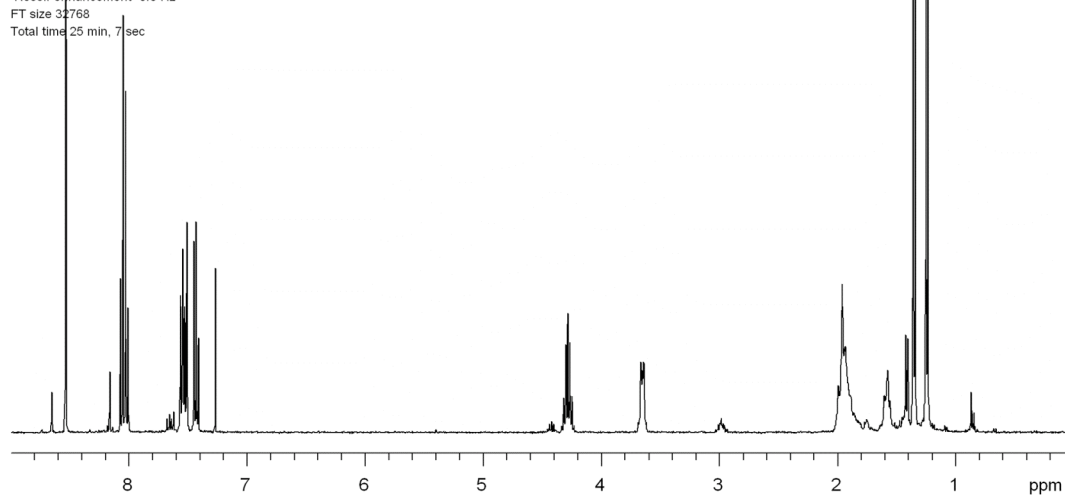
Resol. enhancement -0.0 Hz

FT size 32768

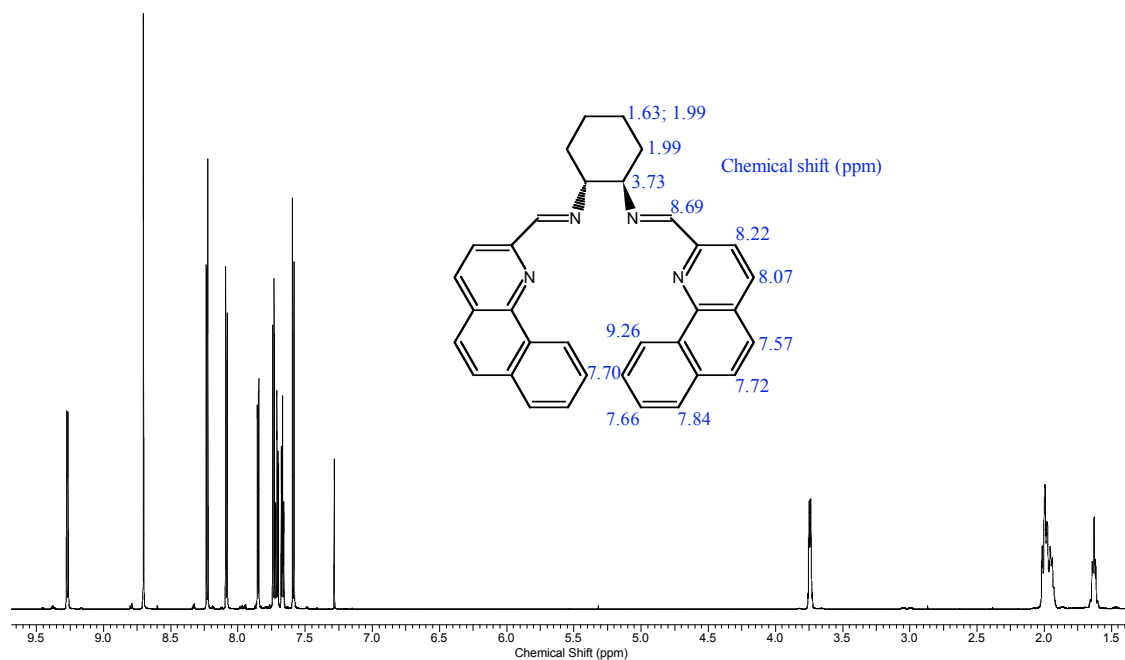
Total time 25 min, 7 sec



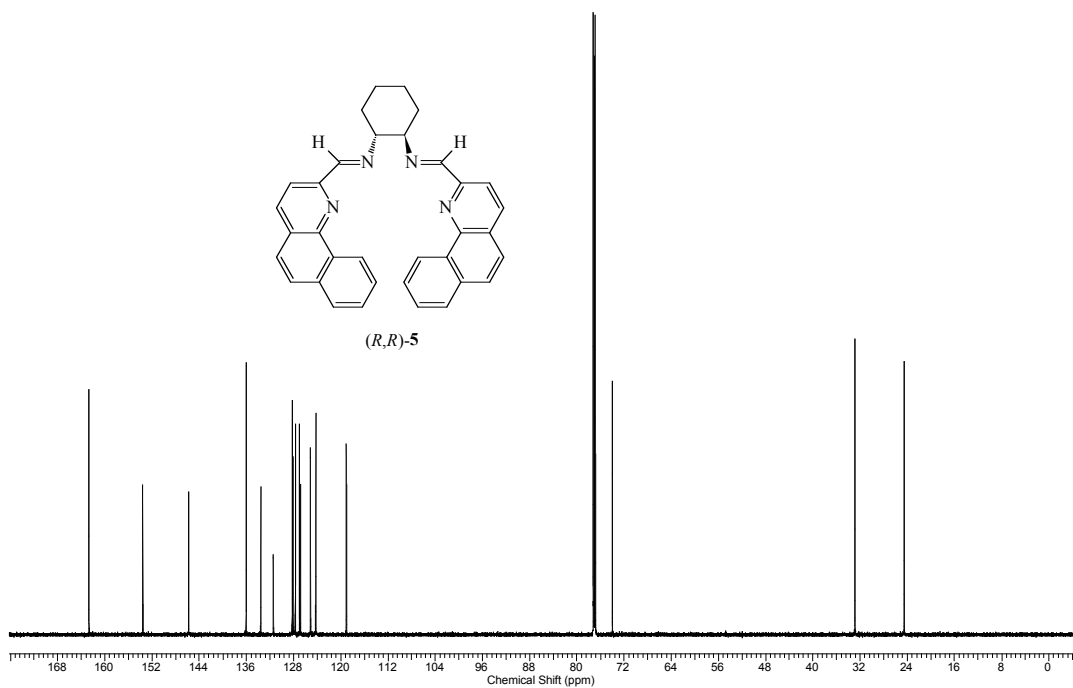
(*R,R*)-**35**



^1H and ^{13}C Spectra of (*R, R*)-6 in CDCl_3



Acquisition Time (sec)	0.6802	Date	21 Nov 2006 21:20:00	Date Stamp	21 Nov 2006 21:20:00
File Name		Nucleus	^{13}C	Number of Transients	512
Frequency (MHz)	201.22	Owner	nmr@su	Points Count	32768
Original Points Count	32701	SW(cyclical) (Hz)	48076.92	Solvent	CHLOROFORM-d
Receiver Gain	32768.00	Sweep Width (Hz)	48075.45	Temperature (degree C)	25.000
Spectrum Offset (Hz)	20121.3398				



^1H and ^{13}C Spectra of (*R*)-7 in CDCl_3

^{13}C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-178

UNITYplus-400 "bones"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 1.199 sec

Width 25000.0 Hz

12000 repetitions

OBSERVE C13, 100.6343867 MHz

DECOUPLE H1, 399.8203907 MHz

Power 45 dB

continuously on

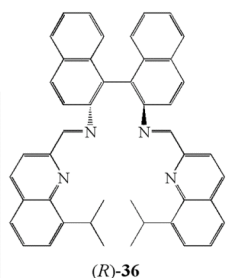
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 22 min, 2 sec



180 160 140 120 100 80 60 40 20 ppm

STANDARD ^1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-178

UNITYplus-400 "bones"

Relax. delay 1.000 sec

Pulse 90.0 degrees

Acq. time 3.701 sec

Width 6000.6 Hz

56 repetitions

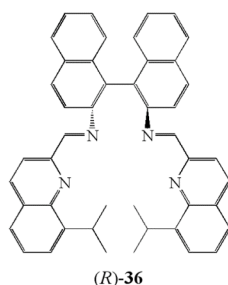
OBSERVE H1, 399.8183757 MHz

DATA PROCESSING

Resol. enhancement -0.0 Hz

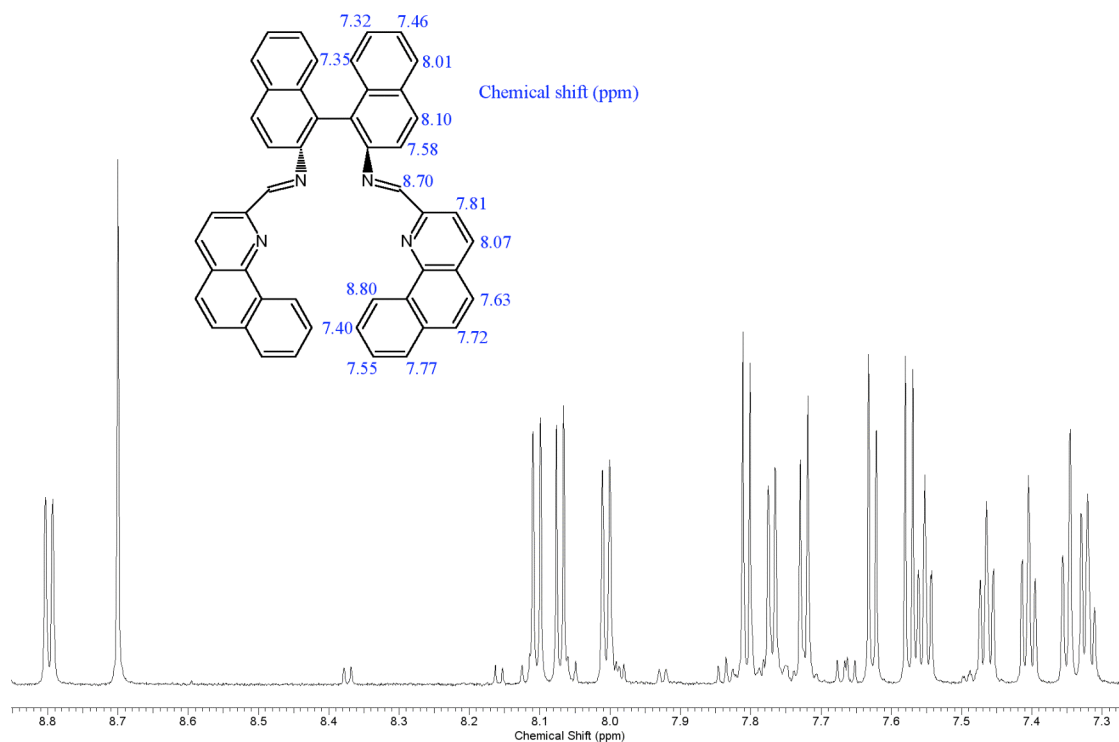
FT size 32768

Total time 25 min, 7 sec

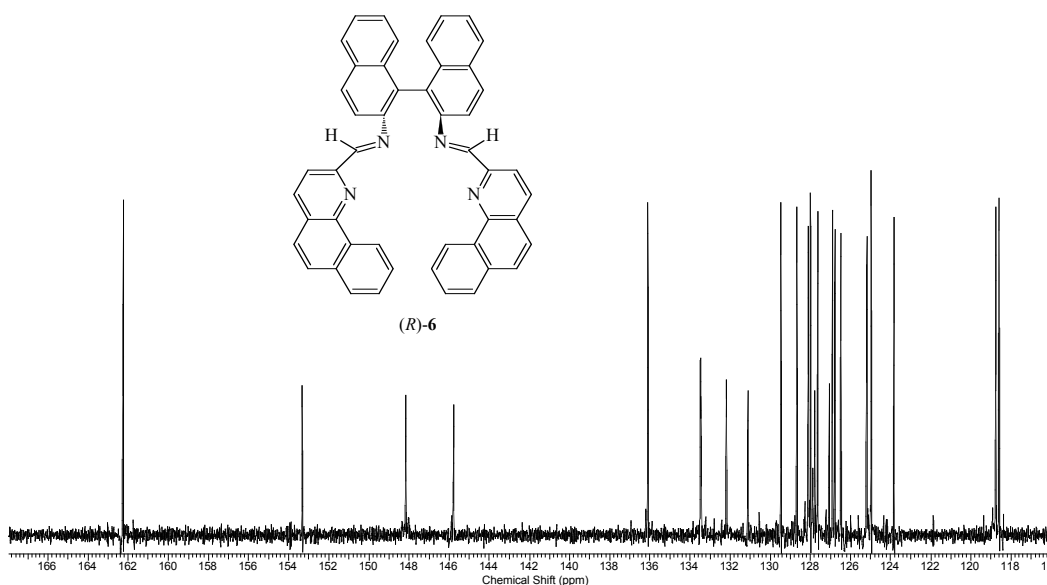


9 8 7 6 5 4 3 2 1 ppm

^1H and ^{13}C Spectra of (*R*)-**8** in CD_2Cl_2



Acquisition Time (sec)	0.6802	Date	22 Nov 2006 20:35:12	Date Stamp	22 Nov 2006 20:35:12
File Name		Nucleus	^{13}C	Number of Transients	2000
Frequency (MHz)	201.22	Owner	nmrsu	Points Count	32768
Original Points Count	32701	SW(cyclical) (Hz)	48076.92	Solvent	DICHLOROMETHANE-d2
Receiver Gain	32768.00	Sweep Width (Hz)	48075.45	Temperature (degree C)	25.000
Spectrum Offset (Hz)	20121.3398				



^1H and ^{13}C Spectra of (*R,R*)-**9** in CDCl_3

^{13}C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-190

UNITYplus-400 "bones"

Pulse 90.0 degrees

Acq. time 1.199 sec

Width 25000.0 Hz

30096 repetitions

OBSERVE C13, 100.5343844 MHz

DECOUPLE H1, 399.8203910 MHz

Power 45 dB

continuously on

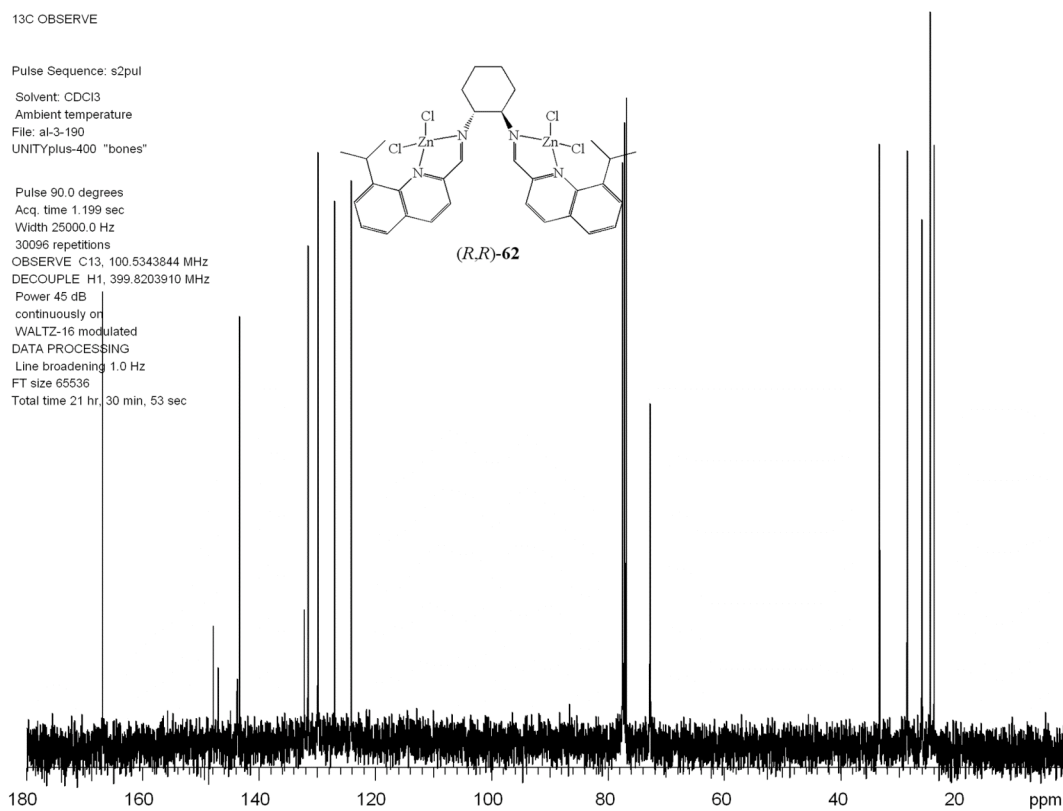
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 21 hr, 30 min, 53 sec



STANDARD ^1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl_3

Ambient temperature

File: al-3-190

UNITYplus-400 "bones"

Relax. delay 1.000 sec

Pulse 27.3 degrees

Acq. time 3.701 sec

Width 6000.6 Hz

532 repetitions

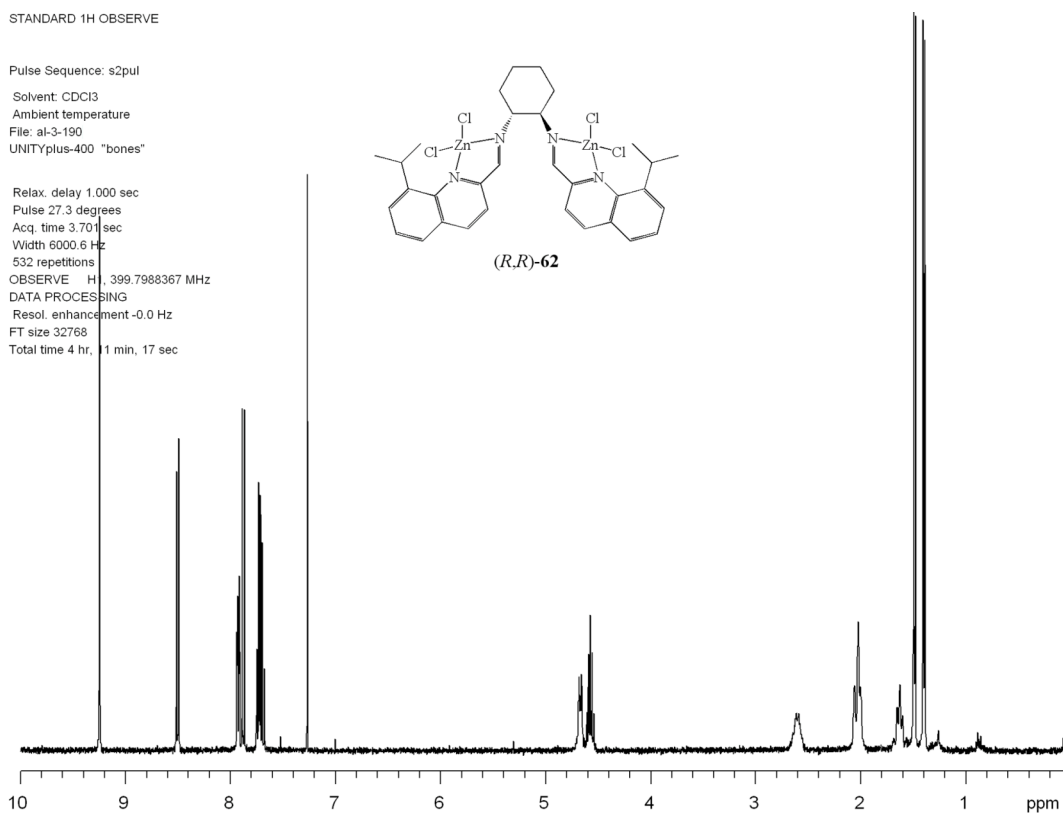
OBSERVE H1, 399.7988367 MHz

DATA PROCESSING

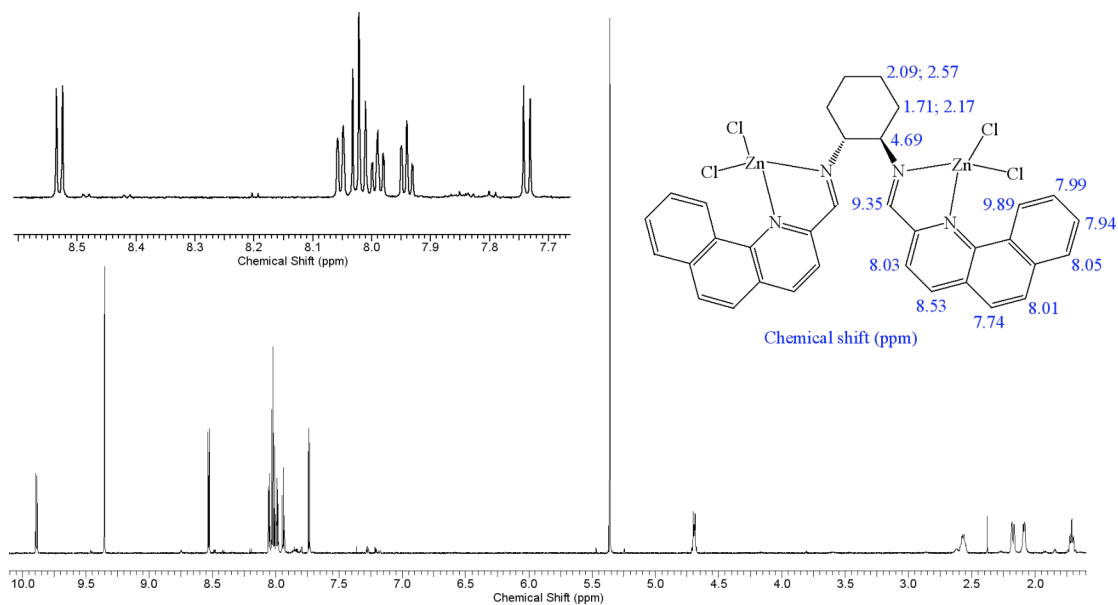
Resol. enhancement -0.0 Hz

FT size 32768

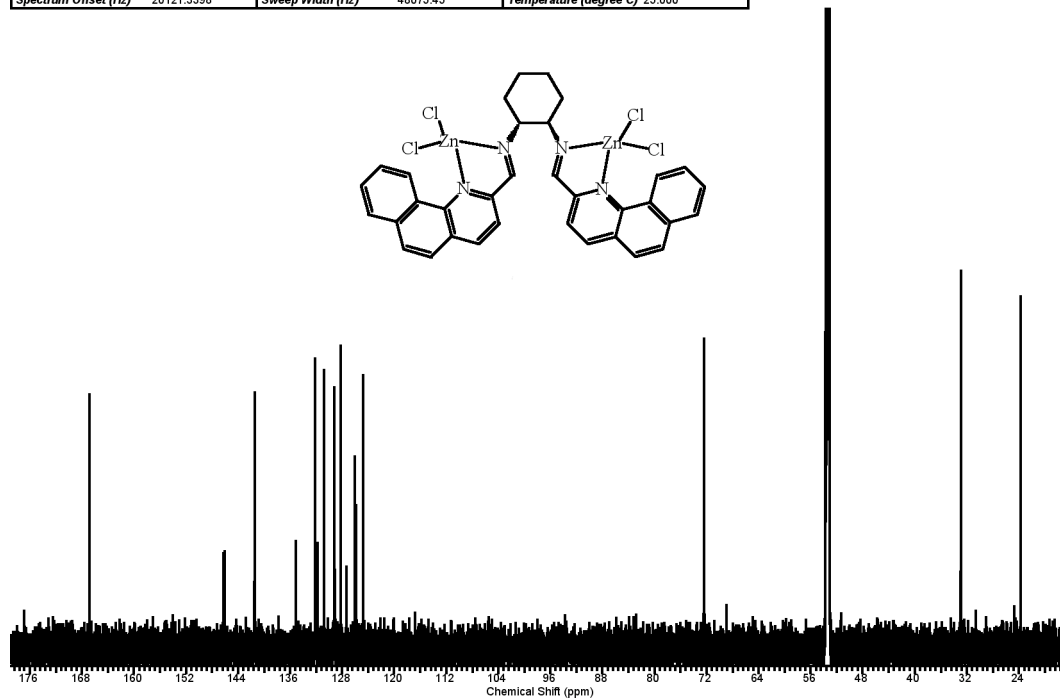
Total time 4 hr, 11 min, 17 sec



¹H and ¹³C Spectra of (R, R)-**10** in CD₂Cl₂



Acquisition Time (sec)	0.6802	Date	22 Nov 2006 17:10:24	Date Stamp	22 Nov 2006 17:10:24
File Name					
Frequency (MHz)	201.22	Nucleus	¹³ C	Number of Transients	1024
Original Points Count	32701	Owner	nmrsu	Points Count	32768
Receiver Gain	32768.00	SW(cyclical) (Hz)	48076.92	Solvent	DICHLOROMETHANE-d2
Spectrum Offset (Hz)	20121.3398	Sweep Width (Hz)	48075.45	Temperature (degree C)	25.000

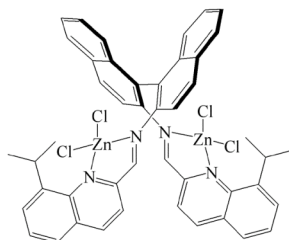


^1H and ^{13}C Spectra of (*R,R*)-11 in CDCl_3

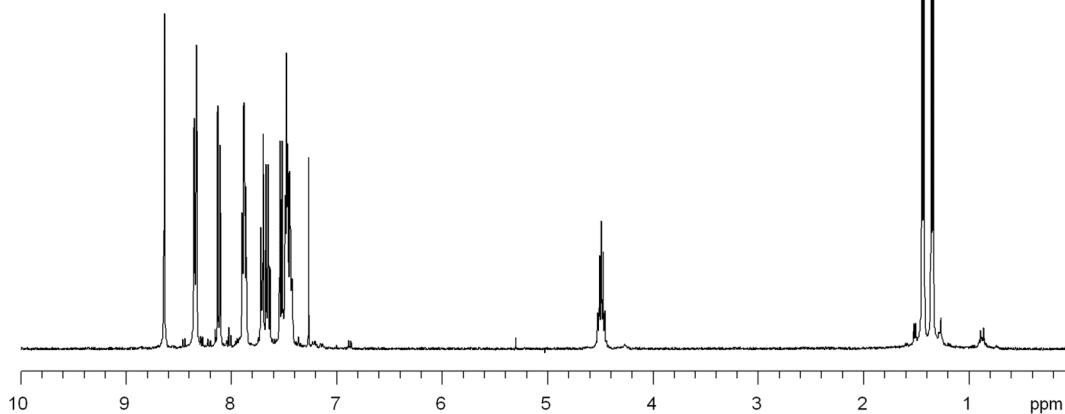
STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl_3
Ambient temperature
File: al-3-163
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
224 repetitions
OBSERVE H1, 399.7988363 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 4 hr, 11 min, 17 sec



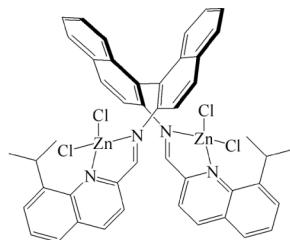
(*R,R*)-63



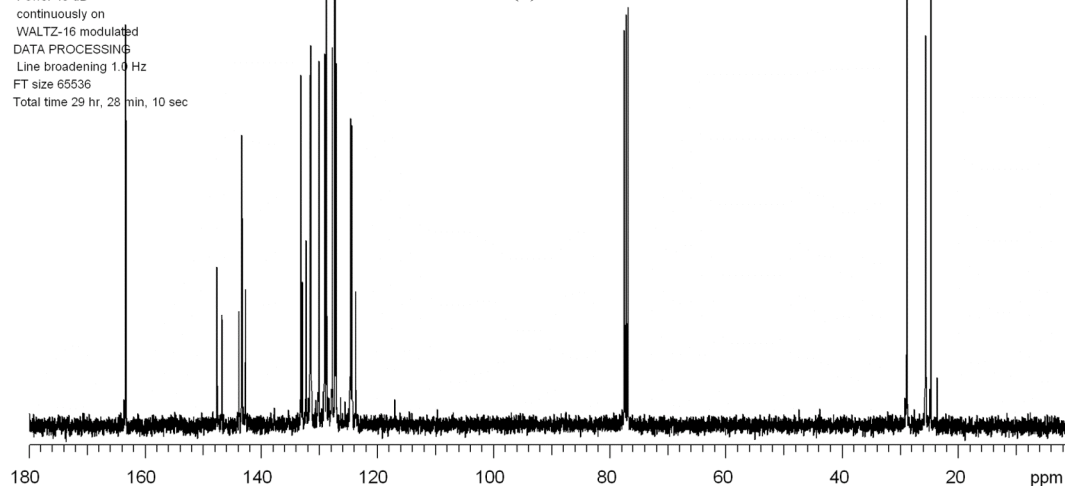
^{13}C OBSERVE

Pulse Sequence: s2pul
Solvent: CDCl_3
Ambient temperature
File: al-3-163
UNITYplus-400 "bones"

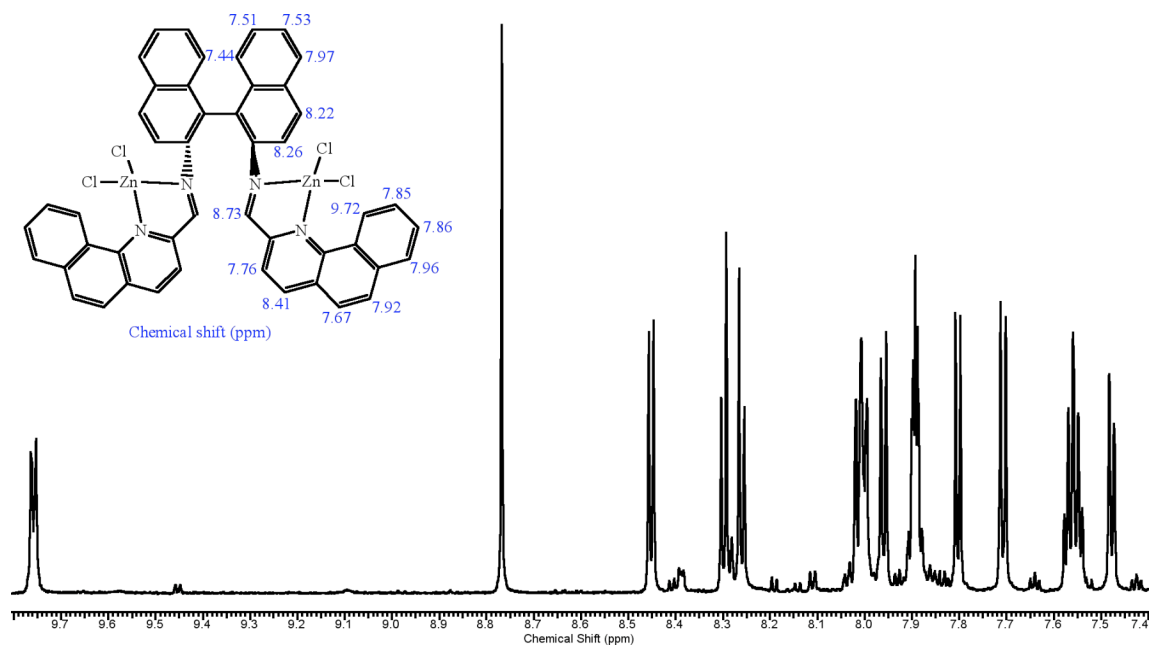
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
27616 repetitions
OBSERVE C13, 100.5294718 MHz
DECOUPLE H1, 399.8008479 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 29 hr, 28 min, 10 sec



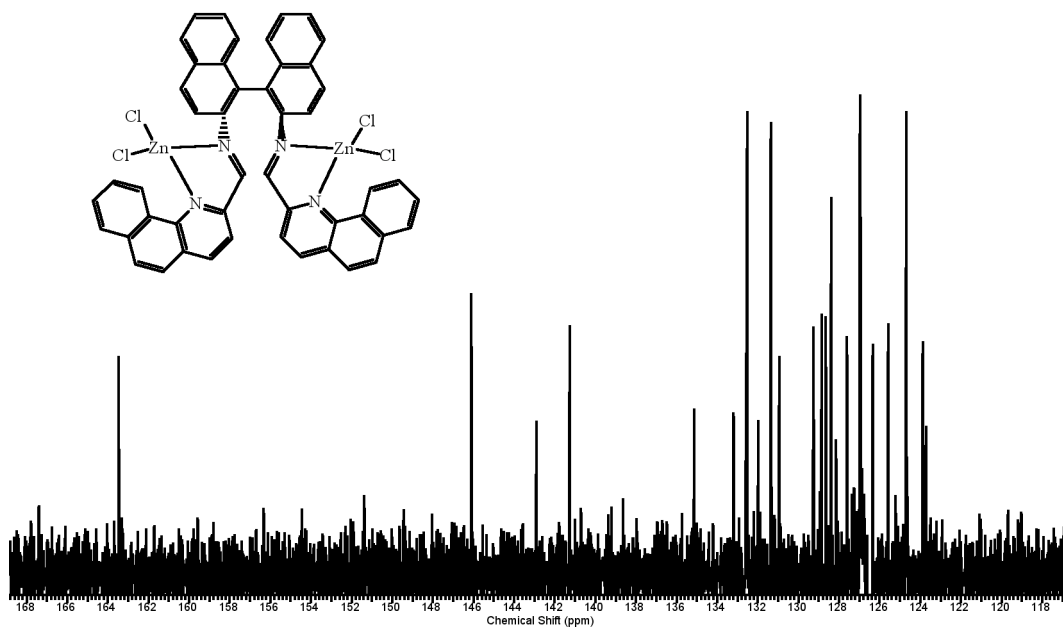
(*R,R*)-63

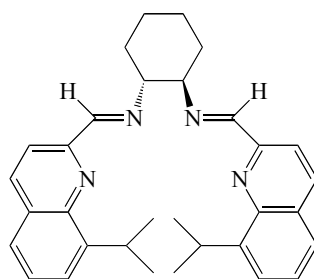


^1H and ^{13}C Spectra of (*R, R*)- **12** in CD_2Cl_2



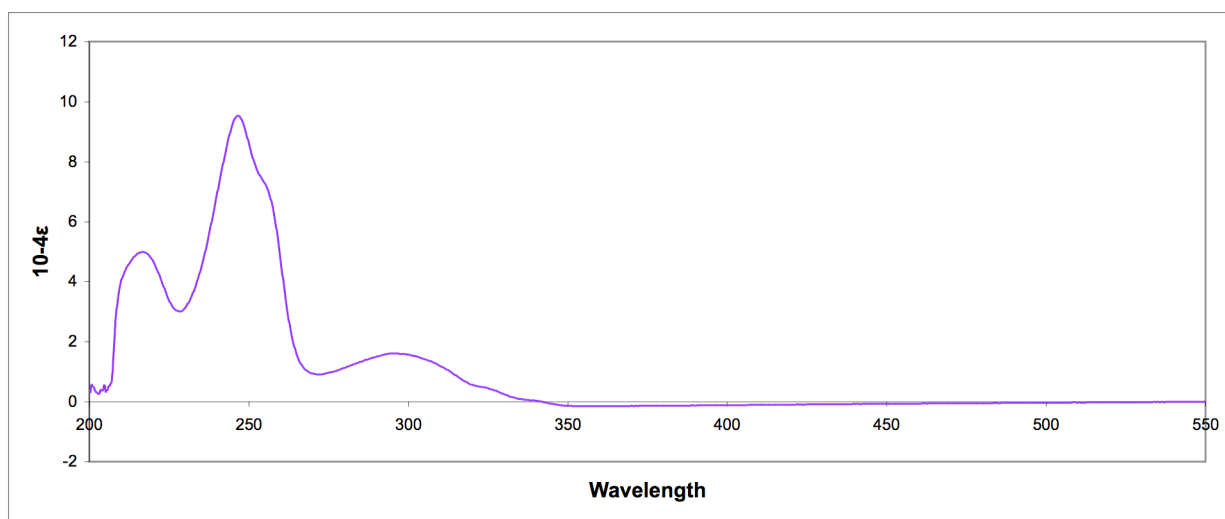
Acquisition Time (sec)	0.6802	Date	23 Nov 2006 18:05:52	Date Stamp	23 Nov 2006 18:05:52
File Name				Frequency (MHz)	201.22
Nucleus	^{13}C	Number of Transients	1024	Origin	spect
Owner	nmrsu	Points Count	32768	Pulse Sequence	zgpg30
SW(cyclical) (Hz)	48076.92	Solvent	DICHLOROMETHANE-d2	Receiver Gain	32768.00
Sweep Width (Hz)	48076.45	Temperature (degree C)	25.000	Spectrum Offset (Hz)	20121.3398



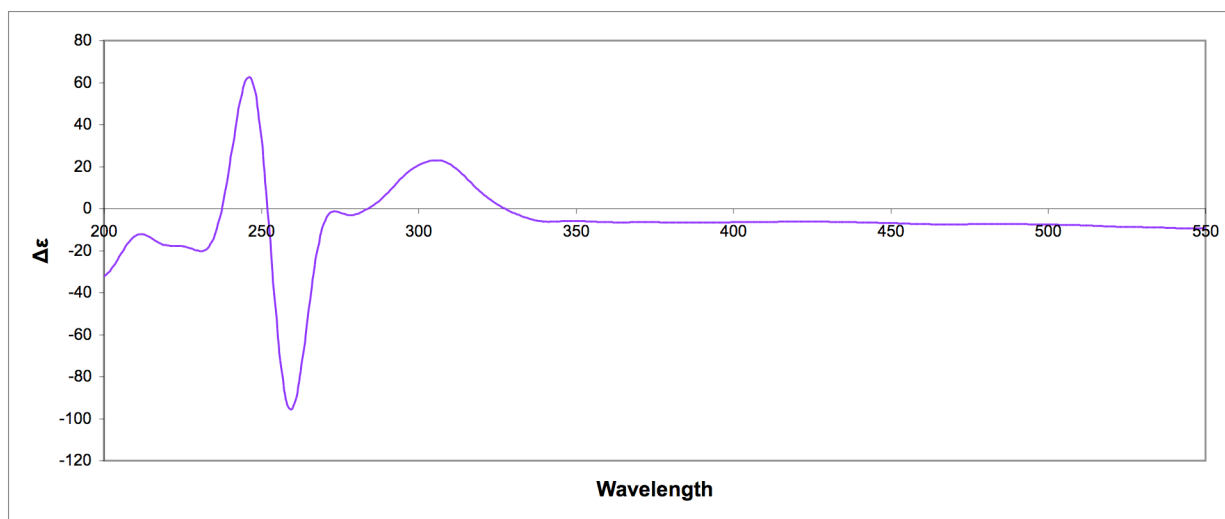


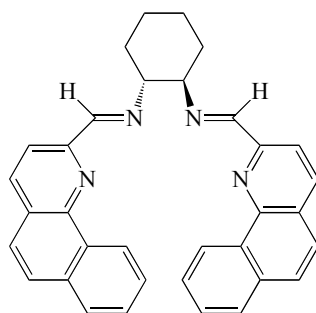
(*R,R*)-**5**

UV-Vis spectrum of (*R,R*)-**5** (2.5×10^{-5} M in THF)



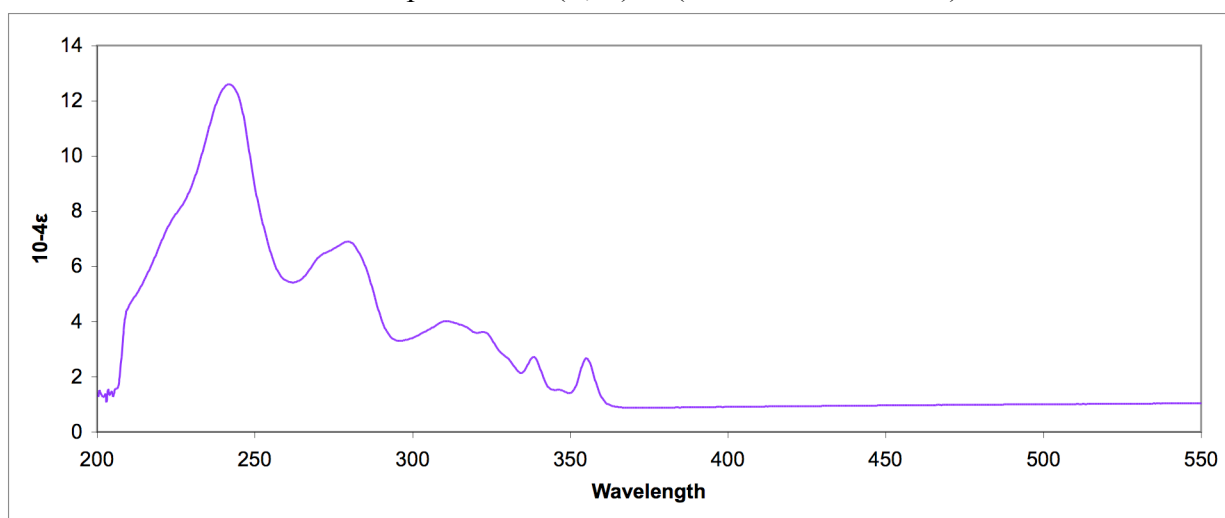
ECD spectrum of (*R,R*)-**5** (2.5×10^{-5} M in THF)



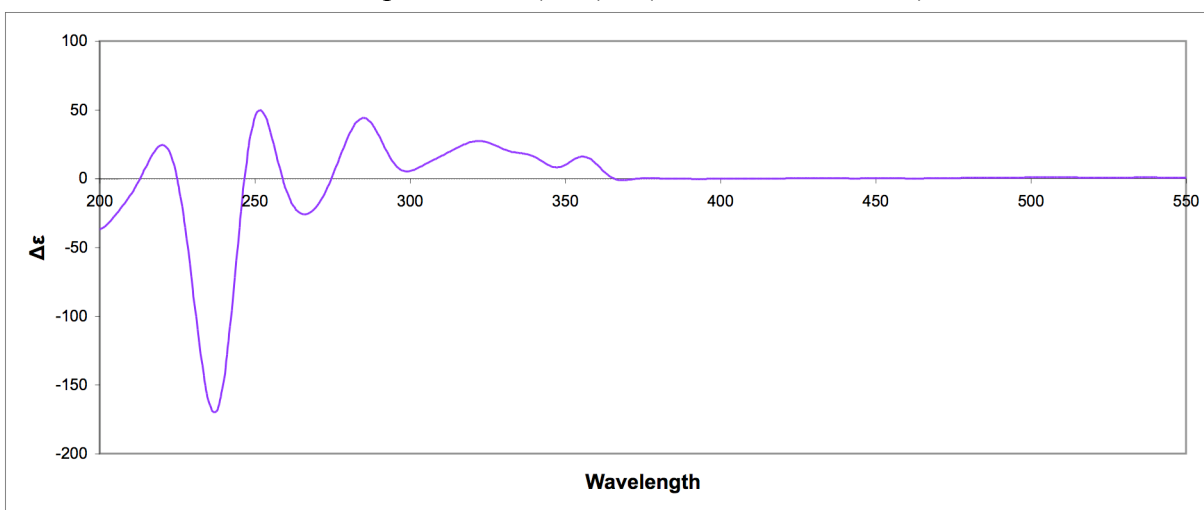


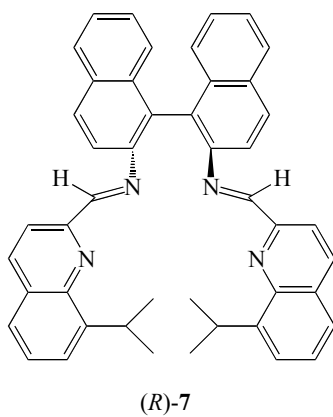
(*R,R*)-**6**

UV-Vis spectrum of (*R,R*)-**6** (1.0×10^{-5} M in THF)

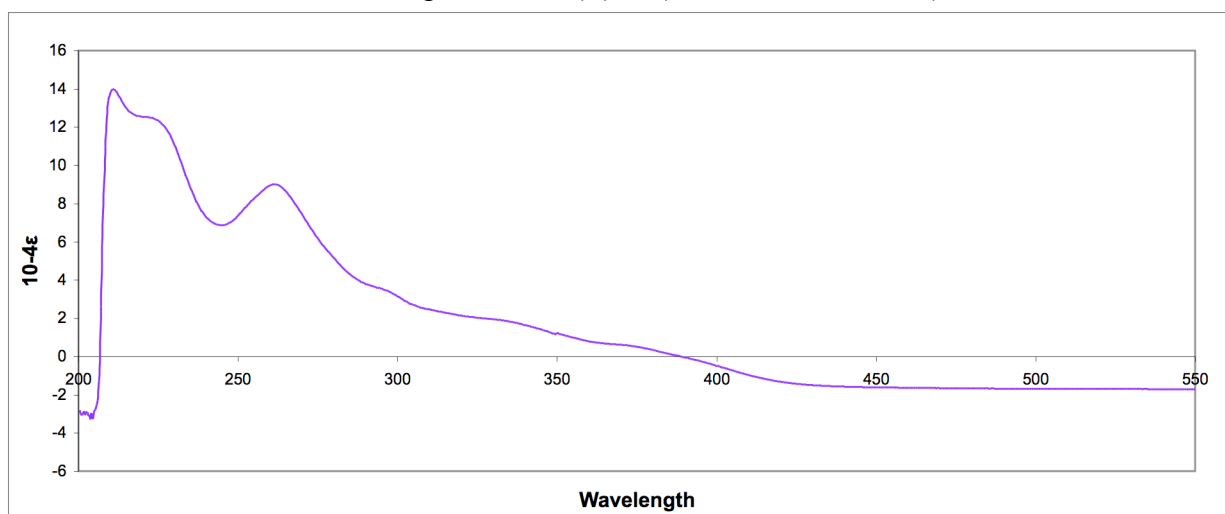


ECD spectrum of (*R,R*)-**6** (2.5×10^{-5} M in THF)

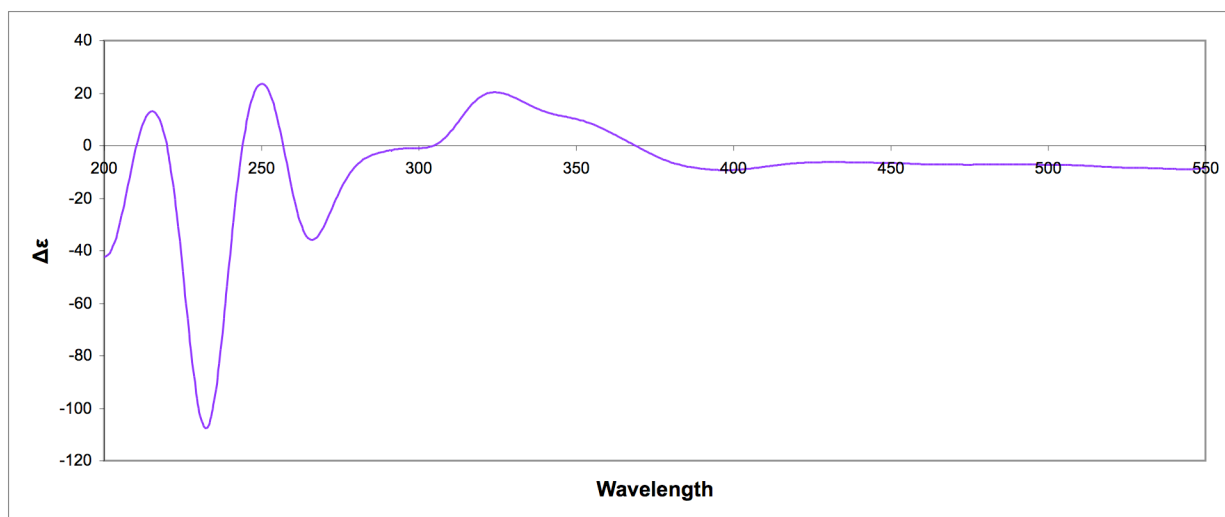


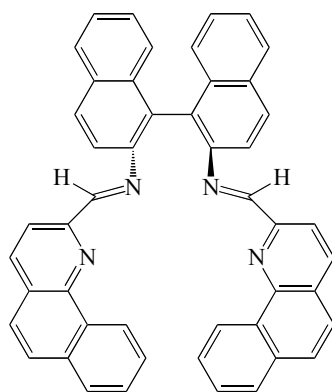


UV-Vis spectrum of *(R)*-7 (1.0×10^{-5} M in THF)



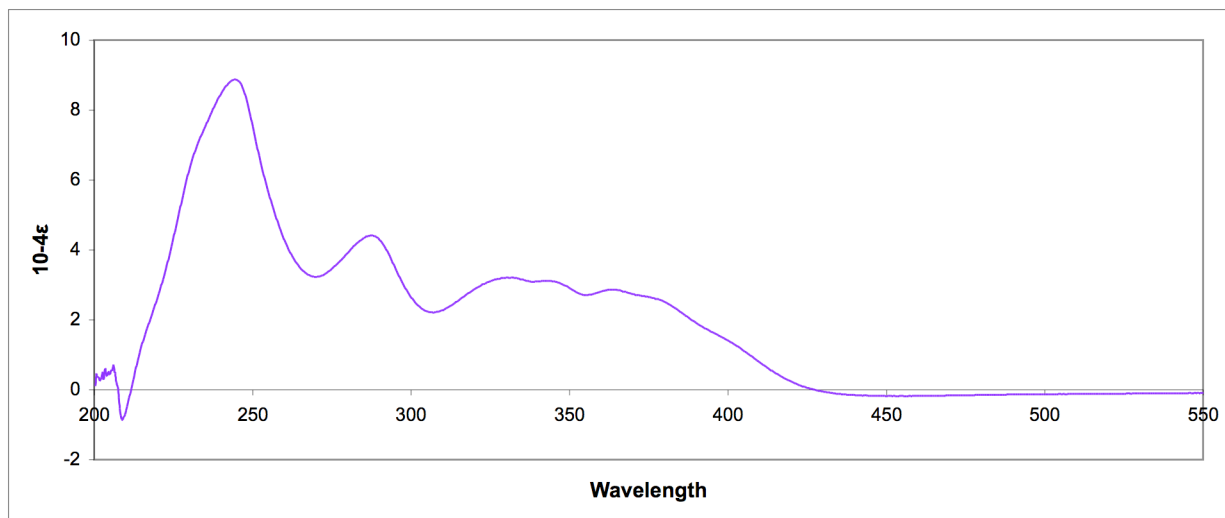
ECD spectrum of *(R)*-7 (2.5×10^{-5} M in THF)



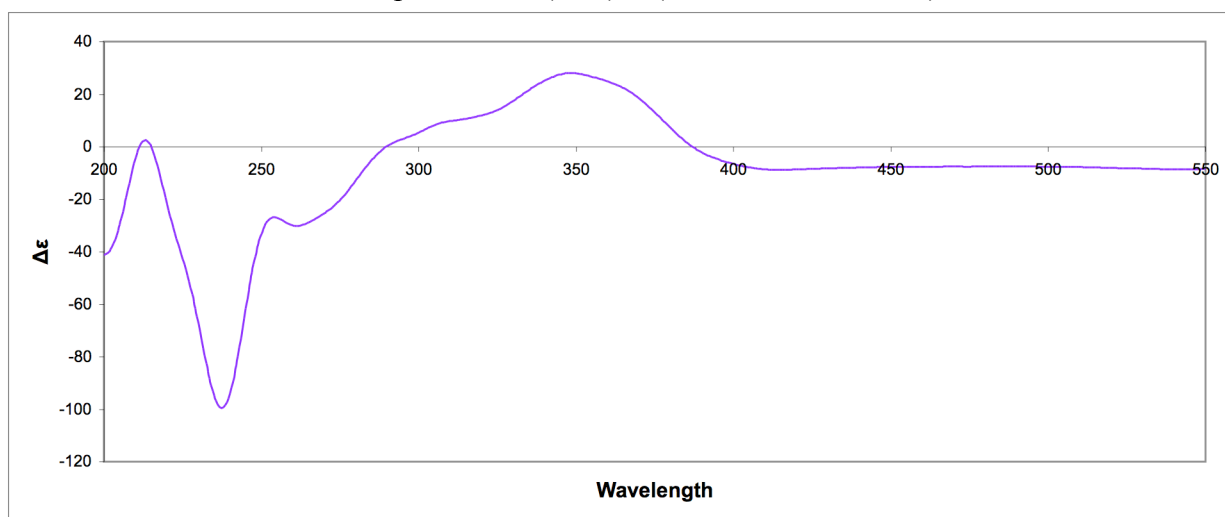


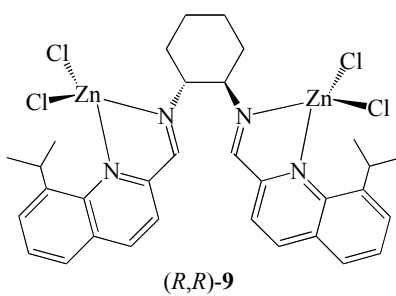
(*R*)-**8**

UV-Vis spectrum of (*R*, *R*)-**8** (1.0×10^{-5} M in THF)

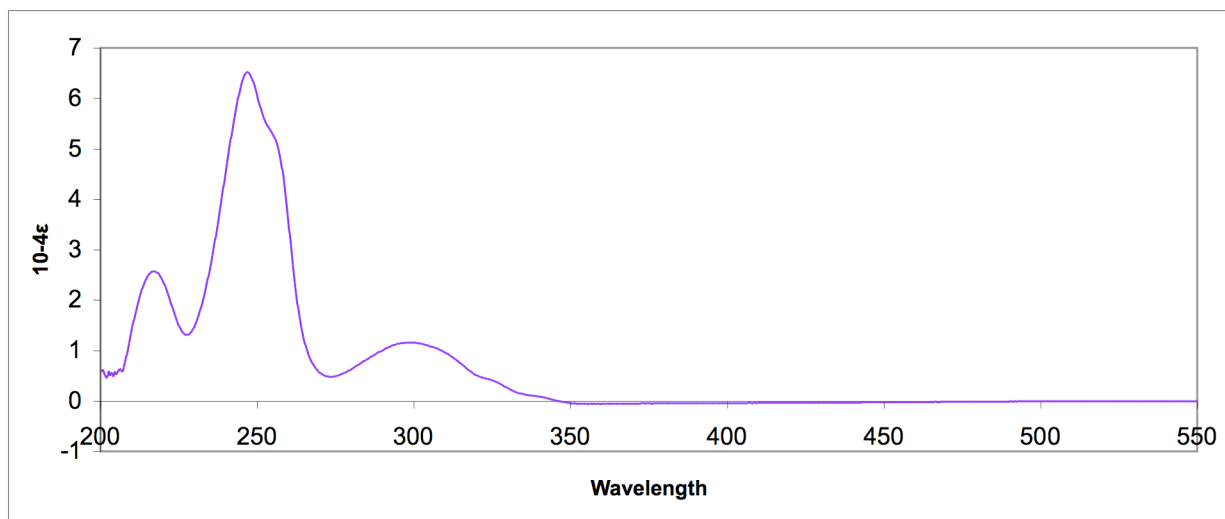


ECD spectrum of (*R*, *R*)-**8** (2.5×10^{-5} M in THF)

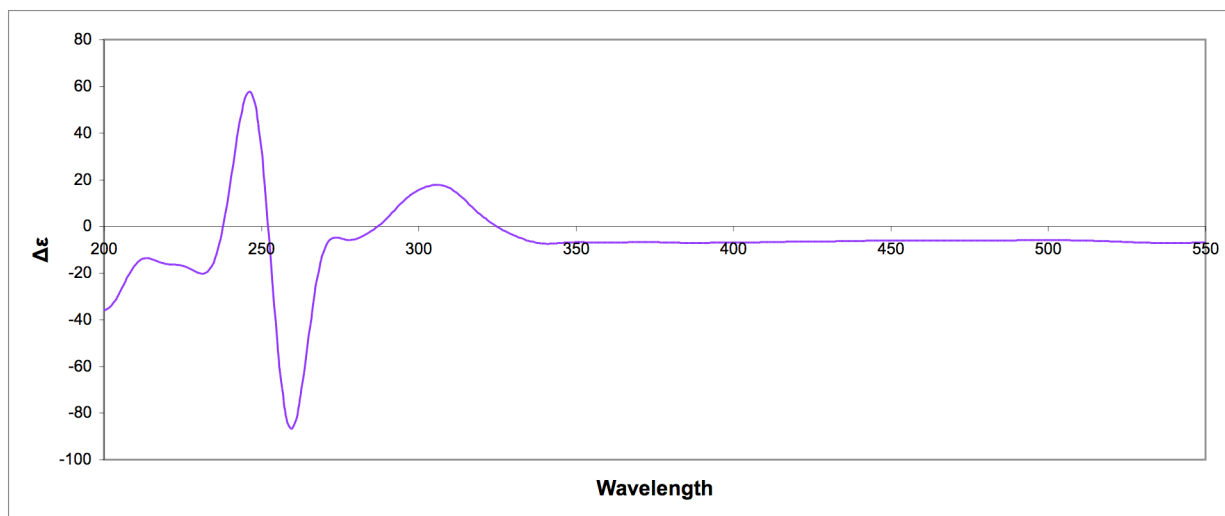


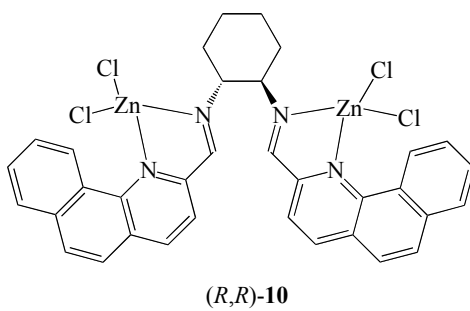


UV-Vis spectrum of (R, R)-9 (2.5×10^{-5} M in THF)

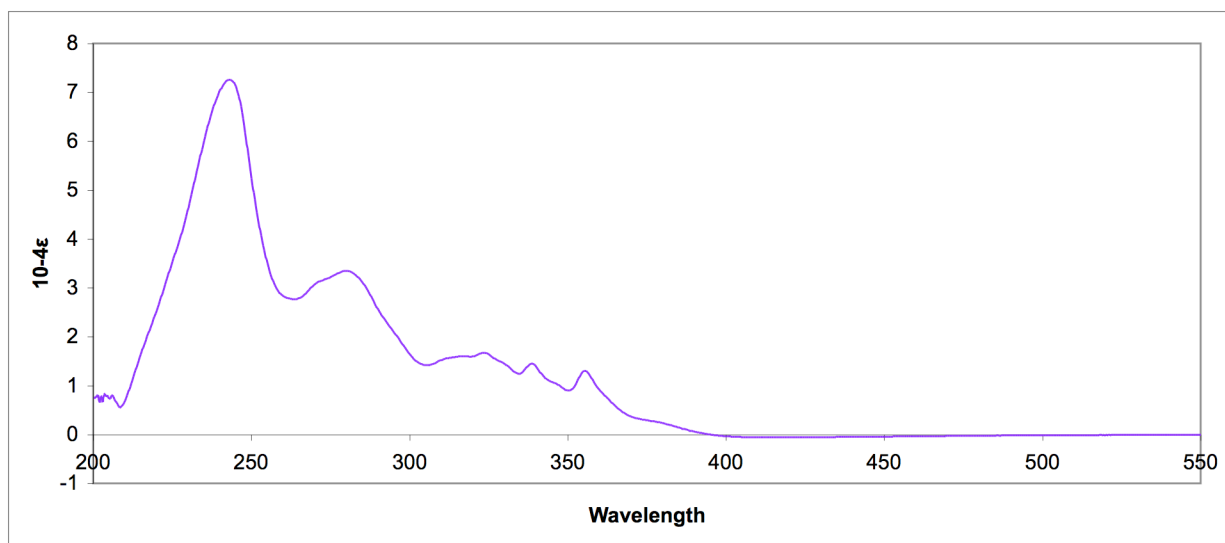


ECD spectrum of (R, R)-9 (2.5×10^{-5} M in THF)

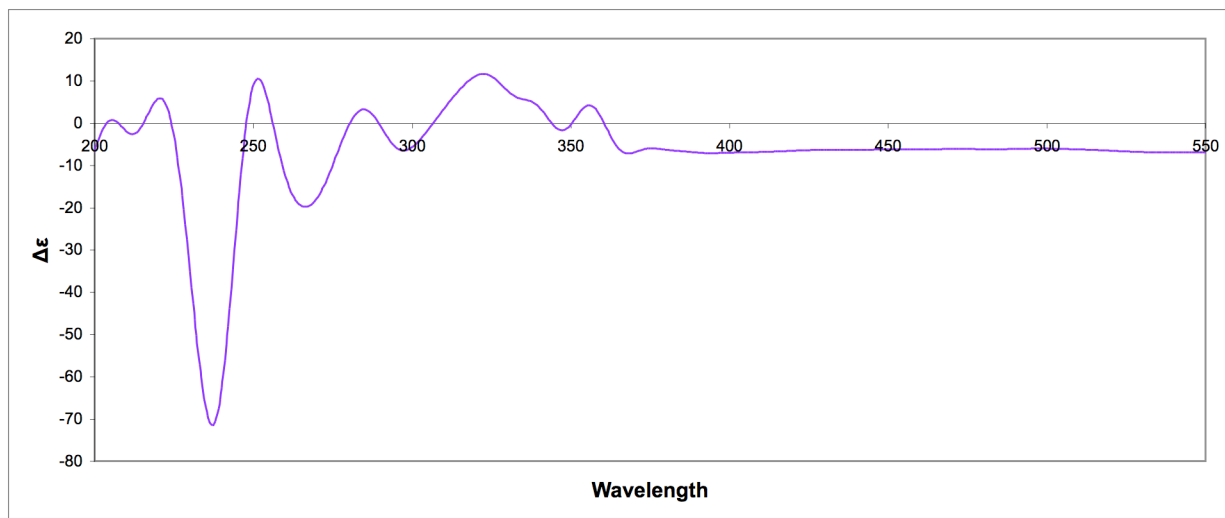


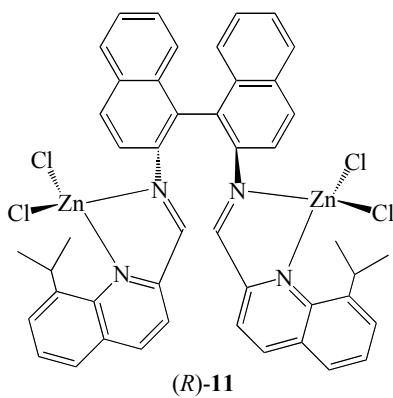


UV-Vis spectrum of (*R, R*)-10 (2.5×10^{-5} M in THF)

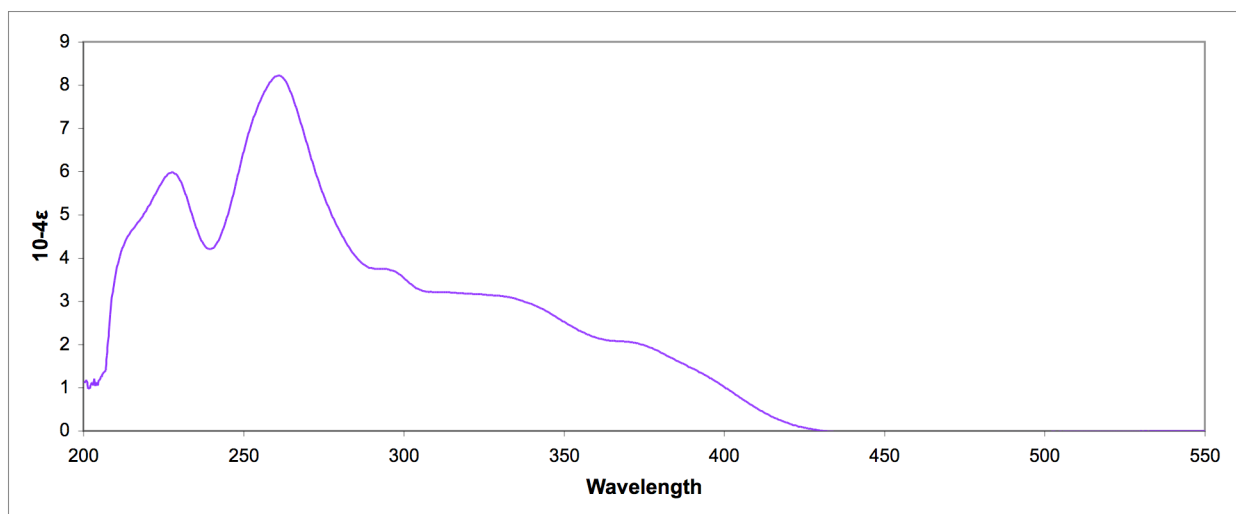


ECD spectrum of (*R, R*)-10 (2.5×10^{-5} M in THF)

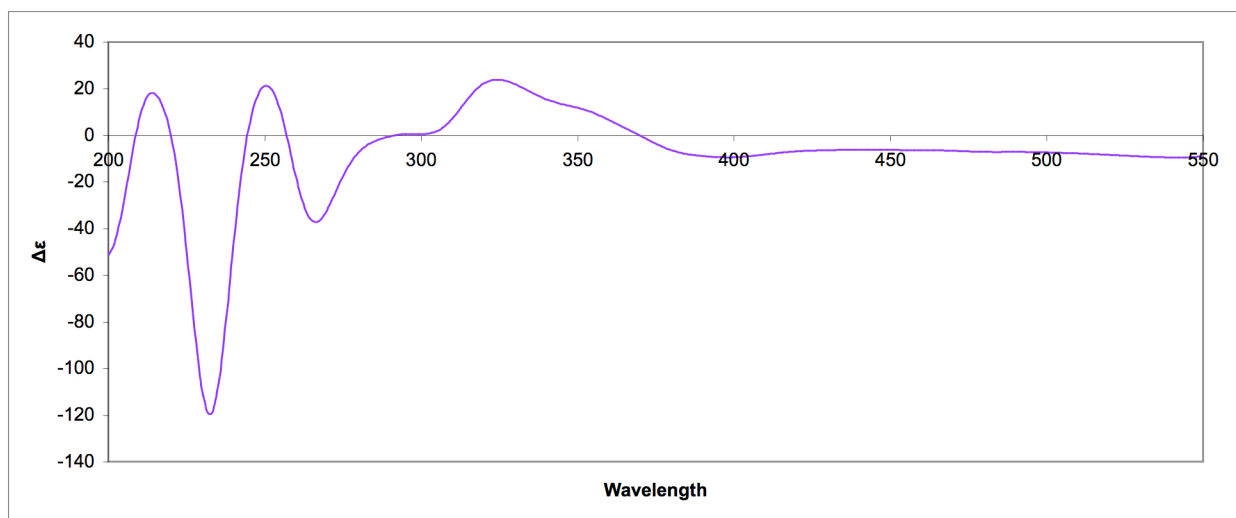


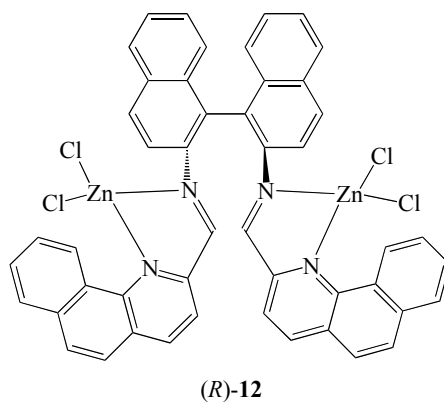


UV-Vis spectrum of (R)-11 (1.3×10^{-5} M in THF)

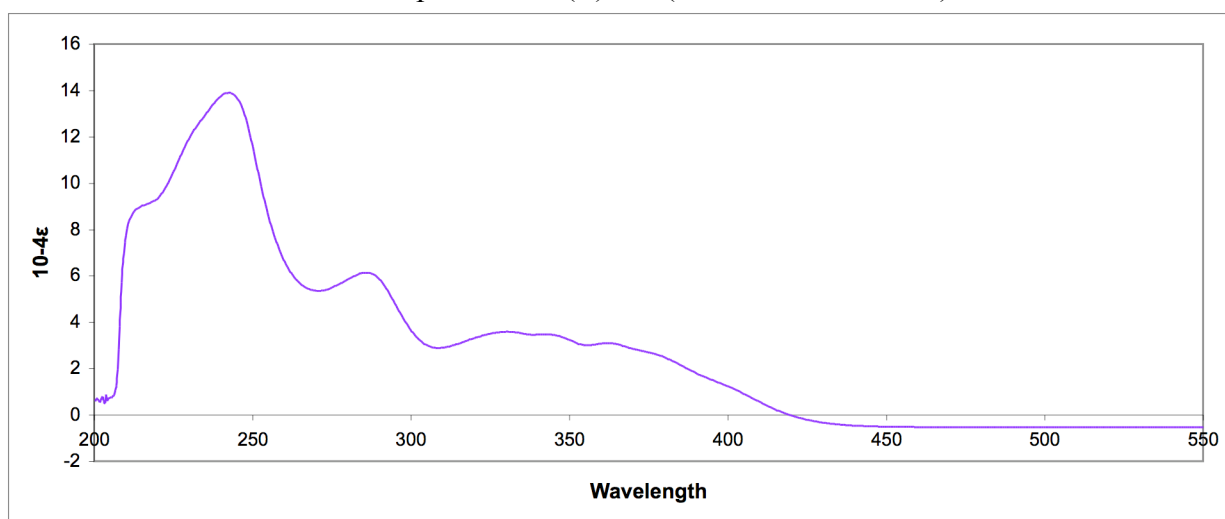


ECD spectrum of (R)-11 (2.5×10^{-5} M in THF)





UV-Vis spectrum of (R)-12 (1.0×10^{-5} M in THF)



ECD spectrum of (R)-12 (2.5×10^{-5} M in THF)

