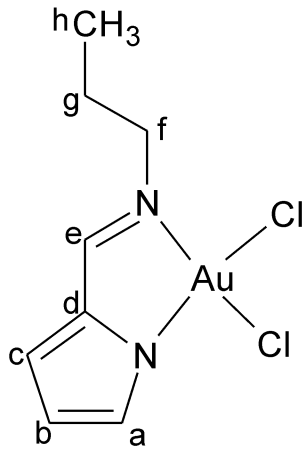
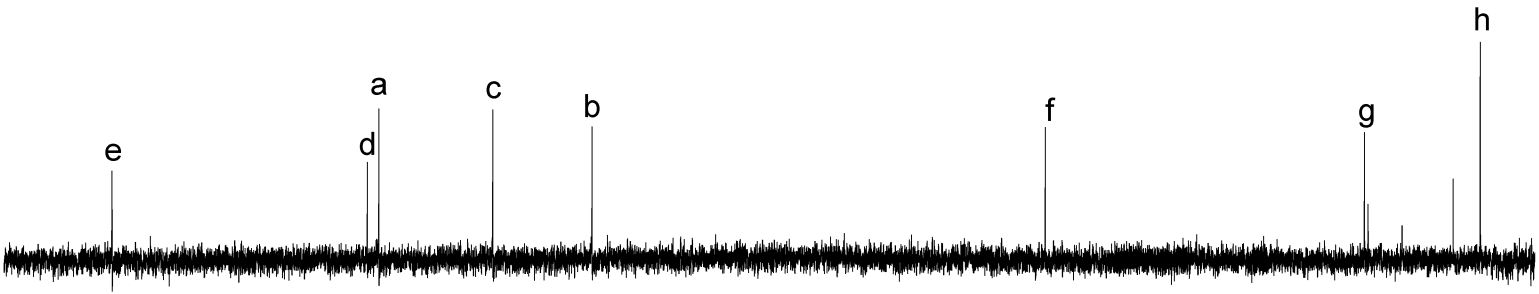
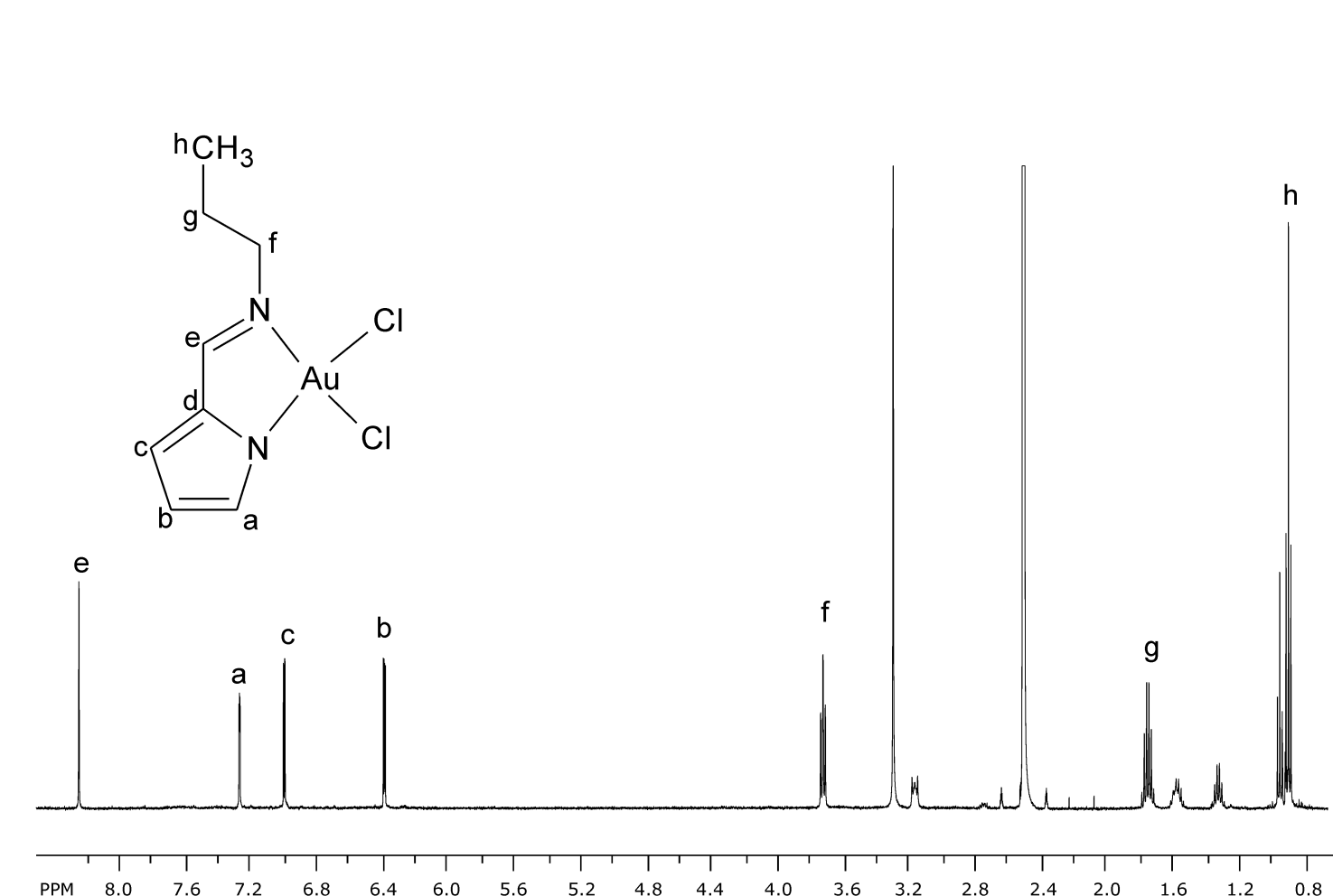
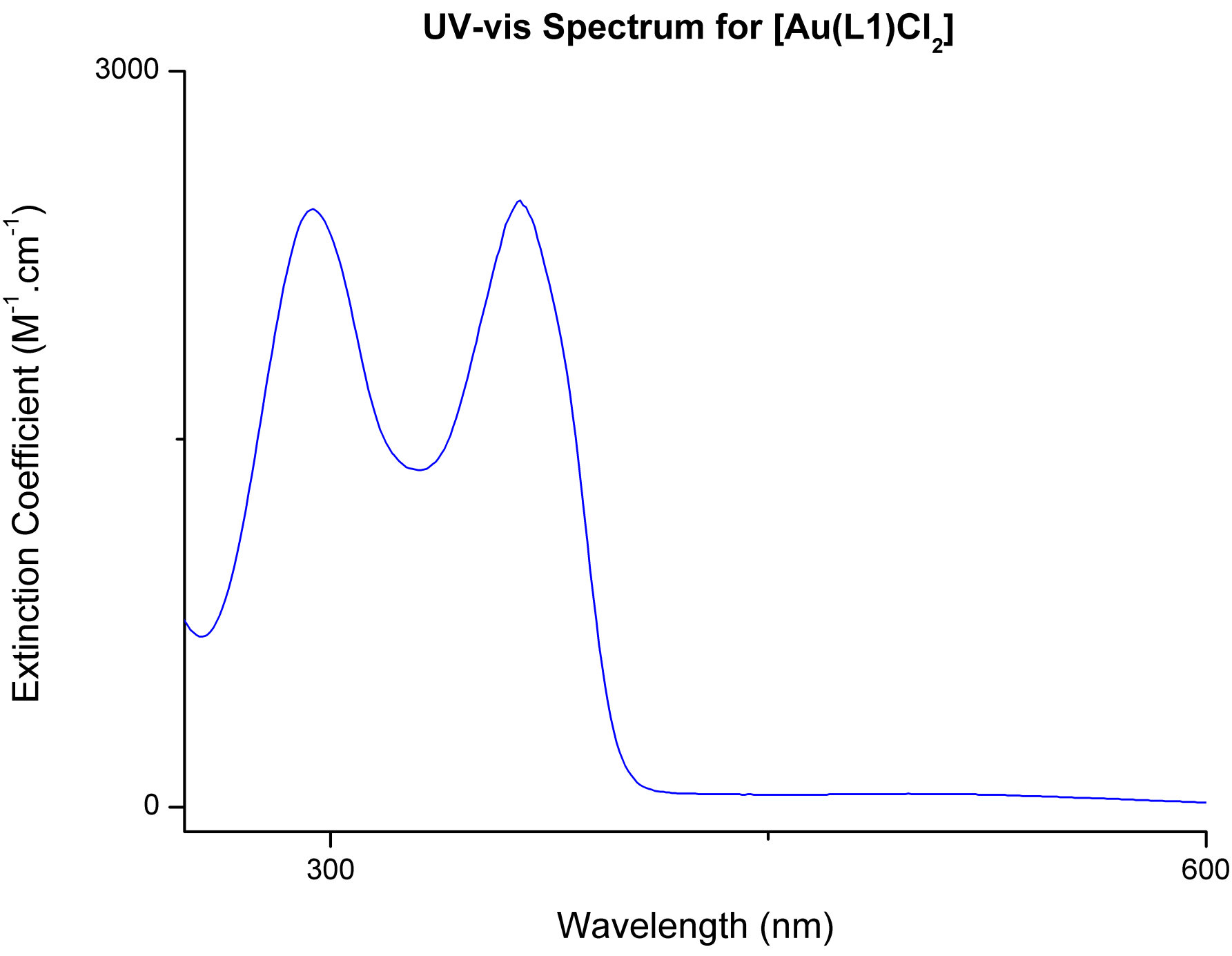
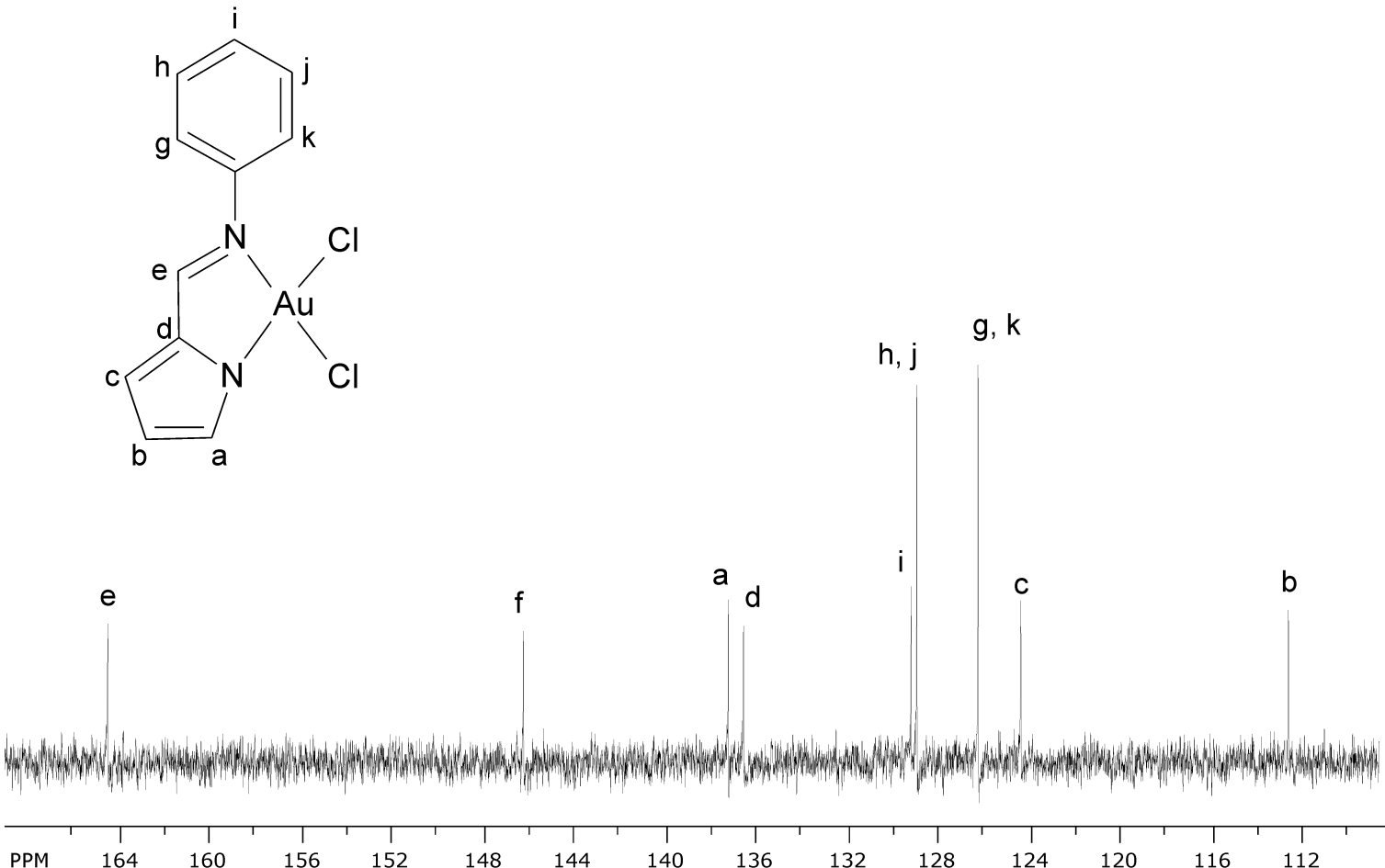
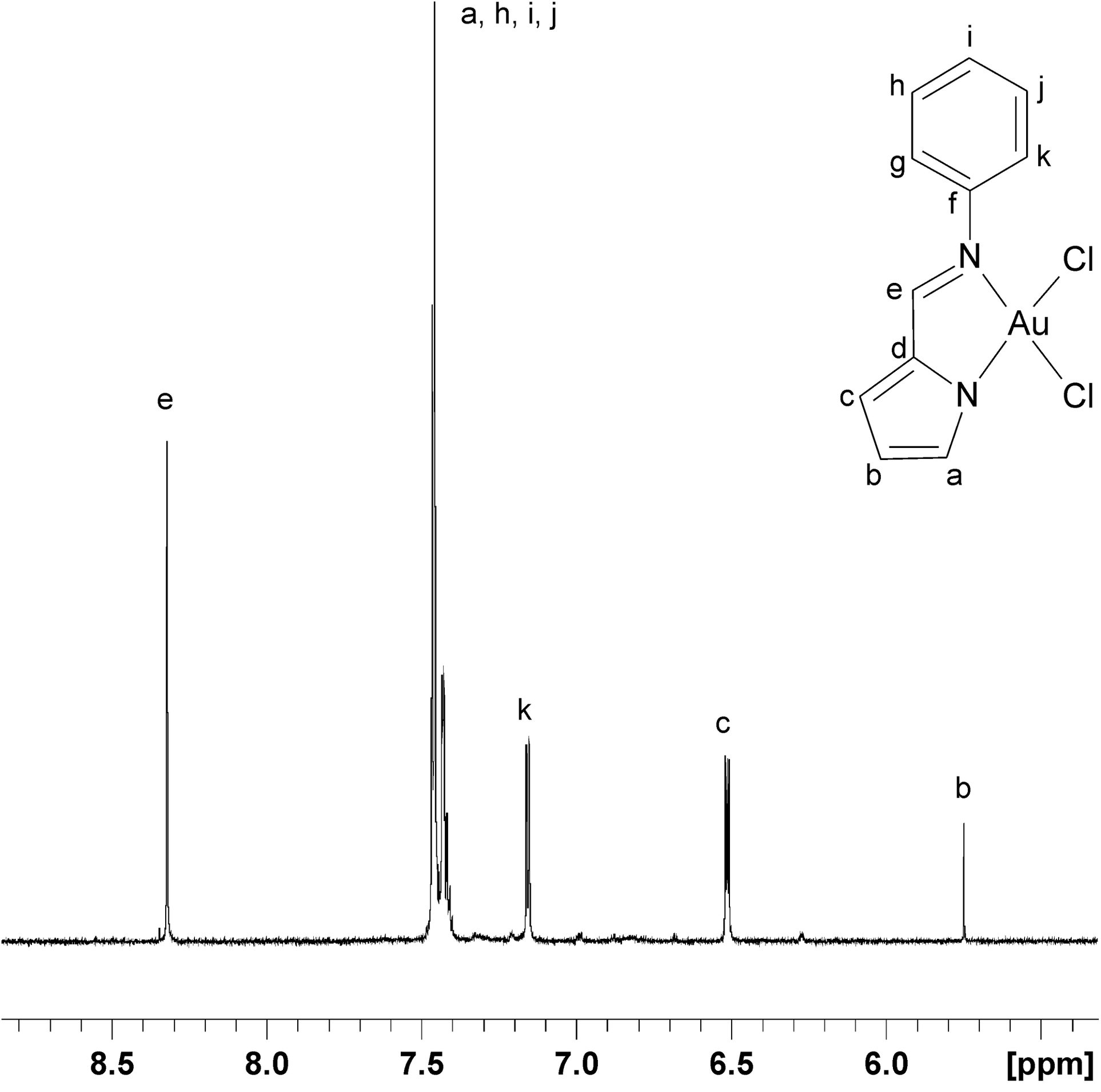

h
CH3
g
f
N
e
Cl
Au
d
Cl
c
N
b
a

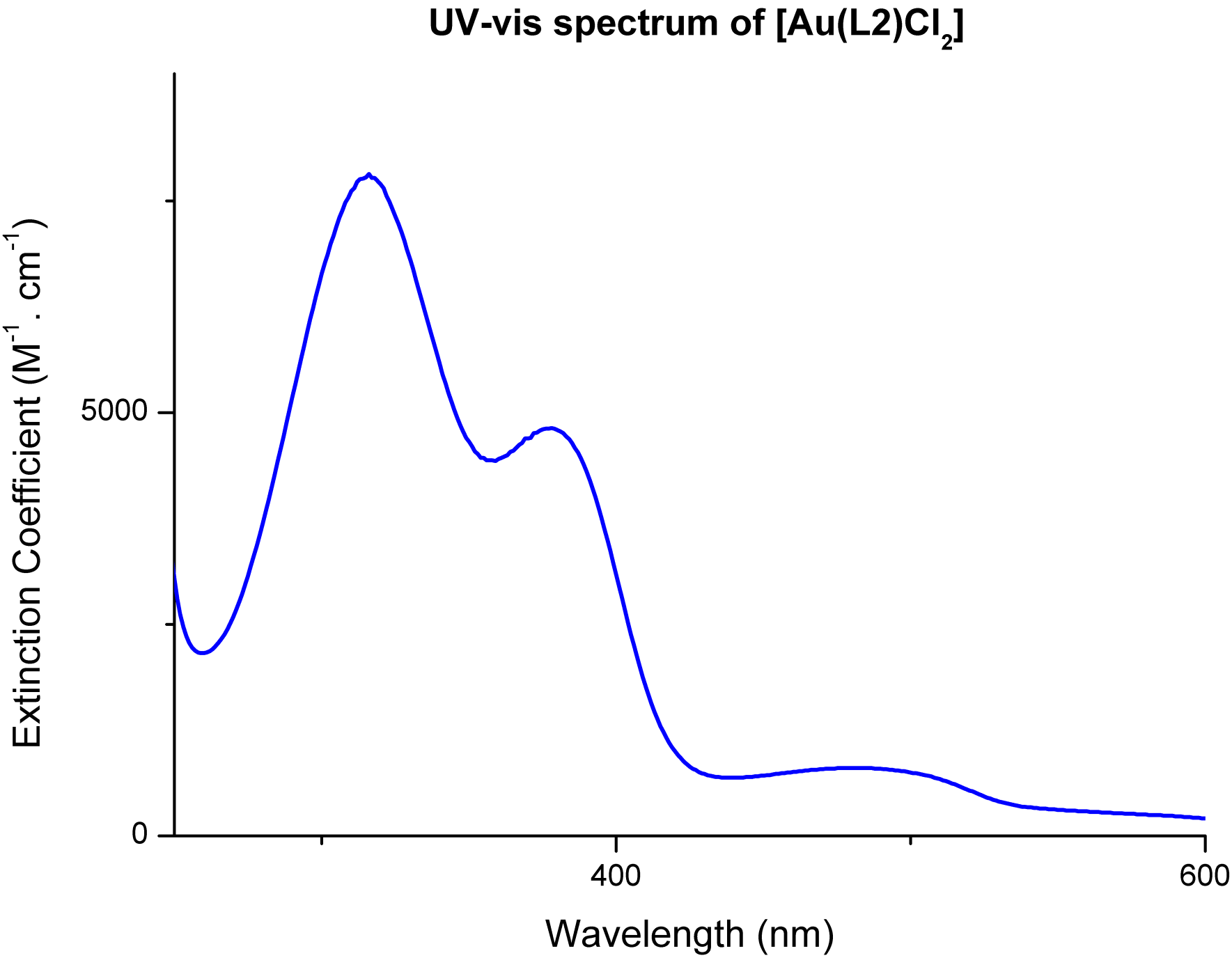

h
a
c
b
f
g
e
d
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

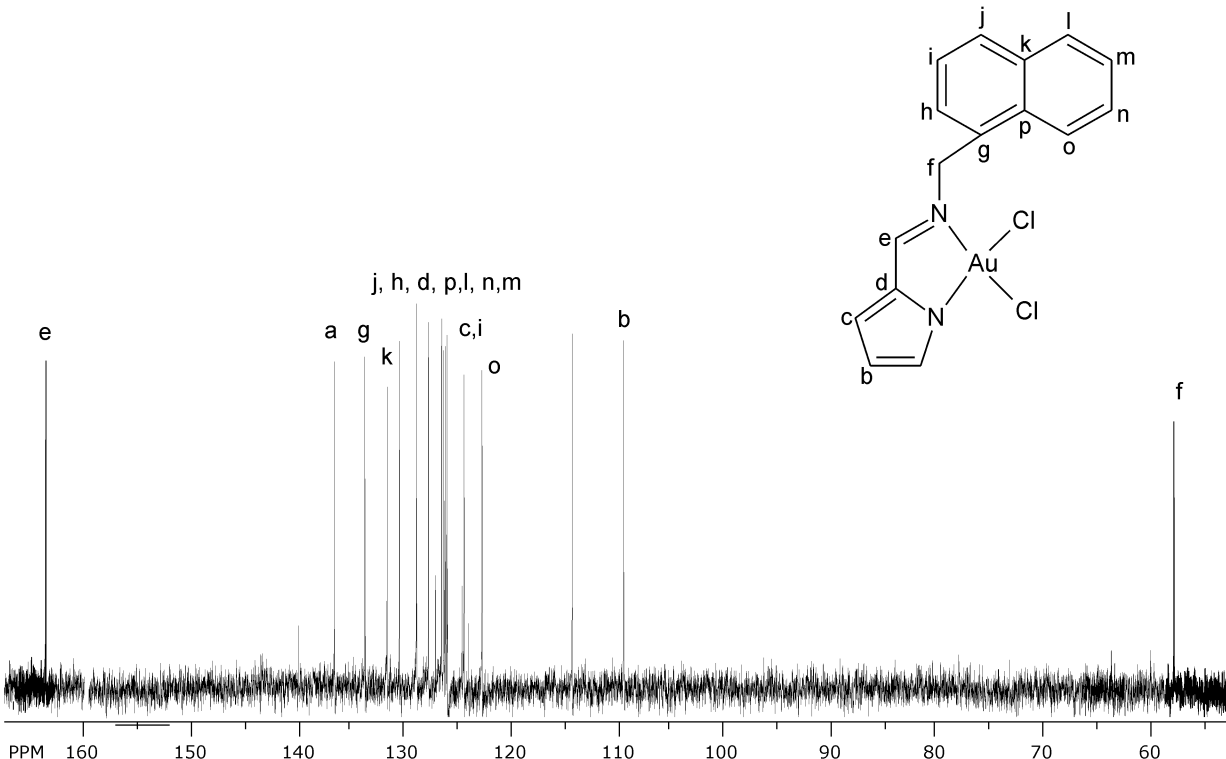

hCH3
g
f
N
e
Cl
Au
d
Cl
c
N
b
a
e
a
c
b
f
g
h
PPM
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
2.0
1.6
1.2
0.8

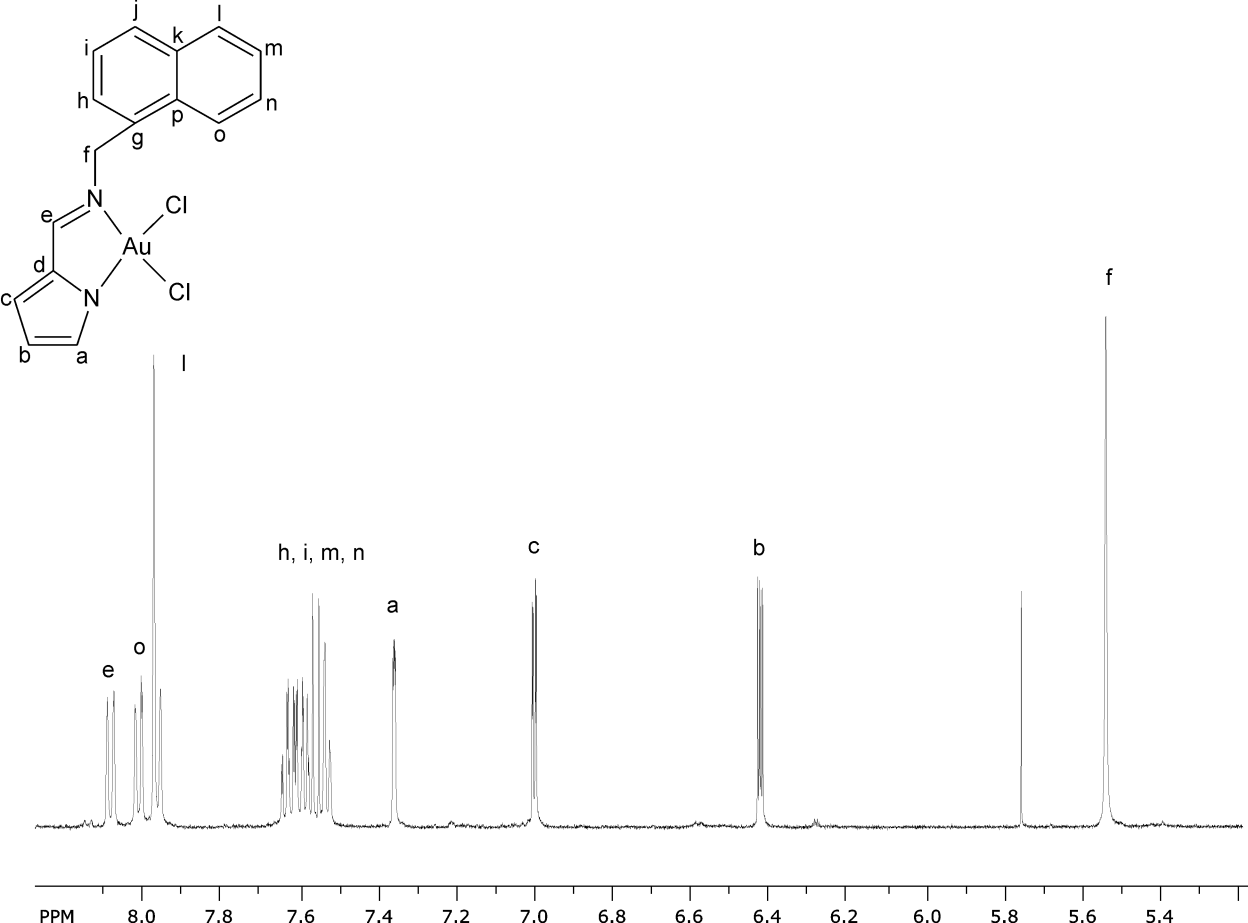

UV-vis Spectrum for [Au(L1)Cl2]
3000
0
Extinction Coefficient (M-1.cm-1)
300
600
Wavelength (nm)

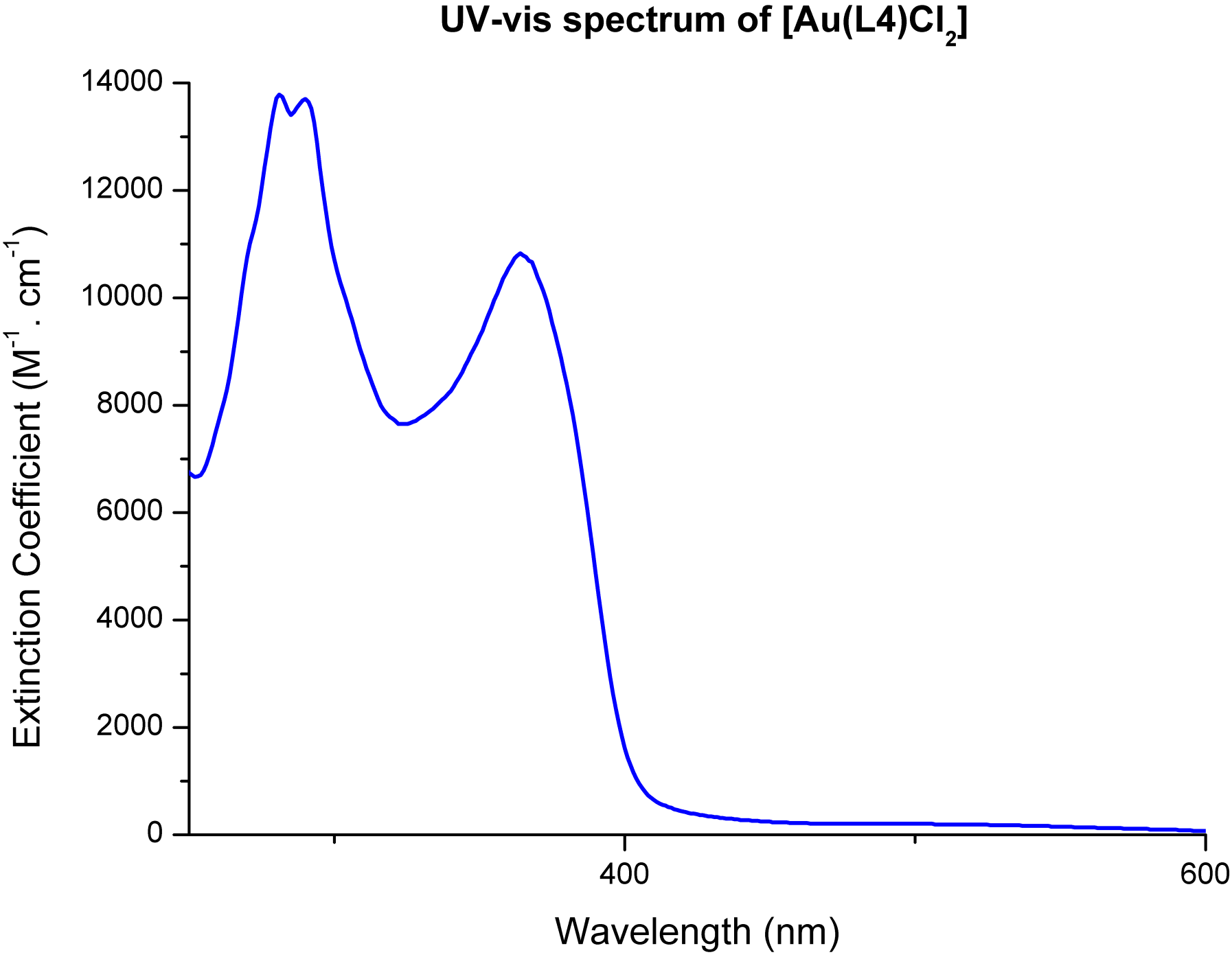

i
h
j
g
k
N
Cl
e
Au
d
c
N
Cl
b
a
e
f
a
d
i
h, j
g, k
c
b
PPM
164
160
156
152
148
144
140
136
132
128
124
120
116
112

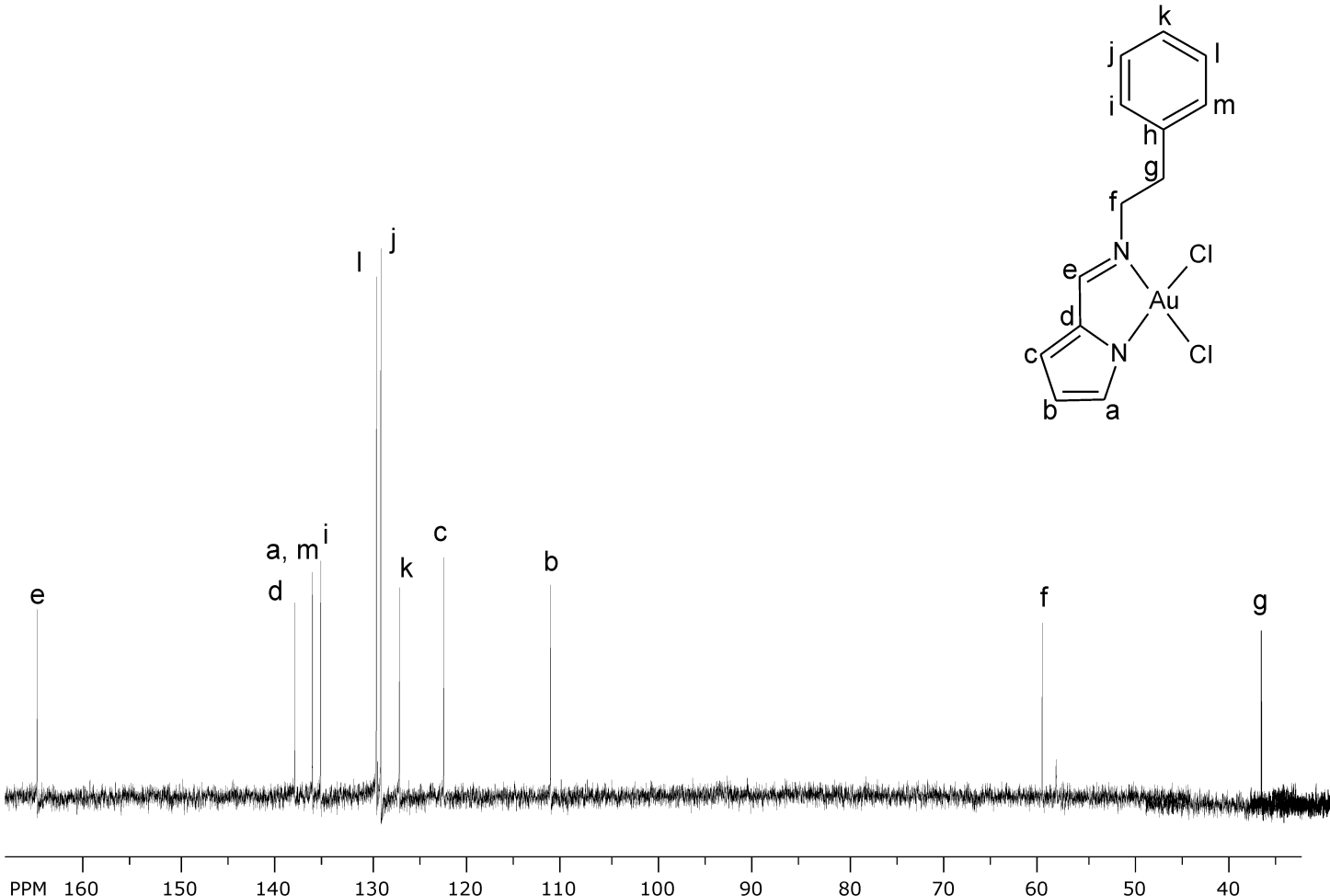

a, h, i, j
e
k
c
b
i
h
j
g
k
f
N
Cl
e
Au
d
c
N
Cl
b
a
8.5
8.0
7.5
7.0
6.5
6.0
[ppm]

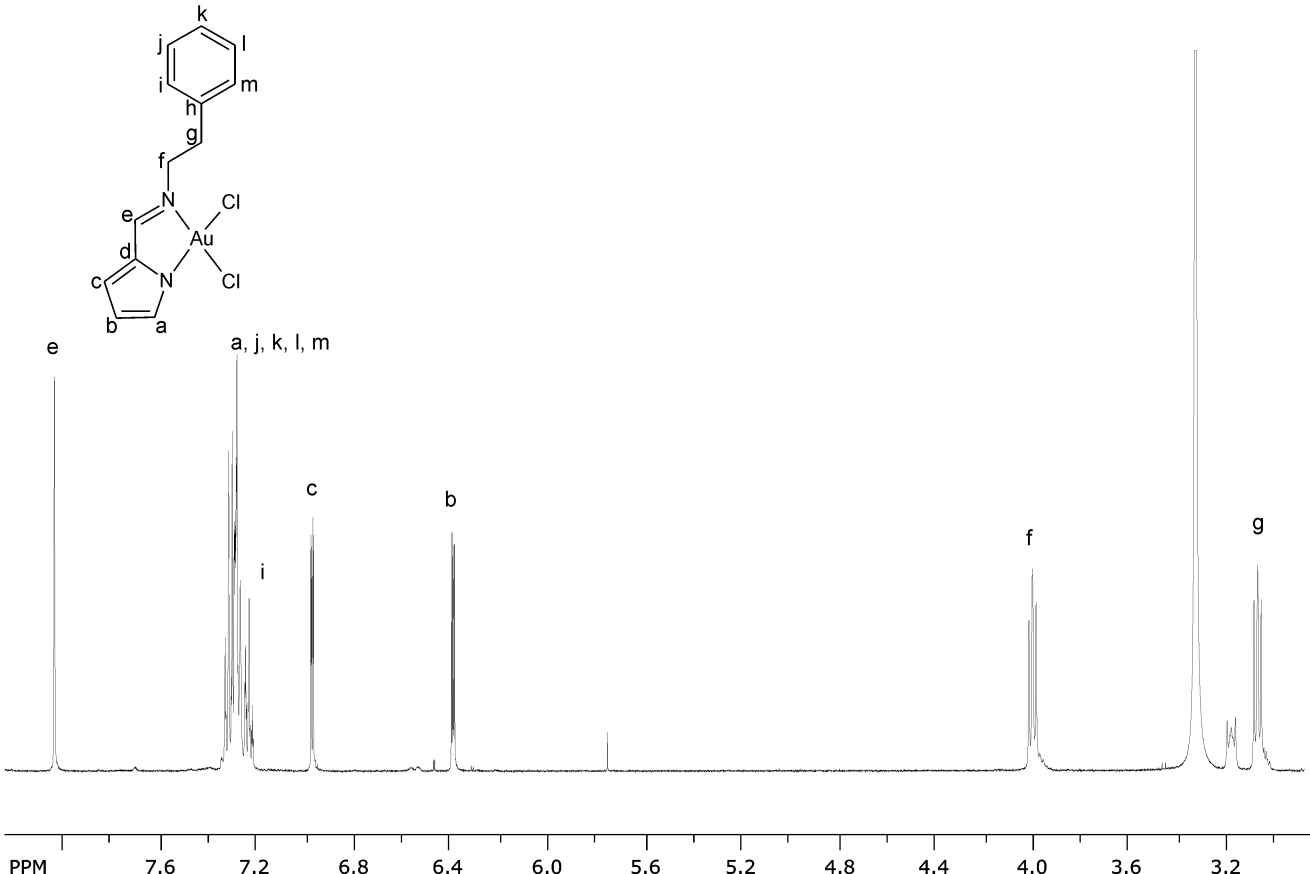

UV-vis spectrum of [Au(L2)Cl2]
Extinction Coefficient (M-1 . cm-1)
5000
0
400
600
Wavelength (nm)

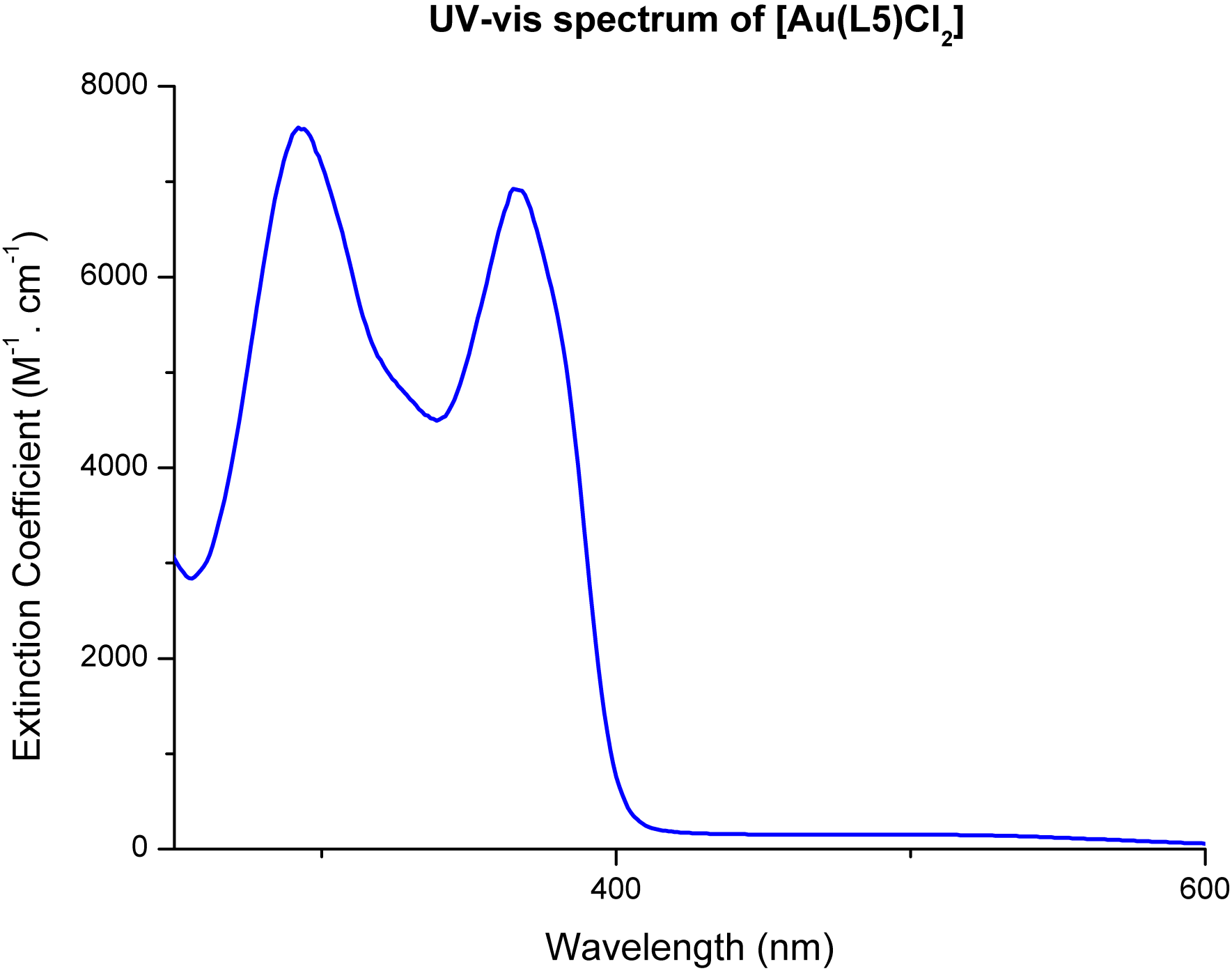

e
a
g
k
j, h, d, p,l, n,m
c,i
o
b
f
PPM
160
150
140
130
120
110
100
90
80
70
60
j
k
l
i
m
h
n
p
g
o
f
N
e
Cl
Au
d
Cl
c
N
b


j
k
l
i
m
h
n
p
g
o
f
N
e
Cl
Au
d
Cl
c
N
b
a
l
f
h, i, m, n
c
b
a
e
o
PPM
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4


UV-vis spectrum of [Au(L4)Cl2]
Extinction Coefficient (M-1 . cm-1)
14000
12000
10000
8000
6000
4000
2000
0
400
600
Wavelength (nm)


k
j
l
i
m
h
g
f
N
Cl
e
Au
d
Cl
c
N
b
a
e
a, m
d
i
l
j
k
c
b
f
g
PPM
160
150
140
130
120
110
100
90
80
70
60
50
40


k
j
l
i
m
h
g
f
N
Cl
e
Au
d
Cl
c
N
b
a
e
a, j, k, l, m
c
b
i
f
g
PPM
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2

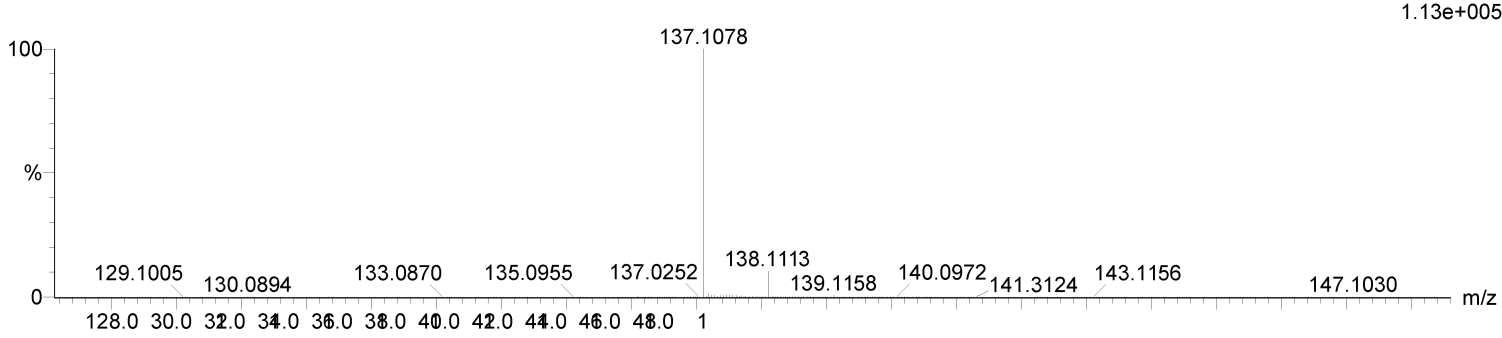

UV-vis spectrum of [Au(L5)Cl2]
8000
6000
4000
2000
0
Extinction Coefficient (M-1 . cm-1)
400
600
Wavelength (nm)

Single Mass Analysis

Tolerance = 500.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 5-10 H: 10-15 N: 0-5 Au: 0-1

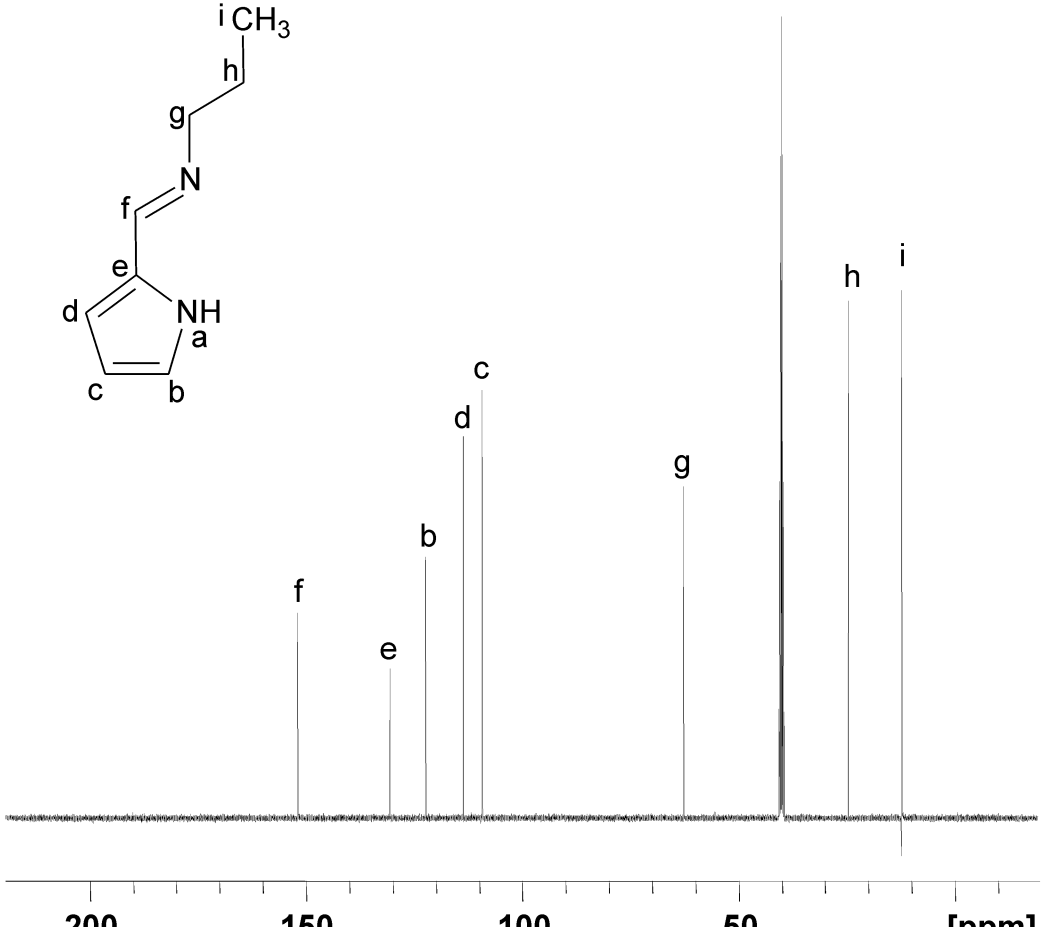
Propyl Ligand 24 (0.392) Cm (1:30)
TOF MS ES+

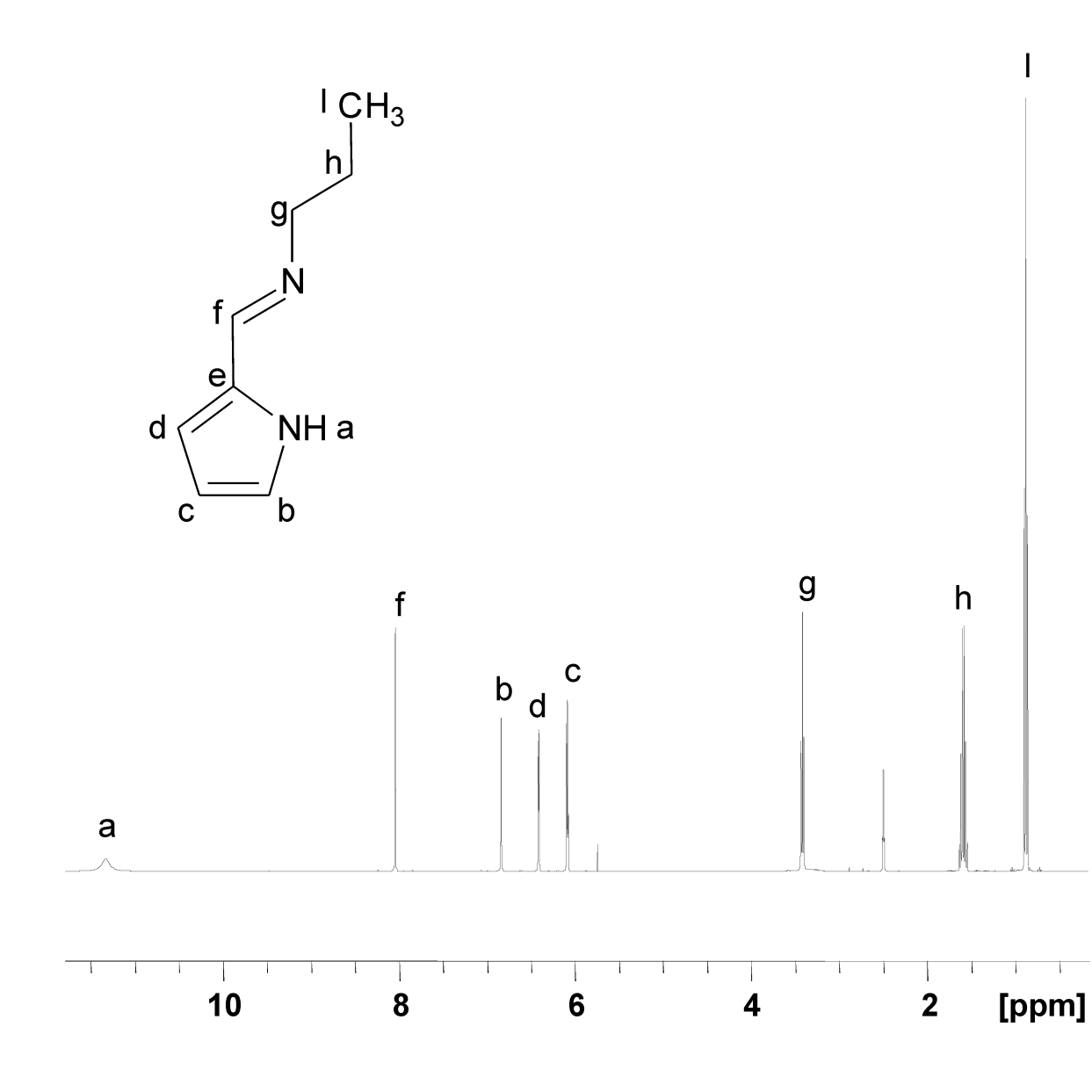


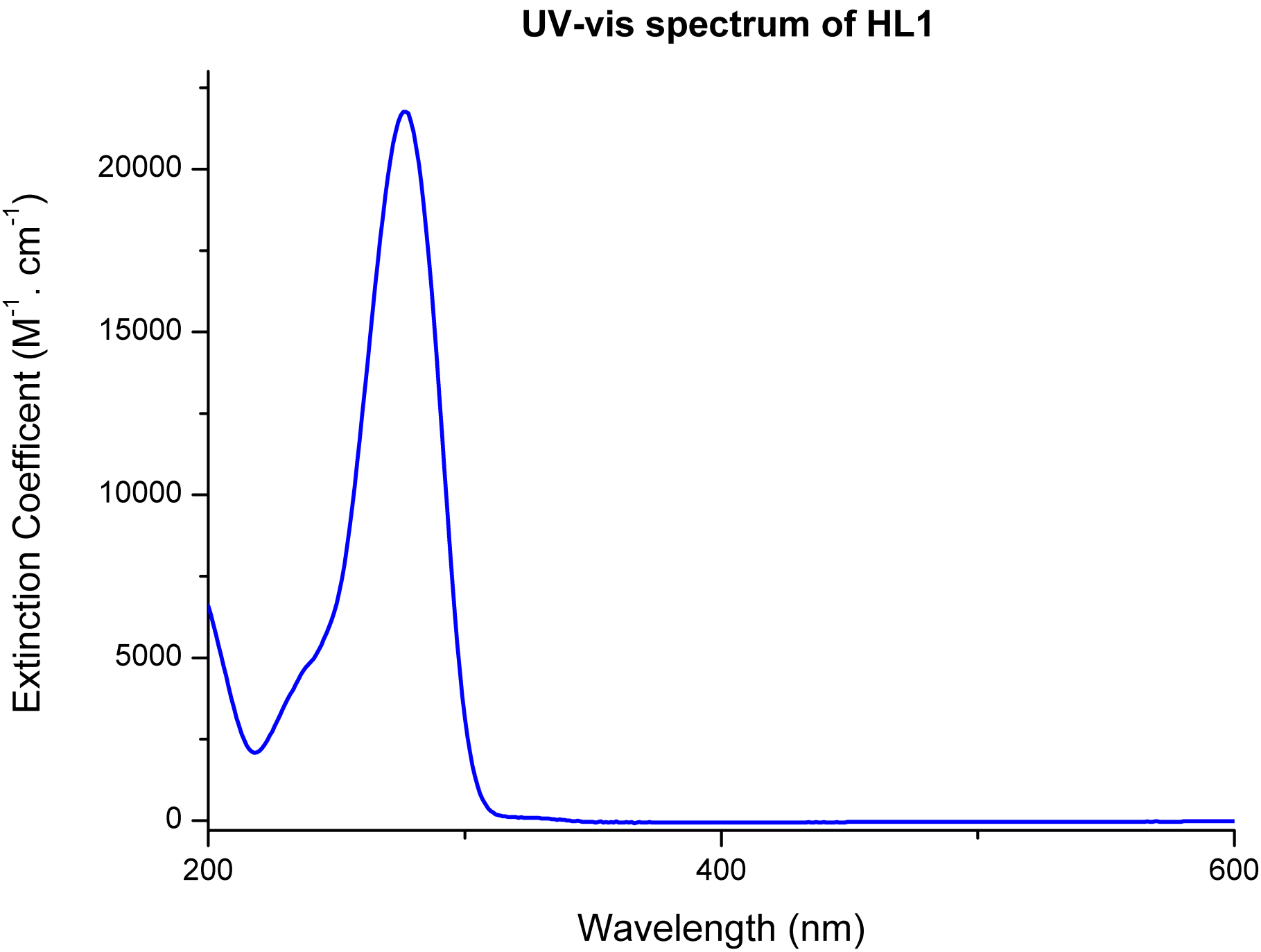
Minimum:			-1.5	
Maximum:		5.0	500.0	50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
137.1078	137.1079	-0.1	-0.7	3.5	660.1	0.0	C8 H13 N2

i CH3
h
g
N
f
e
d
NH
a
c
b


f
e
b
d
c
g
h
i
200
150
100
50
[ppm]


l
CH3
h
g
N
f
e
d
NH a
c
b
a
f
b
d
c
g
h
l
10
8
6
4
2
[ppm]

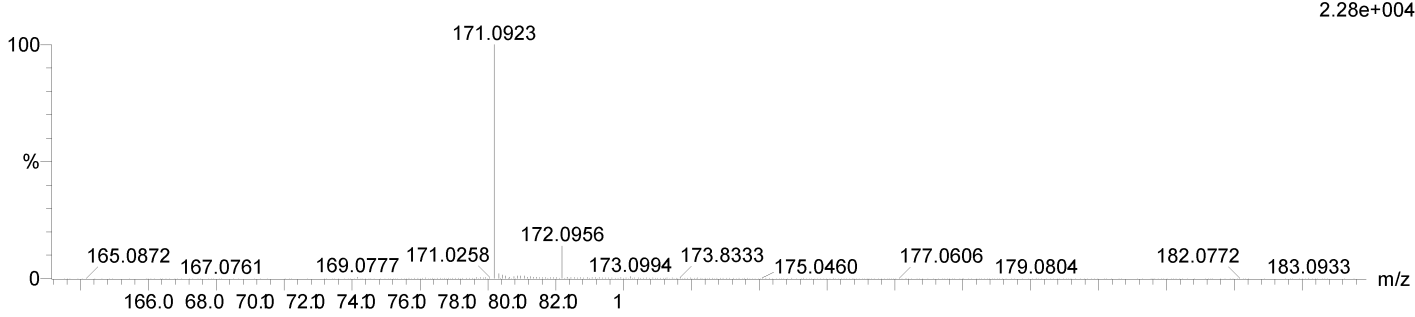

UV-vis spectrum of HL1
Extinction Coefficent (M-1 . cm-1)
20000
15000
10000
5000
0
200
400
600
Wavelength (nm)

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

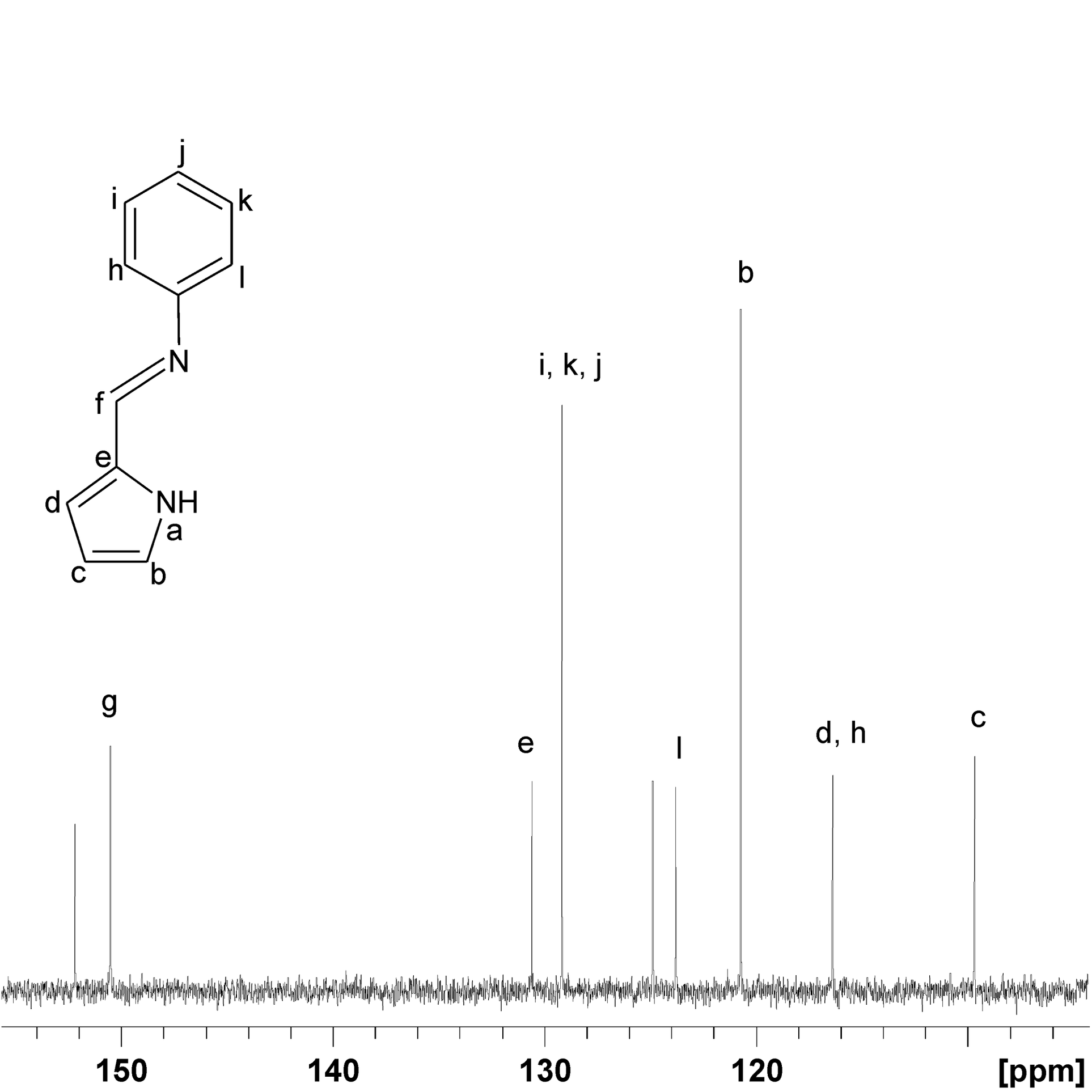
Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 0-5

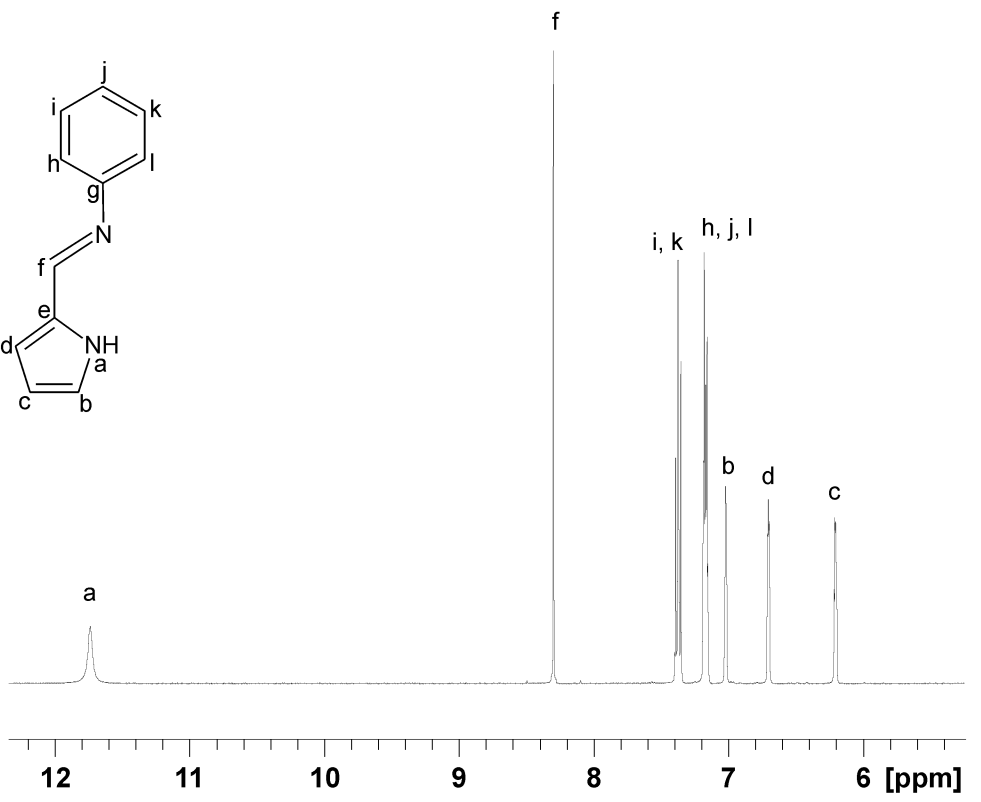
Aniline Ligand 10 (0.154) Cm (1:31)
TOF MS ES+

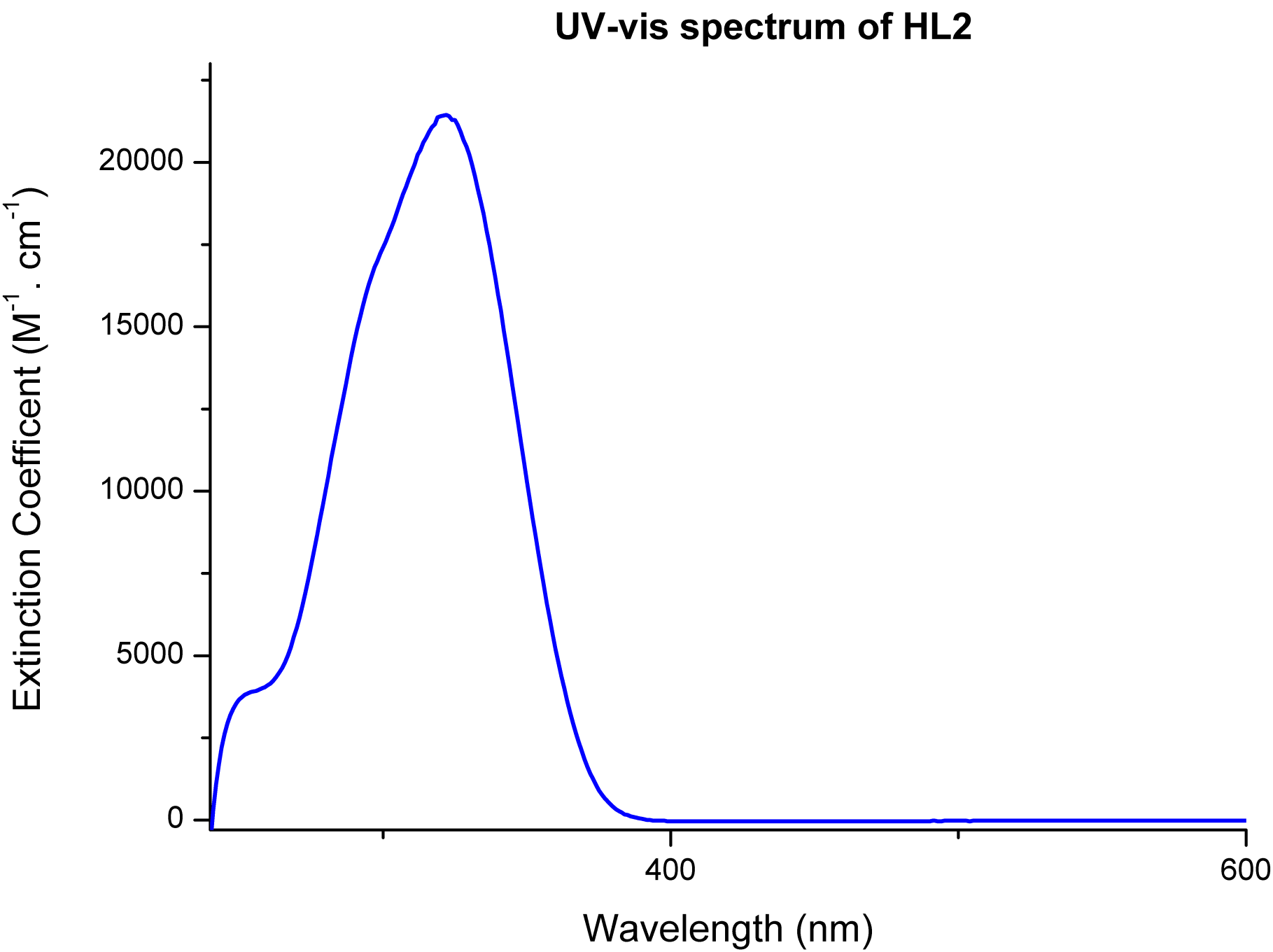


Minimum:		-1.5		
Maximum:	5.0	5.0	50.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
171.0923	171.0922	0.1	0.6	7.5	500.9	0.0	C11 H11 N2


j
i
k
h
l
N
f
e
d
NH
a
c
b
g
e
i, k, j
l
b
d, h
c
150
140
130
120
[ppm]


f
i, k
h, j, l
b
d
c
a
12
11
10
9
8
7
6 [ppm]
j
i
k
h
l
g
N
f
e
d
NH
a
c
b

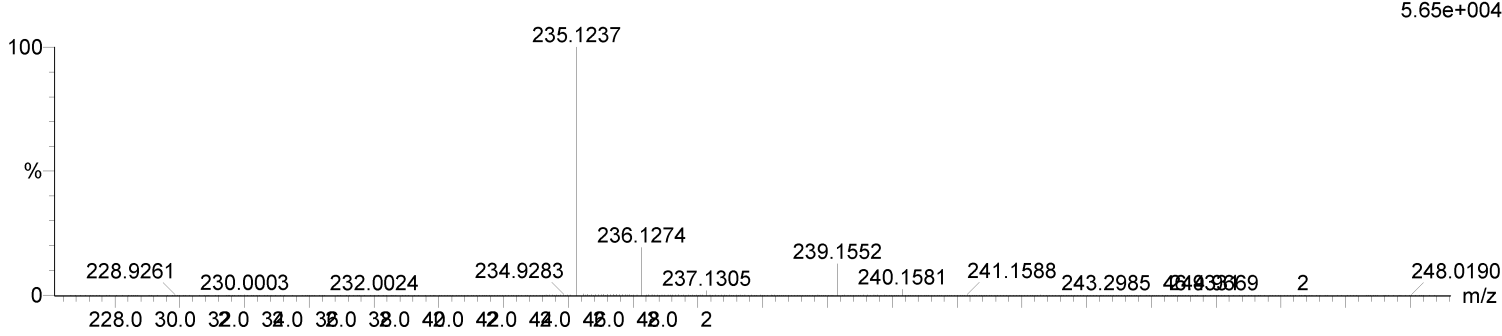

UV-vis spectrum of HL2
Extinction Coefficent (M-1 . cm-1)
20000
15000
10000
5000
0
400
600
Wavelength (nm)

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

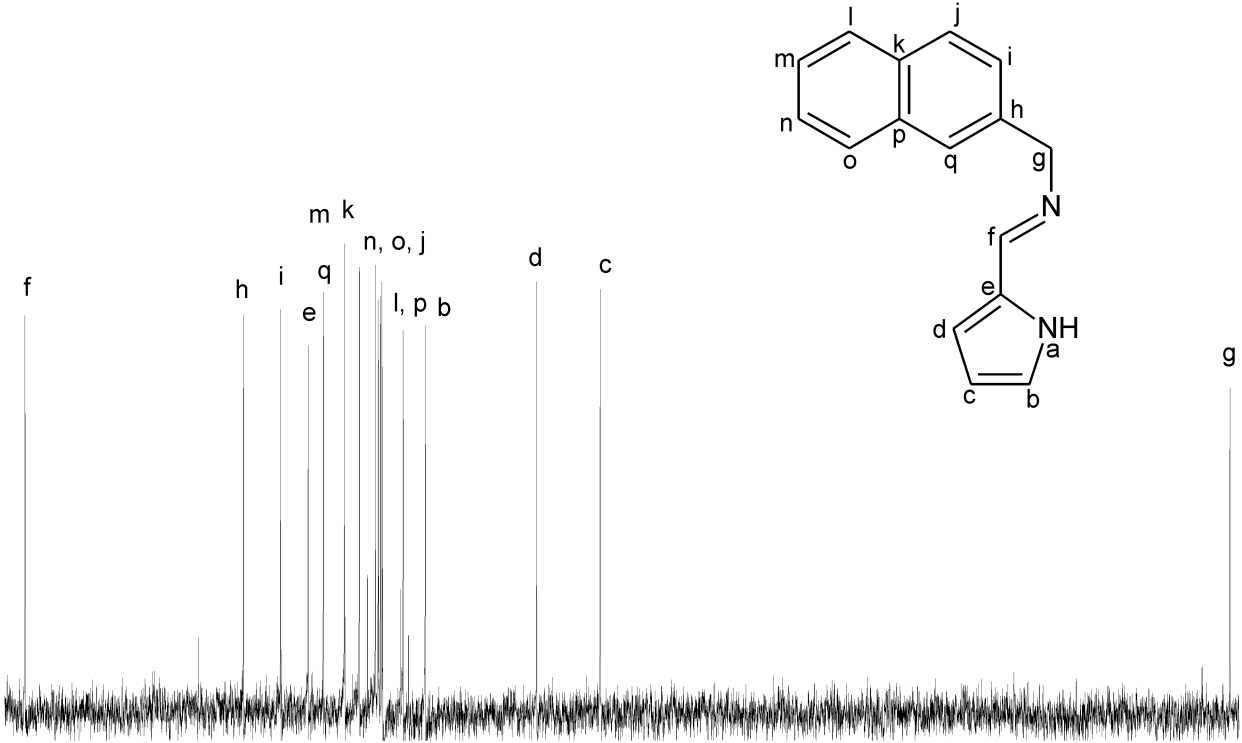
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-20 H: 10-15 N: 0-5

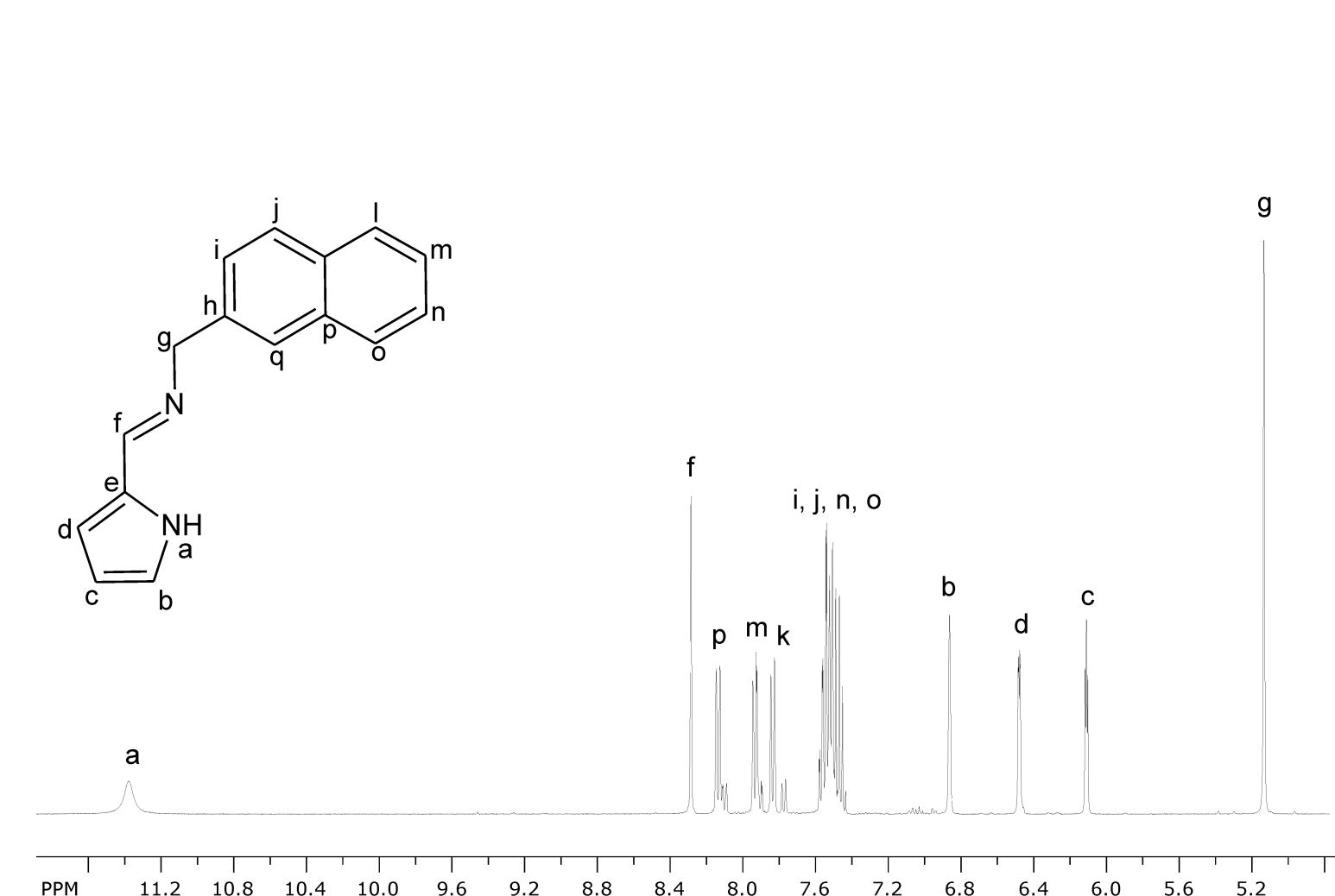
Naphthylmethyl ligand 4 (0.052) Cm (1:30)
TOF MS ES+

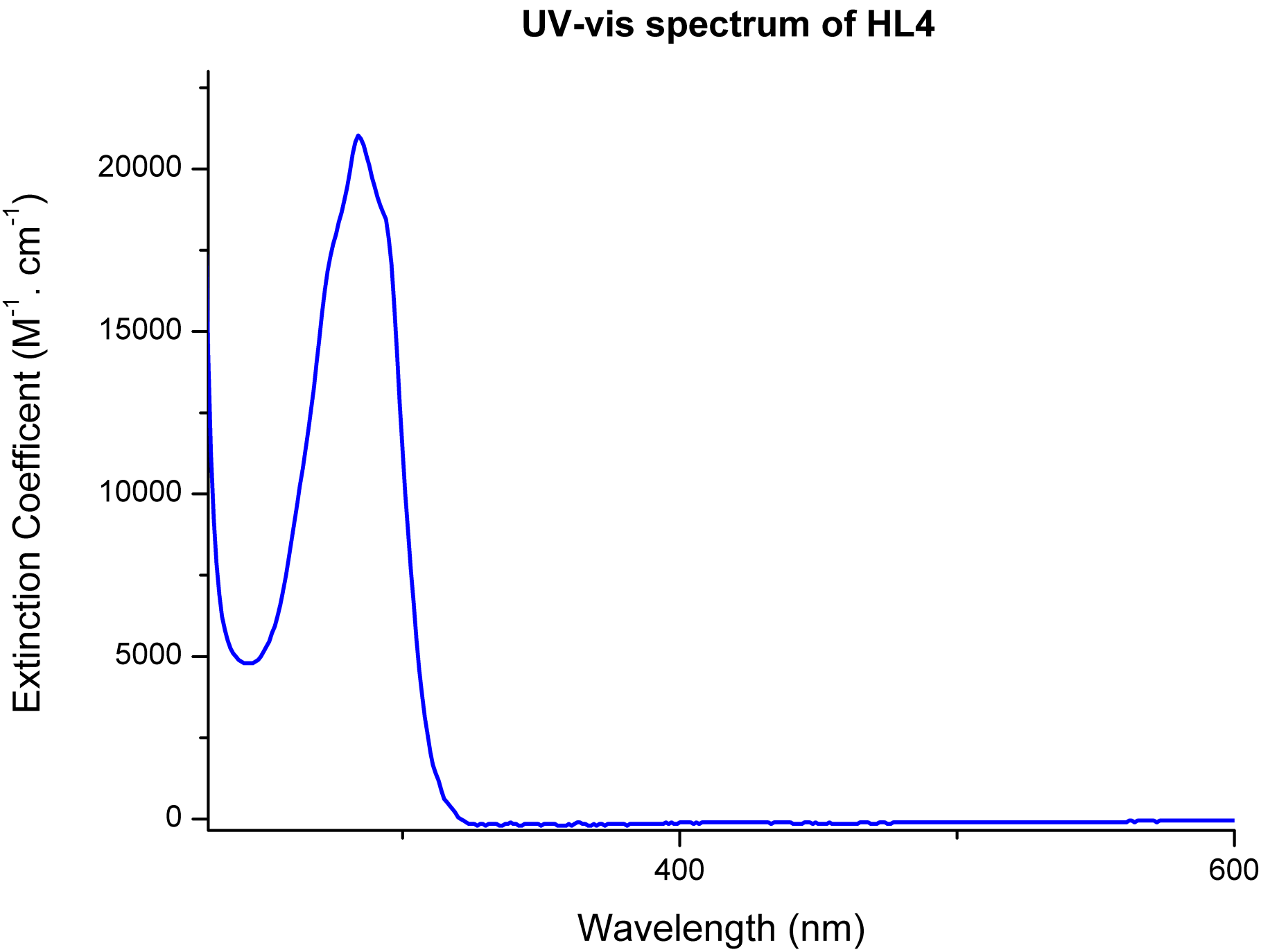


Minimum:		-1.5		
Maximum:	5.0	5.0	100.0	

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
235.1237	235.1235	0.2	0.9	10.5	485.2	0.0	C16 H15 N2


f
h
i
e
q
m
k
n, o, j
l, p
b
d
c
g
l
j
k
m
i
h
n
p
o
q
g
N
f
e
d
NH
a
c
b
PPM
146
142
138
134
130
126
122
118
114
110
106
102
98
94
90
86
82
78
74
70
66
62


j
l
i
m
h
n
g
p
q
o
N
f
e
d
NH
a
c
b
g
f
i, j, n, o
b
c
d
p
m
k
a
PPM
11.2
10.8
10.4
10.0
9.6
9.2
8.8
8.4
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2

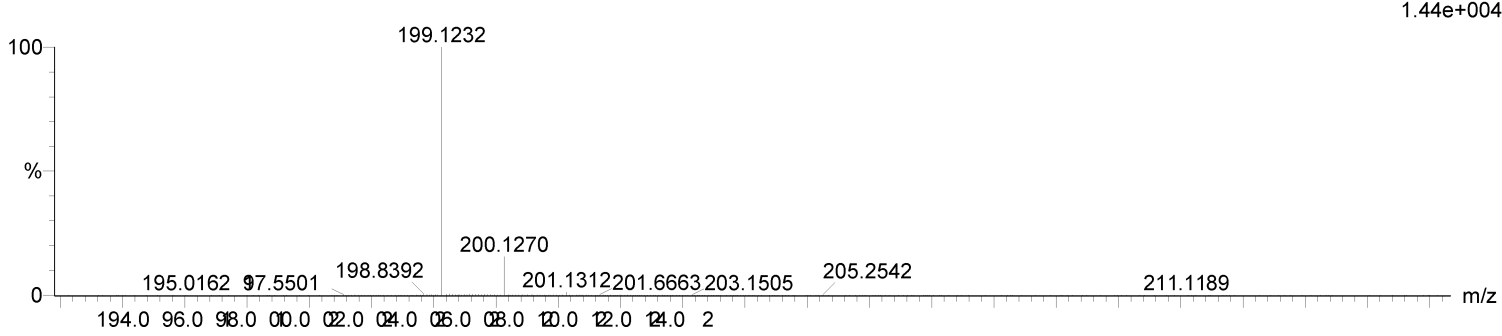

UV-vis spectrum of HL4
Extinction Coefficent (M-1 . cm-1)
20000
15000
10000
5000
0
400
600
Wavelength (nm)

Single Mass Analysis

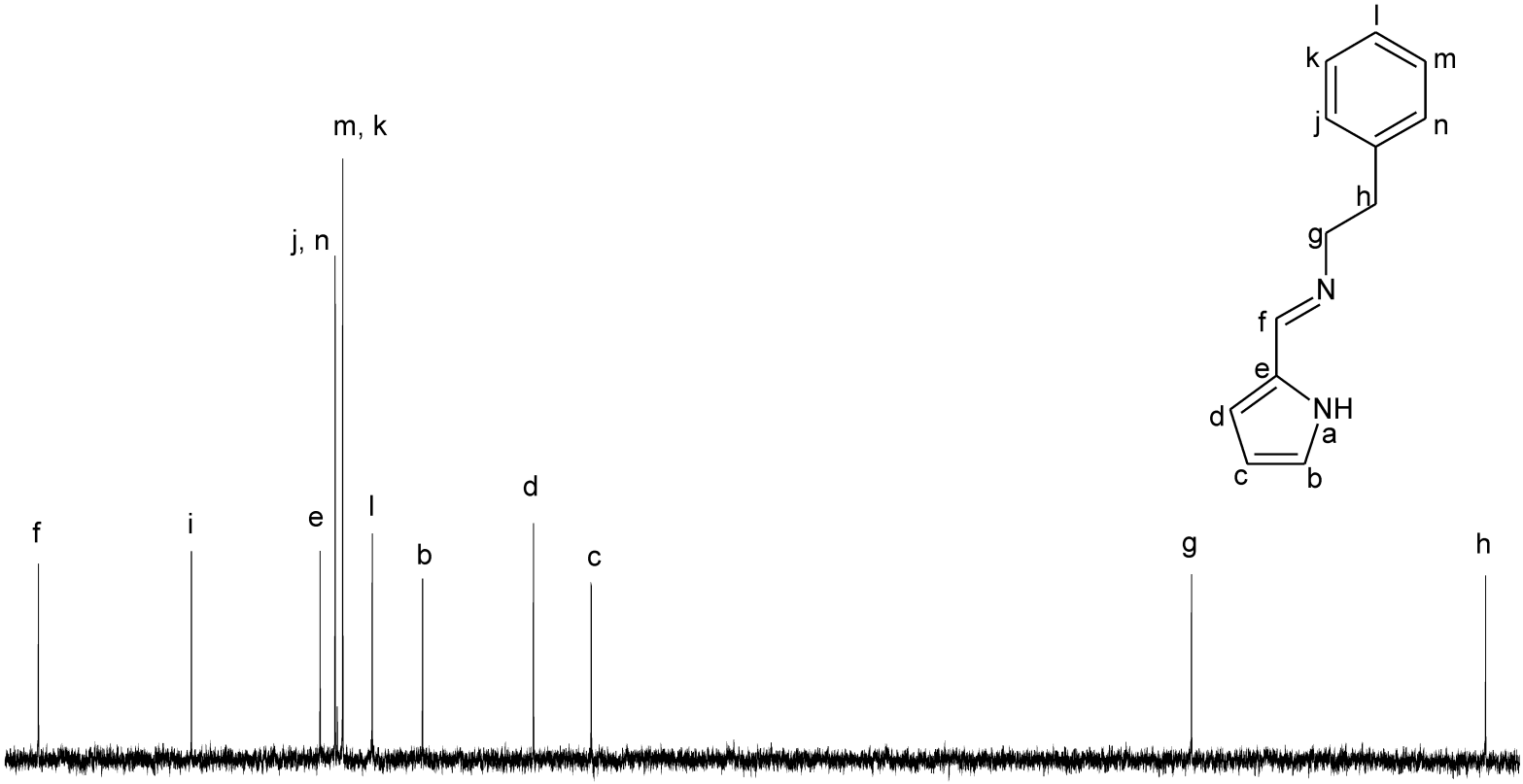
Tolerance = 3.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 10-15 H: 10-15 N: 0-5

Phenyl ethyl ligand 28 (0.461) Cm (1:31)
TOF MS ES+



Minimum:			-1.5				
Maximum:		5.0	3.0	100.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
199.1232	199.1235	-0.3	-1.5	7.5	325.7	0.0	C13 H15 N2


m, k
j, n
f
i
e
l
b
d
c
g
h
l
k
m
j
n
h
g
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f
e
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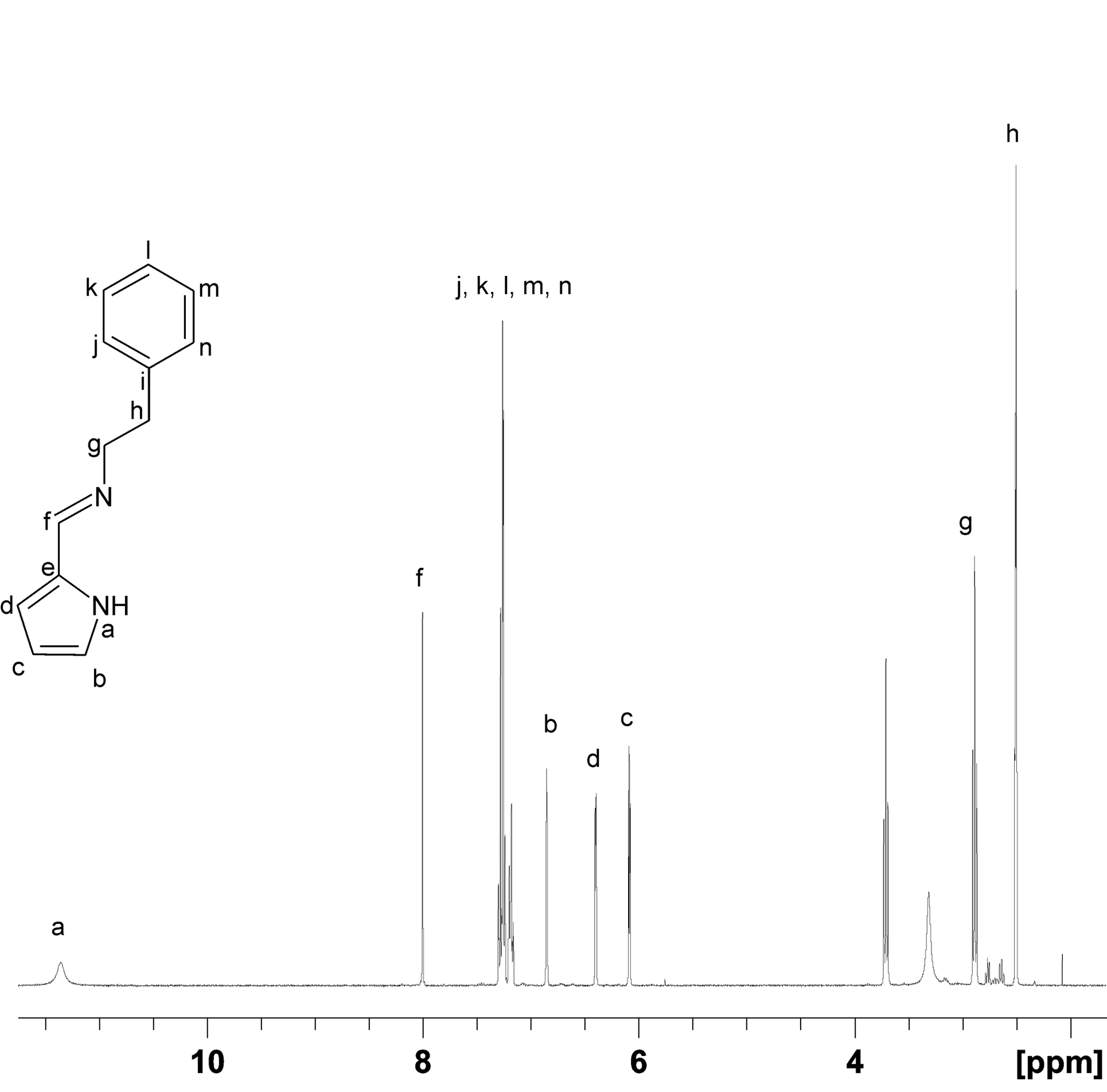
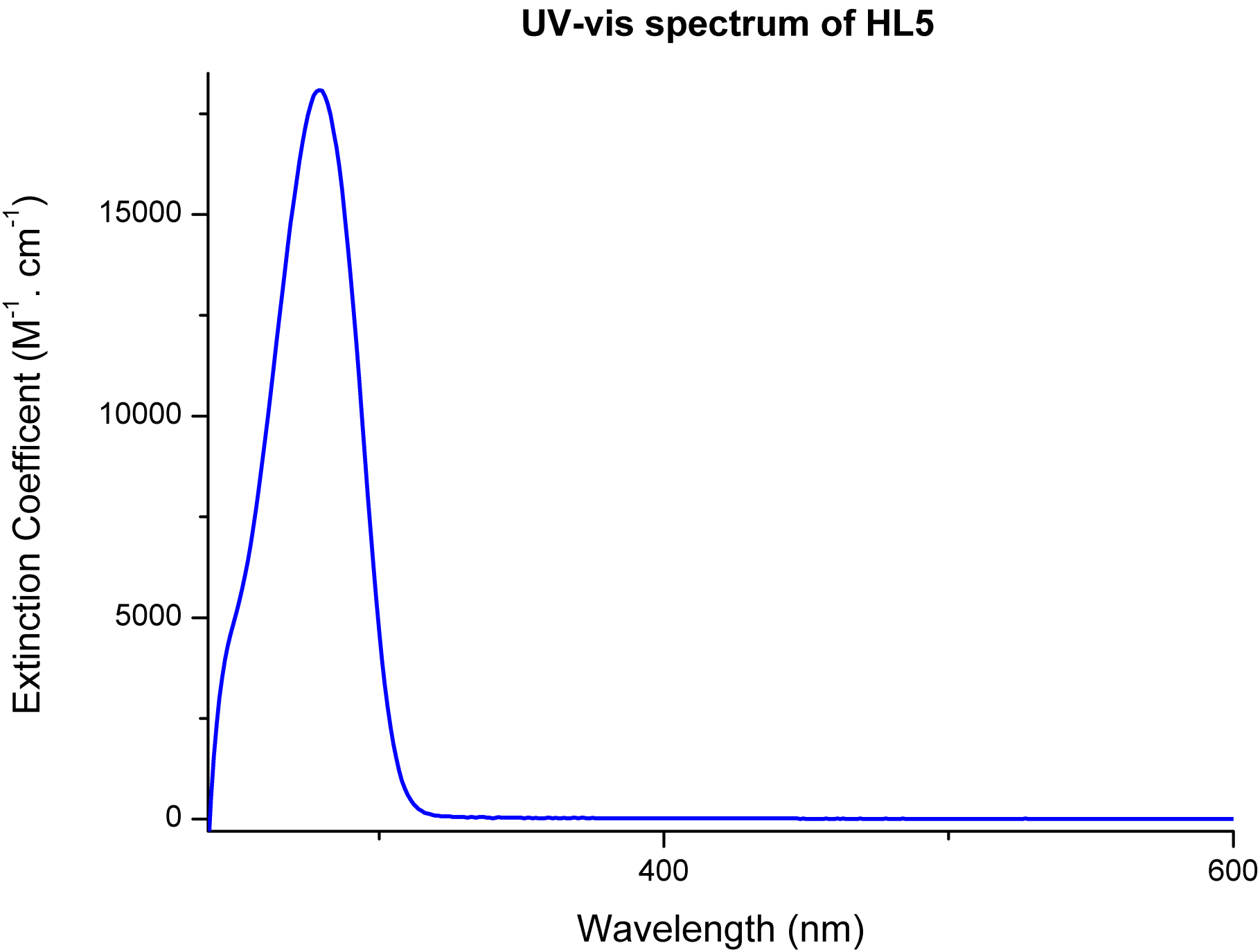
130
120
110
100
90
80
70
60
50
40


l
k
m
j
n
i
h
g
N
f
e
d
NH
a
c
b
j, k, l, m, n
h
g
f
b
d
c
a
10
8
6
4
[ppm]


UV-vis spectrum of HL5
Extinction Coefficent (M-1 . cm-1)
15000
10000
5000
0
400
600
Wavelength (nm)

A.1: Crystallographic Data Tables for [Au(L1)Cl_2]

Table A.1.1: Crystal data and structure refinement for [Au(L1)Cl_2].

Identification code	aupropyl_f	
Empirical formula	C8 H11 Au Cl2 N2	
Formula weight	403.05	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P ca21	
Unit cell dimensions	a = 19.6184(9) Å	□= 90°.
	b = 7.3679(4) Å	□= 90°.
	c = 7.2571(3) Å	□ = 90°.
Volume	1048.99(9) $Å^3$	
Z	4	
Density (calculated)	2.552 Mg/m^3	
Absorption coefficient	14.488 mm^{-1}	
F(000)	744	
Crystal size	0.55 x 0.20 x 0.03 mm^3	
Theta range for data collection	2.08 to 26.42°.	
Index ranges	-24<=h<=24, -9<=k<=9, -8<=l<=8	
Reflections collected	15023	
Independent reflections	2051 [R(int) = 0.0318]	
Completeness to theta = 26.42°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6704 and 0.0463	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2051 / 7 / 119	
Goodness-of-fit on F^2	0.752	
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0559	
R indices (all data)	R1 = 0.0223, wR2 = 0.0566	
Absolute structure parameter	0.277(14)	
Largest diff. peak and hole	1.038 and -1.057 $e.Å^{-3}$	

Table A.1.2: Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for [Au(L1)Cl_2]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	**x**	**y**	**z**	**U(eq)**
Au(1)	1676(1)	5807(1)	10018(1)	12(1)
Cl(1)	581(1)	6821(2)	9912(4)	22(1)
Cl(2)	2035(1)	8503(2)	11202(2)	21(1)
N(1)	2620(2)	4820(7)	9891(15)	17(1)
N(2)	1461(3)	3290(8)	9022(7)	12(1)
C(1)	2643(3)	3075(10)	9177(9)	16(1)
C(2)	3329(3)	2640(11)	8949(11)	21(2)
C(3)	3705(4)	4144(10)	9489(10)	21(2)
C(4)	3252(3)	5478(8)	10010(20)	16(1)
C(5)	2010(3)	2297(10)	8734(10)	18(1)
C(6)	781(3)	2558(10)	8622(10)	18(1)
C(7)	396(3)	2024(9)	10374(10)	16(2)
C(8)	-311(3)	1305(9)	9830(15)	18(2)

Table A.1.3: Bond lengths [Å] for [Au(L1)Cl_2].

Bond	**Length(Å)**	**Bond**	**Length(Å)**
Au(1)-N(1)	1.993(5)	C(3)-H(1)	0.9500
Au(1)-N(2)	2.034(6)	C(4)-H(2)	0.9500
Au(1)-Cl(2)	2.2760(17)	C(5)-H(11)	0.9500
Au(1)-Cl(1)	2.2754(13)	C(6)-C(7)	1.530(10)
N(1)-C(4)	1.334(8)	C(6)-H(4)	0.9900
N(1)-C(1)	1.387(10)	C(6)-H(10)	0.9900
N(2)-C(5)	1.319(9)	C(7)-C(8)	1.537(9)
N(2)-C(6)	1.469(8)	C(7)-H(9)	0.9900
C(1)-C(2)	1.392(9)	C(7)-H(8)	0.9900
C(1)-C(5)	1.404(10)	C(8)-H(7)	0.9800
C(2)-C(3)	1.388(11)	C(8)-H(6)	0.9800
C(2)-H(3)	0.9500	C(8)-H(5)	0.9800
C(3)-C(4)	1.378(10)		

Table A.1.4: Bond angles [°] for [Au(L1)Cl_2].

Bond	**Angle (°)**	**Bond**	**Angle (°)**
N(1)-Au(1)-N(2)	81.0(2)	C(2)-C(3)-H(1)	126.2
N(1)-Au(1)-Cl(2)	92.75(19)	N(1)-C(4)-C(3)	108.8(7)
N(2)-Au(1)-Cl(2)	173.54(16)	N(1)-C(4)-H(2)	125.6
N(1)-Au(1)-Cl(1)	174.9(3)	C(3)-C(4)-H(2)	125.6
N(2)-Au(1)-Cl(1)	95.29(16)	N(2)-C(5)-C(1)	117.4(7)
Cl(2)-Au(1)-Cl(1)	91.08(7)	N(2)-C(5)-H(11)	121.3
C(4)-N(1)-C(1)	109.3(6)	C(1)-C(5)-H(11)	121.3
C(4)-N(1)-Au(1)	136.8(5)	N(2)-C(6)-C(7)	112.2(6)
C(1)-N(1)-Au(1)	112.7(4)	N(2)-C(6)-H(4)	109.2
C(5)-N(2)-C(6)	120.5(6)	C(7)-C(6)-H(4)	109.2
C(5)-N(2)-Au(1)	113.2(5)	N(2)-C(6)-H(10)	109.2
C(6)-N(2)-Au(1)	126.3(4)	C(7)-C(6)-H(10)	109.2
C(2)-C(1)-N(1)	106.8(6)	H(4)-C(6)-H(10)	107.9
C(2)-C(1)-C(5)	137.1(7)	C(8)-C(7)-C(6)	108.6(6)
N(1)-C(1)-C(5)	115.8(6)	C(8)-C(7)-H(9)	110.0
C(3)-C(2)-C(1)	107.3(7)	C(6)-C(7)-H(9)	110.0
C(3)-C(2)-H(3)	126.4	C(8)-C(7)-H(8)	110.0
C(1)-C(2)-H(3)	126.4	C(6)-C(7)-H(8)	110.0
C(4)-C(3)-C(2)	107.7(6)	H(9)-C(7)-H(8)	108.3

Table A.1.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [au(l1)cl2]. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	10(1)	12(1)	13(1)	1(1)	1(1)	1(1)
Cl(1)	12(1)	24(1)	30(1)	1(1)	0(1)	7(1)
Cl(2)	24(1)	14(1)	25(1)	-2(1)	1(1)	-2(1)
N(1)	14(2)	22(2)	15(3)	1(4)	-3(4)	3(2)
N(2)	14(3)	13(3)	9(3)	-4(2)	-1(2)	1(2)
C(1)	15(3)	24(4)	10(3)	0(3)	-3(2)	2(3)
C(2)	14(3)	28(4)	20(4)	5(3)	-1(2)	9(3)
C(3)	12(3)	30(4)	21(5)	7(3)	-1(2)	2(3)
C(4)	14(2)	24(3)	11(3)	-3(5)	6(5)	-5(2)
C(5)	18(3)	21(4)	16(4)	0(3)	2(3)	-2(3)
C(6)	15(3)	18(3)	20(4)	-1(3)	0(3)	-1(3)
C(7)	18(3)	11(3)	17(5)	0(3)	0(3)	-2(2)
C(8)	12(2)	20(3)	22(5)	-1(4)	-3(3)	0(2)

A.2: Crystallograhic Data Tables for $[Au(L2)Cl_2]$.

Table A.2.1: Crystal data and structure refinement for $[Au(L2)Cl_2]$.

Identification code	ma_vc_auaniline	
Empirical formula	C11 H9 Au Cl2 N2	
Formula weight	437.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 18.4739(10) Å	□= 90°.
	b = 4.1151(2) Å	□= 99.534(2)°.
	c = 15.1775(8) Å	□ = 90°.
Volume	1137.89(10) $Å^3$	
Z	4	
Density (calculated)	2.551 Mg/m^3	
Absorption coefficient	13.368 mm^{-1}	
F(000)	808	
Crystal size	0.60 x 0.08 x 0.04 mm^3	
Theta range for data collection	2.24 to 26.07°.	
Index ranges	-20<=h<=22, -1<=k<=5, -17<=l<=18	
Reflections collected	8873	
Independent reflections	2214 [R(int) = 0.0226]	
Completeness to theta = 26.07°	98.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6169 and 0.0460	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2214 / 0 / 145	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0171, wR2 = 0.0402	
R indices (all data)	R1 = 0.0189, wR2 = 0.0411	
Largest diff. peak and hole	1.188 and -1.200 $e.Å^{-3}$	

Table A.2.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Au(L2)Cl_2]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
Au(1)	2849(1)	6855(1)	23(1)	12(1)
Cl(1)	1945(1)	10191(2)	-676(1)	17(1)
Cl(2)	3465(1)	7388(3)	-1147(1)	20(1)
N(1)	2408(2)	6051(8)	1162(2)	13(1)
N(2)	3634(2)	4114(8)	696(2)	13(1)
C(1)	1718(2)	7205(9)	1350(2)	13(1)
C(2)	1082(2)	6709(9)	733(3)	16(1)
C(3)	421(2)	7796(10)	922(3)	18(1)
C(4)	385(2)	9396(10)	1720(3)	18(1)
C(5)	1017(2)	9821(10)	2338(3)	17(1)
C(6)	1685(2)	8750(9)	2153(2)	14(1)
C(7)	2853(2)	4427(9)	1762(2)	13(1)
C(8)	3523(2)	3322(9)	1548(2)	15(1)
C(9)	4289(2)	2931(10)	578(3)	17(1)
C(10)	4605(2)	1322(10)	1356(3)	20(1)
C(11)	4129(2)	1558(9)	1966(3)	17(1)

Table A.2.3: Bond lengths [Å] for [Au(L2)Cl_2].

Bond	**Length(Å)**	**Bond**	**Length(Å)**
Au(1)-N(2)	1.982(3)	C(3)-C(4)	1.390(6)
Au(1)-N(1)	2.056(3)	C(3)-H(4)	0.9500
Au(1)-Cl(2)	2.2731(9)	C(4)-C(5)	1.383(5)
Au(1)-Cl(1)	2.2833(9)	C(4)-H(3)	0.9500
N(1)-C(7)	1.306(5)	C(5)-C(6)	1.382(5)
N(1)-C(1)	1.432(5)	C(5)-H(2)	0.9500
N(2)-C(9)	1.343(5)	C(6)-H(1)	0.9500
N(2)-C(8)	1.382(5)	C(7)-C(8)	1.406(5)
C(1)-C(6)	1.385(5)	C(7)-H(9)	0.9500
C(1)-C(2)	1.391(5)	C(8)-C(11)	1.396(5)
C(2)-C(3)	1.375(6)	C(9)-C(10)	1.395(6)

Table A.2.4: Bond angles [°] for [Au(L2)Cl_2].

Bond	Angle (°)	Bond	Angle (°)
N(2)-Au(1)-N(1)	80.42(12)	C(5)-C(4)-H(3)	120.2
N(2)-Au(1)-Cl(2)	92.25(9)	C(3)-C(4)-H(3)	120.2
N(1)-Au(1)-Cl(2)	172.66(9)	C(6)-C(5)-C(4)	120.2(4)
N(2)-Au(1)-Cl(1)	176.59(9)	C(6)-C(5)-H(2)	119.9
N(1)-Au(1)-Cl(1)	97.25(9)	C(4)-C(5)-H(2)	119.9
Cl(2)-Au(1)-Cl(1)	90.05(3)	C(5)-C(6)-C(1)	119.8(3)
C(7)-N(1)-C(1)	120.6(3)	C(5)-C(6)-H(1)	120.1
C(7)-N(1)-Au(1)	112.2(2)	C(1)-C(6)-H(1)	120.1
C(1)-N(1)-Au(1)	127.1(2)	N(1)-C(7)-C(8)	118.7(3)
C(9)-N(2)-C(8)	108.5(3)	N(1)-C(7)-H(9)	120.6
C(9)-N(2)-Au(1)	137.4(3)	C(8)-C(7)-H(9)	120.6
C(8)-N(2)-Au(1)	114.0(2)	N(2)-C(8)-C(11)	108.3(3)
C(6)-C(1)-C(2)	120.3(3)	N(2)-C(8)-C(7)	114.4(3)
C(6)-C(1)-N(1)	119.9(3)	C(11)-C(8)-C(7)	137.2(4)
C(2)-C(1)-N(1)	119.8(3)	N(2)-C(9)-C(10)	108.6(4)
C(3)-C(2)-C(1)	119.5(4)	N(2)-C(9)-H(8)	125.7
C(3)-C(2)-H(5)	120.3	C(10)-C(9)-H(8)	125.7
C(1)-C(2)-H(5)	120.3	C(11)-C(10)-C(9)	108.1(4)
C(2)-C(3)-C(4)	120.6(4)	C(11)-C(10)-H(7)	126.0
C(2)-C(3)-H(4)	119.7	C(9)-C(10)-H(7)	126.0
C(4)-C(3)-H(4)	119.7		

Table A.2.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L2)Cl_2]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	13(1)	13(1)	9(1)	0(1)	1(1)	-2(1)
Cl(1)	19(1)	17(1)	15(1)	2(1)	0(1)	2(1)
Cl(2)	20(1)	31(1)	12(1)	4(1)	6(1)	0(1)
N(1)	15(2)	16(2)	7(2)	0(1)	1(1)	-6(1)
N(2)	11(1)	14(2)	14(2)	-2(1)	1(1)	-3(1)
C(1)	14(2)	14(2)	13(2)	1(2)	5(2)	-3(2)
C(2)	18(2)	18(2)	14(2)	-2(2)	1(2)	-5(2)
C(3)	12(2)	20(2)	21(2)	2(2)	-1(2)	-4(2)
C(4)	16(2)	13(2)	27(2)	1(2)	9(2)	0(2)
C(5)	24(2)	17(2)	13(2)	-1(2)	7(2)	-2(2)
C(6)	19(2)	12(2)	12(2)	2(2)	3(2)	-4(2)
C(7)	17(2)	14(2)	9(2)	-2(2)	0(1)	-8(2)
C(8)	18(2)	15(2)	11(2)	0(2)	1(2)	-7(2)
C(9)	14(2)	19(2)	18(2)	-3(2)	2(2)	-5(2)
C(10)	15(2)	19(2)	24(2)	-1(2)	-2(2)	-1(2)
C(11)	18(2)	15(2)	14(2)	0(2)	-4(2)	-7(2)

A.3: Crystallographic Data Tables for [Au(L3)Cl_2]

Table A.3.1: Crystal data and structure refinement for [Au(L3)Cl_2].

Identification code	ma_vc_aubenzyl	
Empirical formula	C12 H11 Au Cl2 N2	
Formula weight	451.09	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21	
Unit cell dimensions	a = 7.096(5) Å	□= 90°.
	b = 4.557(5) Å	□= 99.298(5)°.
	c = 19.792(5) Å	□ = 90°.
Volume	631.6(8) $Å^3$	
Z	2	
Density (calculated)	2.372 Mg/m^3	
Absorption coefficient	12.046 mm^{-1}	
F(000)	420	
Crystal size	0.60 x 0.08 x 0.04 mm^3	
Theta range for data collection	2.09 to 26.51°.	
Index ranges	-8<=h<=8, -3<=k<=5, -24<=l<=24	
Reflections collected	5254	
Independent reflections	2029 [R(int) = 0.0241]	
Completeness to theta = 25.00°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6444 and 0.0521	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2029 / 7 / 154	
Goodness-of-fit on F^2	1.204	
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0788	
R indices (all data)	R1 = 0.0361, wR2 = 0.0792	
Absolute structure parameter	0.049(19)	
Largest diff. peak and hole	3.359 and -3.655 $e.Å^{-3}$	

Table A.3.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Au(L3)Cl_2] U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
C(1)	2990(16)	-2800(30)	9395(6)	15(3)
C(2)	1838(17)	-4830(30)	9663(6)	16(3)
C(3)	77(16)	-4930(30)	9220(6)	14(3)
C(4)	245(15)	-3020(30)	8693(6)	11(3)
C(5)	-928(17)	-1910(30)	8106(6)	13(3)
C(6)	-1510(14)	1360(60)	7134(5)	15(3)
C(7)	-1925(17)	-670(30)	6545(6)	14(3)
C(8)	-3712(19)	-1970(30)	6385(7)	20(3)
C(9)	-4078(16)	-3980(70)	5843(6)	27(3)
C(10)	-2670(20)	-4580(30)	5456(6)	26(4)
C(11)	-890(20)	-3350(50)	5612(6)	27(5)
C(12)	-490(20)	-1420(30)	6147(6)	19(3)
N(1)	2076(13)	-1740(30)	8812(5)	12(2)
N(2)	-296(13)	50(30)	7731(5)	10(2)
Cl(1)	5579(4)	1933(7)	8591(2)	17(1)
Cl(2)	2891(4)	4176(8)	7216(2)	18(1)
Au(1)	2517(1)	1074(2)	8090(1)	11(1)

Table A.3.3: Bond lengths [Å] for [Au(L3)Cl_2].

Bond	Length(Å)	Bond	Length(Å)
C(1)-N(1)	1.320(16)	C(7)-C(12)	1.426(18)
C(1)-C(2)	1.394(18)	C(8)-C(9)	1.40(3)
C(2)-C(3)	1.407(16)	C(9)-C(10)	1.38(2)
C(3)-C(4)	1.378(17)	C(10)-C(11)	1.37(2)
C(4)-N(1)	1.408(15)	C(11)-C(12)	1.37(2)
C(4)-C(5)	1.409(17)	N(1)-Au(1)	1.983(12)
C(5)-N(2)	1.288(17)	N(2)-Au(1)	2.061(9)
C(6)-N(2)	1.474(17)	Cl(1)-Au(1)	2.272(3)
C(6)-C(7)	1.48(2)	Cl(2)-Au(1)	2.283(3)
C(7)-C(8)	1.390(18)		

Table A.3.4: Bond lengths [Å] for [Au(L3)Cl_2].

Bond	Angle (°)	Bond	Angle (°)
N(1)-C(1)-C(2)	109.8(11)	C(10)-C(11)-C(12)	120.4(14)
C(1)-C(2)-C(3)	107.6(11)	C(11)-C(12)-C(7)	120.3(14)
C(4)-C(3)-C(2)	105.9(11)	C(1)-N(1)-C(4)	107.8(11)
C(3)-C(4)-N(1)	109.0(10)	C(1)-N(1)-Au(1)	138.9(9)
C(3)-C(4)-C(5)	137.6(11)	C(4)-N(1)-Au(1)	113.3(8)
N(1)-C(4)-C(5)	113.3(11)	C(5)-N(2)-C(6)	122.2(11)
N(2)-C(5)-C(4)	120.6(12)	C(5)-N(2)-Au(1)	111.5(8)
N(2)-C(6)-C(7)	113.0(18)	C(6)-N(2)-Au(1)	126.3(9)
C(8)-C(7)-C(12)	118.6(13)	N(1)-Au(1)-N(2)	81.1(4)
C(8)-C(7)-C(6)	120.3(11)	N(1)-Au(1)-Cl(1)	92.8(3)
C(12)-C(7)-C(6)	121.1(11)	N(2)-Au(1)-Cl(1)	173.7(3)
C(7)-C(8)-C(9)	120.2(13)	N(1)-Au(1)-Cl(2)	176.7(3)
C(10)-C(9)-C(8)	119.4(14)	N(2)-Au(1)-Cl(2)	96.0(3)
C(11)-C(10)-C(9)	121.2(15)	Cl(1)-Au(1)-Cl(2)	90.21(12)

Table A.3.4: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L3)Cl_2]. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	9(5)	22(8)	14(6)	-7(5)	2(5)	0(5)
C(2)	21(6)	12(7)	12(5)	-3(5)	-4(5)	6(5)
C(3)	12(5)	12(7)	19(6)	-1(5)	5(4)	0(5)
C(4)	8(5)	8(8)	19(6)	-5(5)	4(4)	-4(4)
C(5)	15(6)	5(7)	18(6)	-5(5)	3(5)	4(5)
C(6)	12(4)	17(7)	16(4)	7(7)	1(3)	-7(7)
C(7)	13(6)	10(8)	17(6)	8(5)	-2(5)	0(5)
C(8)	18(6)	10(8)	29(7)	8(6)	-8(5)	-4(6)
C(9)	27(6)	14(8)	34(6)	4(13)	-14(5)	-15(12)
C(10)	51(9)	6(11)	17(6)	0(5)	-8(6)	0(6)
C(11)	42(8)	17(16)	22(6)	2(7)	2(5)	-2(8)
C(12)	30(7)	10(8)	18(6)	0(6)	3(5)	10(6)
N(1)	8(5)	15(7)	15(5)	-6(5)	4(4)	5(5)
N(2)	4(4)	10(6)	17(5)	-1(4)	7(4)	-1(4)
Cl(1)	10(1)	14(2)	27(2)	-3(1)	3(1)	-4(1)
Cl(2)	18(2)	11(2)	26(2)	4(1)	6(1)	-2(1)
Au(1)	11(1)	7(1)	16(1)	-1(1)	3(1)	-1(1)

A.4: Crystallographic Data Tables for [Au(L4)Cl_2].

Table A.4.1: Crystal data and structure refinement for [Au(L4)Cl_2].

Identification code	ma_vc_aumenapth	
Empirical formula	C16 H13 Au Cl2 N2	
Formula weight	501.15	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 4.8648(3) Å	□= 90°.
	b = 13.9634(8) Å	□= 90.0500(10)°.
	c = 21.7386(13) Å	□ = 90°.
Volume	1476.68(15) $Å^3$	
Z	4	
Density (calculated)	2.254 Mg/m^3	
Absorption coefficient	10.317 mm^{-1}	
F(000)	944	
Crystal size	0.45 x 0.12 x 0.07 mm^3	
Theta range for data collection	1.73 to 26.12°.	
Index ranges	-5<=h<=5, -17<=k<=17, -26<=l<=26	
Reflections collected	11020	
Independent reflections	2100 [R(int) = 0.0306]	
Completeness to theta = 26.12°	71.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.5320 and 0.0901	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2100 / 0 / 190	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0188, wR2 = 0.0448	
R indices (all data)	R1 = 0.0221, wR2 = 0.0457	
Largest diff. peak and hole	0.789 and -0.569 e.$Å^{-3}$	

Table A.4.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Au(L4)Cl_2]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
Au(1)	10079(1)	8327(1)	2115(1)	17(1)
Cl(1)	13550(3)	9130(1)	2591(1)	26(1)
Cl(2)	9804(3)	9490(1)	1388(1)	26(1)
N(1)	9888(8)	7238(2)	2743(2)	16(1)
N(2)	7163(9)	7539(2)	1725(2)	20(1)
C(2)	6651(11)	6691(3)	2039(2)	19(1)
C(3)	4576(10)	6213(3)	1717(2)	21(1)
C(4)	3872(11)	6772(3)	1210(2)	20(1)
C(5)	5523(11)	7585(3)	1231(2)	21(1)
C(6)	8122(11)	6575(3)	2579(2)	20(1)
C(7)	11444(10)	7160(3)	3332(2)	20(1)
C(8)	9552(10)	7019(3)	3881(2)	19(1)
C(9)	9488(11)	6156(3)	4175(2)	22(1)
C(10)	7703(11)	5998(3)	4677(2)	25(1)
C(11)	5992(12)	6689(3)	4875(2)	24(1)
C(12)	5936(10)	7606(3)	4583(2)	20(1)
C(13)	4085(12)	8328(3)	4771(2)	25(1)
C(14)	4103(11)	9198(3)	4496(2)	26(1)
C(15)	6049(11)	9400(3)	4029(2)	24(1)
C(16)	7812(10)	8714(3)	3829(2)	20(1)
C(17)	7814(10)	7783(3)	4087(2)	19(1)

Table A.4.3: Bond lengths [Å] for [Au(L4)Cl_2].

Bond	Length(Å)	Bond	Length(Å)
Au(1)-N(2)	1.985(4)	C(11)-C(12)	1.430(6)
Au(1)-N(1)	2.045(3)	C(11)-H(9)	0.9500
Au(1)-Cl(2)	2.2697(11)	C(12)-C(13)	1.412(6)
Au(1)-Cl(1)	2.2748(13)	C(12)-C(17)	1.435(5)
N(1)-C(6)	1.312(6)	C(13)-C(14)	1.353(6)
N(1)-C(7)	1.492(6)	C(13)-H(5)	0.9500
N(2)-C(5)	1.339(6)	C(7)-H(11)	0.9900
N(2)-C(2)	1.390(5)	C(8)-C(9)	1.365(6)
C(2)-C(6)	1.383(7)	C(8)-C(17)	1.433(6)
C(2)-C(3)	1.398(7)	C(9)-C(10)	1.412(5)
C(3)-C(4)	1.393(7)	C(9)-H(10)	0.9500
C(3)-H(1)	0.9500	C(10)-C(11)	1.345(6)
C(4)-C(5)	1.391(6)	C(10)-H(4)	0.9500
C(4)-H(2)	0.9500	C(14)-C(15)	1.417(6)
C(5)-H(3)	0.9500	C(14)-H(6)	0.9500
C(6)-H(13)	0.9500	C(15)-C(16)	1.357(6)
C(7)-C(8)	1.521(5)	C(15)-H(7)	0.9500
C(7)-H(12)	0.9900	C(16)-C(17)	1.416(6)
Au(1)-N(2)	1.985(4)	C(16)-H(8)	0.9500

Table A.4.4: Bond angles [°] for [Au(L4)Cl_2].

Bond	Angle	Bond	Angle	Bond	Angle
N(2)-Au(1)-N(1)	80.79(16)	N(2)-C(5)-C(4)	109.4(4)	C(10)-C(11)-C(12)	120.8(4)
N(2)-Au(1)-Cl(2)	93.29(11)	N(2)-C(5)-H(3)	125.3	C(10)-C(11)-H(9)	119.6
N(1)-Au(1)-Cl(2)	173.58(13)	C(4)-C(5)-H(3)	125.3	C(12)-C(11)-H(9)	119.6
N(2)-Au(1)-Cl(1)	175.84(11)	N(1)-C(6)-C(2)	119.1(4)	C(13)-C(12)-C(11)	121.5(4)
N(1)-Au(1)-Cl(1)	95.59(13)	N(1)-C(6)-H(13)	120.5	C(13)-C(12)-C(17)	120.1(4)
Cl(2)-Au(1)-Cl(1)	90.41(5)	C(2)-C(6)-H(13)	120.5	C(11)-C(12)-C(17)	118.4(4)
C(6)-N(1)-C(7)	120.9(4)	N(1)-C(7)-C(8)	112.1(4)	C(14)-C(13)-C(12)	120.6(4)
C(6)-N(1)-Au(1)	111.9(3)	N(1)-C(7)-H(12)	109.2	C(14)-C(13)-H(5)	119.7
C(7)-N(1)-Au(1)	127.1(3)	C(8)-C(7)-H(12)	109.2	C(12)-C(13)-H(5)	119.7
C(5)-N(2)-C(2)	109.2(4)	N(1)-C(7)-H(11)	109.2	C(13)-C(14)-C(15)	120.0(4)
C(5)-N(2)-Au(1)	137.8(3)	C(8)-C(7)-H(11)	109.2	C(13)-C(14)-H(6)	120.0
C(2)-N(2)-Au(1)	113.0(3)	H(12)-C(7)-H(11)	107.9	C(15)-C(14)-H(6)	120.0
C(6)-C(2)-N(2)	115.1(4)	C(9)-C(8)-C(17)	119.8(4)	C(16)-C(15)-C(14)	120.7(4)
C(6)-C(2)-C(3)	138.0(4)	C(9)-C(8)-C(7)	119.8(4)	C(16)-C(15)-H(7)	119.6
N(2)-C(2)-C(3)	106.8(4)	C(17)-C(8)-C(7)	120.4(4)	C(14)-C(15)-H(7)	119.6
C(4)-C(3)-C(2)	107.9(4)	C(8)-C(9)-C(10)	120.9(4)	C(15)-C(16)-C(17)	121.5(4)
C(4)-C(3)-H(1)	126.1	C(8)-C(9)-H(10)	119.5	C(15)-C(16)-H(8)	119.3
C(2)-C(3)-H(1)	126.1	C(10)-C(9)-H(10)	119.5	C(17)-C(16)-H(8)	119.3
C(5)-C(4)-C(3)	106.8(5)	C(11)-C(10)-C(9)	121.1(4)	C(16)-C(17)-C(8)	124.1(4)
C(5)-C(4)-H(2)	126.6	C(11)-C(10)-H(4)	119.4	C(16)-C(17)-C(12)	117.1(4)
C(3)-C(4)-H(2)	126.6	C(9)-C(10)-H(4)	119.4	C(8)-C(17)-C(12)	118.8(4)

Table A.4.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L4)Cl2]. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	17(1)	16(1)	17(1)	-2(1)	4(1)	1(1)
Cl(1)	22(1)	27(1)	28(1)	-8(1)	5(1)	-4(1)
Cl(2)	34(1)	20(1)	25(1)	4(1)	4(1)	-2(1)
N(1)	17(3)	20(2)	12(2)	1(1)	0(2)	6(2)
N(2)	26(3)	17(2)	18(2)	-3(2)	8(2)	-1(2)
C(2)	23(3)	17(2)	17(2)	-3(2)	5(2)	2(2)
C(3)	20(3)	22(2)	22(2)	-4(2)	4(2)	-3(2)
C(4)	19(3)	27(2)	15(2)	-7(2)	-3(2)	-3(2)
C(5)	26(3)	24(2)	13(2)	0(2)	6(2)	6(2)
C(6)	24(3)	17(2)	20(2)	-1(2)	9(3)	2(2)
C(7)	15(3)	24(2)	21(2)	0(2)	-1(2)	7(2)
C(8)	16(3)	25(2)	17(2)	1(2)	-3(2)	1(2)
C(9)	22(3)	25(2)	21(2)	0(2)	-7(2)	5(2)
C(10)	30(3)	27(2)	17(2)	3(2)	-4(2)	-1(2)
C(11)	22(3)	36(3)	13(2)	3(2)	-5(2)	-6(2)
C(12)	17(3)	29(2)	14(2)	-3(2)	-3(2)	-3(2)
C(13)	21(3)	37(3)	16(2)	-7(2)	3(2)	-4(2)
C(14)	22(3)	25(2)	31(3)	-12(2)	1(3)	-1(2)
C(15)	29(3)	21(2)	22(2)	-2(2)	-1(2)	3(2)
C(16)	21(3)	20(2)	18(2)	2(2)	-2(2)	0(2)
C(17)	17(3)	25(2)	16(2)	-4(2)	-2(2)	-2(2)

A.5: Crystallographic Data Tables for [Au(L5)Cl_2]

Table A.5.1: Crystal data and structure refinement for [Au(L5)Cl_2].

Identification code	ma_vc_auphet	
Empirical formula	C13 H13 Au Cl2 N2	
Formula weight	465.12	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 19.0672(14) Å	□= 90°.
	b = 7.2240(4) Å	□= 92.602(3)°.
	c = 20.2020(14) Å	□ = 90°.
Volume	2779.8(3) $Å^3$	
Z	8	
Density (calculated)	2.223 Mg/m^3	
Absorption coefficient	10.951 mm^{-1}	
F(000)	1744	
Crystal size	0.60 x 0.21 x 0.15 mm^3	
Theta range for data collection	1.44 to 28.27°.	
Index ranges	-25<=h<=23, -9<=k<=6, -26<=l<=26	
Reflections collected	27670	
Independent reflections	6757 [R(int) = 0.0408]	
Completeness to theta = 28.27°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2904 and 0.0585	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6757 / 6 / 325	
Goodness-of-fit on F^2	1.141	
Final R indices [I>2sigma(I)]	R1 = 0.0656, wR2 = 0.1762	
R indices (all data)	R1 = 0.0708, wR2 = 0.1788	
Largest diff. peak and hole	6.974 and -3.275 e.$Å^{-3}$	

Table A.5.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Au(L5)Cl_2]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Au(1)	467(1)	10133(1)	3777(1)	12(1)
Au(2)	1258(1)	10383(1)	-453(1)	14(1)
Cl(1)	-412(2)	12108(6)	3427(2)	23(1)
Cl(2)	385(2)	8557(6)	2804(2)	22(1)
Cl(3)	1577(2)	12330(6)	398(2)	24(1)
Cl(4)	2323(2)	8959(6)	-388(2)	26(1)
N(1)	592(6)	11337(18)	4661(6)	14(2)
C(7)	1239(8)	5270(20)	3861(8)	18(3)
C(9)	1278(8)	3640(20)	2762(7)	18(3)
C(4)	1149(8)	10610(20)	5047(7)	14(3)
C(3)	1191(8)	11590(20)	5637(7)	17(3)
C(2)	657(8)	12910(20)	5619(8)	20(3)
C(1)	294(8)	12690(20)	5001(8)	18(3)
C(5)	1515(7)	9150(20)	4744(7)	15(3)
N(2)	1283(6)	8618(17)	4152(6)	16(2)
C(6)	1637(8)	7100(20)	3800(7)	15(3)
C(8)	1534(8)	3810(20)	3425(8)	20(3)
C(10)	1573(9)	2370(30)	2343(9)	26(4)
C(11)	2104(9)	1200(20)	2567(9)	27(4)
C(12)	2373(9)	1400(20)	3215(8)	20(3)
C(13)	2093(8)	2670(20)	3642(8)	18(3)
N(4)	878(7)	8898(18)	-1251(6)	16(2)
C(18)	252(7)	9400(20)	-1452(7)	13(3)
C(17)	-85(8)	10790(20)	-1098(7)	16(3)
N(3)	308(6)	11474(18)	-565(6)	13(2)
C(14)	-76(8)	12755(19)	-255(7)	14(3)
C(15)	-723(8)	12940(20)	-590(7)	18(3)
C(16)	-730(9)	11680(20)	-1134(8)	23(3)
C(19)	1245(8)	7400(20)	-1583(8)	19(3)
C(20)	1143(9)	5530(20)	-1235(7)	19(3)
C(21)	1554(8)	4010(20)	-1553(7)	14(3)
C(22)	1267(8)	3020(20)	-2088(8)	20(3)
C(23)	1652(11)	1640(20)	-2385(8)	30(4)
C(24)	2332(10)	1300(20)	-2158(9)	30(4)

C(25)	2621(9)	2300(30)	-1629(10)	29(4)
C(26)	2240(8)	3660(20)	-1339(8)	18(3)

Table A.5.3: Bond lengths [Å] for $[Au(L5)Cl_2]$.

Bond	**Length(Å)**	**Bond**	**Length(Å)**	**Bond**	**Length(Å)**
Au(1)-N(1)	1.991(13)	C(2)-H(2)	0.9500	C(14)-C(15)	1.39(2)
Au(1)-N(2)	2.021(12)	C(1)-H(1)	0.9500	C(14)-H(14)	0.9500
Au(1)-Cl(2)	2.271(4)	C(5)-N(2)	1.313(18)	C(15)-C(16)	1.42(2)
Au(1)-Cl(1)	2.288(4)	C(5)-H(5)	0.9500	C(15)-H(15)	0.9500
Au(2)-N(3)	1.979(12)	N(2)-C(6)	1.486(19)	C(16)-H(16)	0.9500
Au(2)-N(4)	2.041(13)	C(6)-H(6A)	0.9900	C(19)-C(20)	1.54(2)
Au(2)-Cl(4)	2.276(4)	C(6)-H(6B)	0.9900	C(19)-H(19A)	0.9900
Au(2)-Cl(3)	2.283(4)	C(8)-C(13)	1.40(2)	C(19)-H(19B)	0.9900
N(1)-C(1)	1.33(2)	C(10)-C(11)	1.38(3)	C(20)-C(21)	1.513(19)
N(1)-C(4)	1.392(17)	C(10)-H(10)	0.9500	C(20)-H(20A)	0.9900
C(7)-C(8)	1.50(2)	C(11)-C(12)	1.39(2)	C(20)-H(20B)	0.9900
C(7)-C(6)	1.53(2)	C(11)-H(11)	0.9500	C(21)-C(22)	1.39(2)
C(7)-H(7A)	0.9900	C(12)-C(13)	1.38(2)	C(21)-C(26)	1.38(2)
C(7)-H(7B)	0.9900	C(12)-H(12)	0.9500	C(22)-C(23)	1.39(2)
C(9)-C(10)	1.39(2)	C(13)-H(13)	0.9500	C(22)-H(22)	0.9500
C(9)-C(8)	1.41(2)	N(4)-C(18)	1.296(18)	C(23)-C(24)	1.38(3)
C(9)-H(9)	0.9500	N(4)-C(19)	1.465(18)	C(23)-H(23)	0.9500
C(4)-C(3)	1.39(2)	C(18)-C(17)	1.40(2)	C(24)-C(25)	1.38(3)
C(4)-C(5)	1.42(2)	C(18)-H(18)	0.9500	C(24)-H(24)	0.9500
C(3)-C(2)	1.39(2)	C(17)-N(3)	1.376(18)	C(25)-C(26)	1.37(2)
C(3)-H(3)	0.9500	C(17)-C(16)	1.39(2)	C(25)-H(25)	0.9500
C(2)-C(1)	1.41(2)	N(3)-C(14)	1.351(18)	C(26)-H(26)	0.9500

Table A.5.4: Bond angles [°] for [Au(L5)Cl_2].

Bond	Angle (°)	Bond	Angle (°)	Bond	Angle (°)
(5)-N(2)-C(6)	120.8(12)	C(5)-N(2)-C(6)	120.8(12)	C(14)-C(15)-C(16)	107.1(13)
C(5)-N(2)-Au(1)	113.8(10)	C(5)-N(2)-Au(1)	113.8(10)	C(14)-C(15)-H(15)	126.5
C(6)-N(2)-Au(1)	125.4(9)	C(6)-N(2)-Au(1)	125.4(9)	C(16)-C(15)-H(15)	126.5
N(2)-C(6)-C(7)	111.2(12)	N(2)-C(6)-C(7)	111.2(12)	C(17)-C(16)-C(15)	106.1(14)
N(2)-C(6)-H(6A)	109.4	N(2)-C(6)-H(6A)	109.4	C(17)-C(16)-H(16)	127.0
C(7)-C(6)-H(6A)	109.4	C(7)-C(6)-H(6A)	109.4	C(15)-C(16)-H(16)	126.9
N(2)-C(6)-H(6B)	109.4	N(2)-C(6)-H(6B)	109.4	N(4)-C(19)-C(20)	111.3(12)
C(7)-C(6)-H(6B)	109.4	C(7)-C(6)-H(6B)	109.4	N(4)-C(19)-H(19A)	109.4
H(6A)-C(6)-H(6B)	108.0	H(6A)-C(6)-H(6B)	108.0	C(20)-C(19)-H(19A)	109.4
C(13)-C(8)-C(9)	118.2(14)	C(13)-C(8)-C(9)	118.2(14)	N(4)-C(19)-H(19B)	109.4
C(13)-C(8)-C(7)	122.1(15)	C(13)-C(8)-C(7)	122.1(15)	C(20)-C(19)-H(19B)	109.4
C(9)-C(8)-C(7)	119.6(15)	C(9)-C(8)-C(7)	119.6(15)	H(19A)-C(19)-H(19B)	108.0
C(11)-C(10)-C(9)	121.3(16)	C(11)-C(10)-C(9)	121.3(16)	C(21)-C(20)-C(19)	111.5(11)
C(11)-C(10)-H(10)	119.4	C(11)-C(10)-H(10)	119.4	C(21)-C(20)-H(20A)	109.3
C(9)-C(10)-H(10)	119.4	C(9)-C(10)-H(10)	119.4	C(19)-C(20)-H(20A)	109.3
C(10)-C(11)-C(12)	118.8(15)	C(10)-C(11)-C(12)	118.8(15)	C(21)-C(20)-H(20B)	109.3
C(10)-C(11)-H(11)	120.6	C(10)-C(11)-H(11)	120.6	C(19)-C(20)-H(20B)	109.3
C(12)-C(11)-H(11)	120.6	C(12)-C(11)-H(11)	120.6	H(20A)-C(20)-H(20B)	108.0
C(13)-C(12)-C(11)	121.1(15)	C(13)-C(12)-C(11)	121.1(15)	C(22)-C(21)-C(26)	119.1(14)
C(13)-C(12)-H(12)	119.5	C(13)-C(12)-H(12)	119.5	C(22)-C(21)-C(20)	120.9(14)
C(11)-C(12)-H(12)	119.5	C(11)-C(12)-H(12)	119.5	C(26)-C(21)-C(20)	120.0(14)
C(12)-C(13)-C(8)	120.4(15)	C(12)-C(13)-C(8)	120.4(15)	C(21)-C(22)-C(23)	120.5(15)
C(12)-C(13)-H(13)	119.8	C(12)-C(13)-H(13)	119.8	C(21)-C(22)-H(22)	119.8
C(8)-C(13)-H(13)	119.8	C(8)-C(13)-H(13)	119.8	C(23)-C(22)-H(22)	119.8
C(18)-N(4)-C(19)	121.1(13)	C(18)-N(4)-C(19)	121.1(13)	C(24)-C(23)-C(22)	119.5(16)
C(18)-N(4)-Au(2)	112.8(10)	C(18)-N(4)-Au(2)	112.8(10)	C(24)-C(23)-H(23)	120.3
C(19)-N(4)-Au(2)	126.1(10)	C(19)-N(4)-Au(2)	126.1(10)	C(22)-C(23)-H(23)	120.3
N(4)-C(18)-C(17)	118.5(13)	N(4)-C(18)-C(17)	118.5(13)	C(25)-C(24)-C(23)	119.9(15)
N(4)-C(18)-H(18)	120.7	N(4)-C(18)-H(18)	120.7	C(25)-C(24)-H(24)	120.0
C(17)-C(18)-H(18)	120.7	C(17)-C(18)-H(18)	120.7	C(23)-C(24)-H(24)	120.0
N(3)-C(17)-C(16)	108.8(13)	N(3)-C(17)-C(16)	108.8(13)	C(26)-C(25)-C(24)	120.4(16)
N(3)-C(17)-C(18)	114.3(13)	N(3)-C(17)-C(18)	114.3(13)	C(26)-C(25)-H(25)	119.8
C(16)-C(17)-C(18)	136.9(14)	C(16)-C(17)-C(18)	136.9(14)	C(24)-C(25)-H(25)	119.8
C(14)-N(3)-C(17)	108.8(12)	C(14)-N(3)-C(17)	108.8(12)	C(25)-C(26)-C(21)	120.5(15)
C(14)-N(3)-Au(2)	137.1(10)	C(14)-N(3)-Au(2)	137.1(10)	C(25)-C(26)-H(26)	119.8

C(17)-N(3)-Au(2)	114.1(10)	C(17)-N(3)-Au(2)	114.1(10)	C(21)-C(26)-H(26)	119.8
N(3)-C(14)-C(15)	109.2(13)	N(3)-C(14)-C(15)	109.2(13)		
N(3)-C(14)-H(14)	125.4	N(3)-C(14)-H(14)	125.4		

Table A.5.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L5)Cl_2]. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	9(1)	15(1)	13(1)	0(1)	-1(1)	-1(1)
Au(2)	12(1)	16(1)	14(1)	3(1)	2(1)	3(1)
Cl(1)	18(2)	24(2)	26(2)	3(2)	-6(1)	5(1)
Cl(2)	22(2)	27(2)	15(2)	-4(1)	-6(1)	-2(2)
Cl(3)	20(2)	27(2)	24(2)	-4(2)	-5(1)	0(2)
Cl(4)	16(2)	34(2)	28(2)	3(2)	0(1)	11(2)
N(1)	3(5)	17(6)	23(6)	3(5)	0(4)	-1(4)
C(7)	19(7)	13(7)	23(7)	-3(6)	8(6)	3(6)
C(9)	11(6)	22(6)	21(6)	2(5)	3(5)	-11(5)
C(4)	15(7)	13(6)	13(6)	-1(5)	-7(5)	0(5)
C(3)	16(7)	19(7)	16(7)	2(6)	3(5)	-2(6)
C(2)	14(7)	24(8)	22(7)	-5(6)	6(6)	-4(6)
C(1)	21(7)	12(7)	21(7)	3(6)	4(6)	-2(6)
C(5)	12(7)	20(7)	14(6)	-3(5)	3(5)	2(5)
N(2)	14(6)	13(6)	19(6)	-3(5)	-4(5)	1(5)
C(6)	13(7)	16(7)	17(7)	-3(5)	0(5)	-4(5)
C(8)	19(7)	16(7)	24(8)	-1(6)	8(6)	0(6)
C(10)	18(8)	33(9)	27(8)	-8(7)	9(6)	-11(7)
C(11)	32(9)	21(8)	29(9)	-13(7)	17(7)	-4(7)
C(12)	23(8)	13(7)	25(8)	6(6)	8(6)	3(6)
C(13)	18(7)	13(7)	22(7)	1(6)	8(6)	0(6)
N(4)	21(6)	17(6)	11(5)	0(5)	2(5)	8(5)
C(18)	15(7)	14(6)	10(6)	1(5)	-3(5)	5(5)
C(17)	18(7)	20(7)	10(6)	3(5)	0(5)	-2(6)
N(3)	6(5)	18(6)	16(6)	-1(5)	3(4)	2(4)
C(14)	16(7)	8(6)	19(7)	2(5)	4(5)	-1(5)
C(15)	21(7)	16(7)	17(7)	1(6)	5(6)	5(6)
C(16)	28(8)	27(8)	13(7)	4(6)	2(6)	5(7)
C(19)	23(8)	15(7)	19(7)	4(6)	3(6)	11(6)
C(20)	25(8)	18(7)	15(7)	2(6)	13(6)	7(6)
C(21)	18(7)	10(6)	15(6)	6(5)	4(5)	4(5)
C(22)	9(6)	28(8)	23(7)	1(6)	2(5)	-5(6)
C(23)	53(12)	20(8)	19(8)	-10(6)	16(8)	-20(8)
C(24)	35(10)	16(7)	42(10)	2(7)	31(8)	6(7)
C(25)	14(8)	29(9)	45(11)	14(8)	10(7)	7(7)
C(26)	13(7)	20(7)	19(7)	3(6)	1(5)	1(6)

A.1: Crystallographic Data Tables for HL2

Table A.1.1: Crystal data and structure refinement for HL2.

Identification code	HL2	
Empirical formula	$C_{11} H_{10} N_2$	
Formula weight	170.21	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P bca	
Unit cell dimensions	a = 9.4092(8) Å	α = 90°.
	b = 18.1595(16) Å	β = 90°.
	c = 21.2310(18) Å	γ = 90°.
Volume	3627.7(5) $Å^3$	
Z	16	
Density (calculated)	1.247 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	1440	
Crystal size	0.56 x 0.42 x 0.30 mm^3	
Theta range for data collection	2.44 to 26.00°.	
Index ranges	-11<=h<=8, -22<=k<=12, -21<=l<=26	
Reflections collected	14939	
Independent reflections	3555 [R(int) = 0.0258]	
Completeness to theta = 26.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.991 and 0.962	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3555 / 0 / 243	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.0879	
R indices (all data)	R1 = 0.0418, wR2 = 0.0922	
Largest diff. peak and hole	0.180 and -0.261 $e.Å^{-3}$	

Table A.1.2: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for HL2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
N(1)	2683(1)	1222(1)	4113(1)	19(1)
N(2)	4374(1)	2264(1)	4853(1)	19(1)
N(3)	3088(1)	65(1)	5105(1)	20(1)
N(4)	4057(1)	1248(1)	5950(1)	21(1)
C(1)	551(1)	-291(1)	2946(1)	24(1)
C(2)	1875(1)	-26(1)	2766(1)	24(1)
C(3)	2588(1)	480(1)	3140(1)	20(1)
C(4)	1974(1)	730(1)	3700(1)	18(1)
C(5)	3308(1)	1783(1)	3868(1)	19(1)
C(6)	4121(1)	2307(1)	4217(1)	19(1)
C(7)	5243(1)	2824(1)	5026(1)	21(1)
C(8)	-61(1)	-46(1)	3502(1)	23(1)
C(9)	644(1)	458(1)	3881(1)	21(1)
C(10)	5544(1)	3245(1)	4506(1)	24(1)
C(11)	4838(1)	2923(1)	3994(1)	24(1)
C(12)	2666(1)	-603(1)	4881(1)	24(1)
C(13)	3639(1)	-25(1)	5698(1)	20(1)
C(14)	4130(1)	561(1)	6091(1)	21(1)
C(15)	4586(1)	1758(1)	6402(1)	23(1)
C(16)	5837(2)	1637(1)	6740(1)	29(1)
C(17)	6288(2)	2152(1)	7181(1)	38(1)
C(18)	5525(2)	2793(1)	7277(1)	40(1)
C(19)	2931(1)	-1129(1)	5333(1)	26(1)
C(20)	3836(2)	2413(1)	6491(1)	28(1)
C(21)	4307(2)	2927(1)	6925(1)	35(1)
C(22)	3544(1)	-768(1)	5847(1)	25(1)

Table A.1.3: Bond lengths [Å] for HL2.

Bond	**Length(Å)**	**Bond**	**Length(Å)**
N(1)-C(5)	1.2862(16)	N(1)-C(5)	1.2862(16)
N(1)-C(4)	1.4198(15)	C(9)-H(9)	0.9300
N(2)-C(7)	1.3553(15)	C(10)-C(11)	1.4029(18)
N(2)-C(6)	1.3746(16)	C(10)-H(10)	0.9300
N(2)-H(101)	0.877(16)	C(11)-H(11)	0.9300
N(3)-C(12)	1.3609(16)	C(12)-C(19)	1.3760(19)
N(3)-C(13)	1.3722(17)	C(12)-H(12)	0.9300
N(3)-H(102)	0.903(16)	C(13)-C(22)	1.3896(17)
N(4)-C(14)	1.2852(16)	C(13)-C(14)	1.4278(18)
N(4)-C(15)	1.4230(16)	C(14)-H(14)	0.9300
C(1)-C(8)	1.3859(18)	C(15)-C(20)	1.3952(19)
C(1)-C(2)	1.3894(19)	C(15)-C(16)	1.3957(19)
C(1)-H(1)	0.9300	C(16)-C(17)	1.390(2)
C(2)-C(3)	1.3870(18)	C(16)-H(16)	0.9300
C(2)-H(2)	0.9300	C(17)-C(18)	1.382(2)
C(3)-C(4)	1.3972(17)	C(17)-H(17)	0.9300
C(3)-H(3)	0.9300	C(18)-C(21)	1.390(2)
C(4)-C(9)	1.3993(17)	C(18)-H(18)	0.9300
C(5)-C(6)	1.4278(17)	C(19)-C(22)	1.398(2)
C(5)-H(5)	0.9300	C(19)-H(19)	0.9300
C(6)-C(11)	1.3885(17)	C(20)-C(21)	1.3856(19)
C(7)-C(10)	1.3726(18)	C(20)-H(20)	0.9300
C(7)-H(7)	0.9300	C(21)-H(21)	0.9300
C(8)-C(9)	1.3864(18)	C(22)-H(22)	0.9300
C(8)-H(8)	0.9300		

Table A.1.4: Bond angles [°] for HL2.

Bond	Angle (°)	Bond	Angle (°)	Bond	Angle (°)
C(5)-N(1)-C(4)	117.61(10)	N(2)-C(7)-C(10)	108.92(11)	C(20)-C(15)-N(4)	117.93(12)
C(7)-N(2)-C(6)	109.17(10)	N(2)-C(7)-H(7)	125.5	C(16)-C(15)-N(4)	122.58(12)
C(7)-N(2)-H(101)	124.1(10)	C(10)-C(7)-H(7)	125.5	C(17)-C(16)-C(15)	119.86(14)
C(6)-N(2)-H(101)	126.5(10)	C(1)-C(8)-C(9)	120.50(12)	C(17)-C(16)-H(16)	120.1
C(12)-N(3)-C(13)	108.99(11)	C(1)-C(8)-H(8)	119.7	C(15)-C(16)-H(16)	120.1
C(12)-N(3)-H(102)	123.9(10)	C(9)-C(8)-H(8)	119.7	C(18)-C(17)-C(16)	120.46(14)
C(13)-N(3)-H(102)	127.1(10)	C(8)-C(9)-C(4)	120.06(12)	C(18)-C(17)-H(17)	119.8
C(14)-N(4)-C(15)	117.20(11)	C(8)-C(9)-H(9)	120.0	C(16)-C(17)-H(17)	119.8
C(8)-C(1)-C(2)	119.66(12)	C(4)-C(9)-H(9)	120.0	C(17)-C(18)-C(21)	119.78(13)
C(8)-C(1)-H(1)	120.2	C(7)-C(10)-C(11)	107.08(11)	C(17)-C(18)-H(18)	120.1
C(2)-C(1)-H(1)	120.2	C(7)-C(10)-H(10)	126.5	C(21)-C(18)-H(18)	120.1
C(3)-C(2)-C(1)	120.40(12)	C(11)-C(10)-H(10)	126.5	C(12)-C(19)-C(22)	107.08(11)
C(3)-C(2)-H(2)	119.8	C(6)-C(11)-C(10)	107.55(11)	C(12)-C(19)-H(19)	126.5
C(1)-C(2)-H(2)	119.8	C(6)-C(11)-H(11)	126.2	C(22)-C(19)-H(19)	126.5
C(2)-C(3)-C(4)	120.11(12)	C(10)-C(11)-H(11)	126.2	C(21)-C(20)-C(15)	120.12(14)
C(2)-C(3)-H(3)	119.9	N(3)-C(12)-C(19)	108.81(12)	C(21)-C(20)-H(20)	119.9
C(4)-C(3)-H(3)	119.9	N(3)-C(12)-H(12)	125.6	C(15)-C(20)-H(20)	119.9
C(3)-C(4)-C(9)	119.27(11)	C(19)-C(12)-H(12)	125.6	C(20)-C(21)-C(18)	120.24(15)
C(3)-C(4)-N(1)	122.41(11)	N(3)-C(13)-C(22)	107.40(11)	C(20)-C(21)-H(21)	119.9
C(9)-C(4)-N(1)	118.23(11)	N(3)-C(13)-C(14)	124.80(11)	C(18)-C(21)-H(21)	119.9
N(1)-C(5)-C(6)	124.24(11)	C(22)-C(13)-C(14)	127.71(12)	C(13)-C(22)-C(19)	107.72(12)
N(1)-C(5)-H(5)	117.9	N(4)-C(14)-C(13)	124.79(12)	C(13)-C(22)-H(22)	126.1
C(6)-C(5)-H(5)	117.9	N(4)-C(14)-H(14)	117.6	C(19)-C(22)-H(22)	126.1
N(2)-C(6)-C(11)	107.27(11)	C(13)-C(14)-H(14)	117.6	C(20)-C(15)-N(4)	117.93(12)
N(2)-C(6)-C(5)	124.37(11)	C(20)-C(15)-C(16)	119.46(13)	C(16)-C(15)-N(4)	122.58(12)

Table A.1.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for HL2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$.

Atom	**U^{11}**	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
N(1)	18(1)	20(1)	18(1)	-3(1)	-1(1)	1(1)
N(2)	20(1)	17(1)	19(1)	0(1)	-1(1)	-1(1)
N(3)	21(1)	19(1)	21(1)	0(1)	1(1)	1(1)
N(4)	21(1)	24(1)	18(1)	1(1)	1(1)	-1(1)
C(1)	24(1)	25(1)	24(1)	-5(1)	-7(1)	-2(1)
C(2)	24(1)	30(1)	19(1)	-6(1)	-1(1)	3(1)
C(3)	17(1)	23(1)	19(1)	0(1)	0(1)	0(1)
C(4)	18(1)	18(1)	17(1)	2(1)	-3(1)	3(1)
C(5)	18(1)	21(1)	17(1)	0(1)	-1(1)	3(1)
C(6)	19(1)	19(1)	19(1)	0(1)	0(1)	2(1)
C(7)	19(1)	21(1)	22(1)	-5(1)	-1(1)	-1(1)
C(8)	18(1)	26(1)	26(1)	2(1)	-2(1)	-2(1)
C(9)	20(1)	24(1)	19(1)	-1(1)	2(1)	2(1)
C(10)	23(1)	21(1)	30(1)	-2(1)	4(1)	-5(1)
C(11)	28(1)	23(1)	22(1)	2(1)	3(1)	-2(1)
C(12)	22(1)	23(1)	29(1)	-6(1)	2(1)	-1(1)
C(13)	15(1)	24(1)	22(1)	4(1)	3(1)	2(1)
C(14)	17(1)	28(1)	18(1)	5(1)	0(1)	-1(1)
C(15)	27(1)	27(1)	14(1)	4(1)	3(1)	-7(1)
C(16)	31(1)	34(1)	22(1)	8(1)	-2(1)	-12(1)
C(17)	40(1)	50(1)	24(1)	6(1)	-6(1)	-24(1)
C(18)	53(1)	47(1)	21(1)	-8(1)	8(1)	-31(1)
C(19)	21(1)	18(1)	41(1)	0(1)	5(1)	1(1)
C(20)	33(1)	30(1)	21(1)	0(1)	6(1)	-6(1)
C(21)	46(1)	32(1)	27(1)	-6(1)	16(1)	-14(1)
C(22)	19(1)	25(1)	31(1)	7(1)	2(1)	3(1)

A.2: Crystallographic Data Tables for HL3

Table A.2.1: Crystal data and structure refinement for HL3.

Identification code	HL3	
Empirical formula	$C_{12} H_{12} N_2$	
Formula weight	184.24	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 9.8555(5) Å	α= 90°.
	b = 17.3532(9) Å	β= 94.184(2)°.
	c = 11.7790(6) Å	γ = 90°.
Volume	2009.13(18) $Å^3$	
Z	8	
Density (calculated)	1.218 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	784	
Crystal size	0.60 x 0.45 x 0.30 mm^3	
Theta range for data collection	2.09 to 26.43°.	
Index ranges	-12<=h<=12, -21<=k<=21, -14<=l<=14	
Reflections collected	31276	
Independent reflections	4118 [R(int) = 0.0259]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9783 and 0.9572	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4118 / 0 / 261	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0981	
R indices (all data)	R1 = 0.0396, wR2 = 0.1016	
Largest diff. peak and hole	0.228 and -0.231 $e.Å^{-3}$	

Table A.2.2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for HL3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
N(2B)	10651(1)	1760(1)	3543(1)	19(1)
N(1B)	8376(1)	1104(1)	2119(1)	19(1)
N(2A)	6789(1)	1774(1)	3988(1)	19(1)
N(1A)	8997(1)	1014(1)	5365(1)	19(1)
C(2B)	8377(1)	730(1)	316(1)	26(1)
C(3B)	9674(1)	1029(1)	653(1)	24(1)
C(4B)	9654(1)	1261(1)	1775(1)	19(1)
C(5B)	10727(1)	1621(1)	2484(1)	19(1)
C(6B)	11825(1)	2160(1)	4110(1)	20(1)
C(7B)	12521(1)	1688(1)	5066(1)	18(1)
C(12B)	12756(1)	902(1)	4945(1)	21(1)
C(11B)	13411(1)	484(1)	5831(1)	26(1)
C(10B)	13836(1)	846(1)	6849(1)	25(1)
C(1B)	7599(1)	789(1)	1232(1)	23(1)
C(8B)	12959(1)	2045(1)	6085(1)	22(1)
C(9B)	13610(1)	1628(1)	6972(1)	25(1)
C(10A)	3623(1)	1074(1)	559(1)	24(1)
C(9A)	4041(1)	1833(1)	469(1)	23(1)
C(8A)	4701(1)	2202(1)	1400(1)	21(1)
C(7A)	4954(1)	1823(1)	2434(1)	18(1)
C(6A)	5673(1)	2234(1)	3440(1)	21(1)
C(5A)	6724(1)	1640(1)	5049(1)	19(1)
C(4A)	7763(1)	1233(1)	5736(1)	19(1)
C(3A)	7739(1)	998(1)	6858(1)	24(1)
C(2A)	8991(1)	629(1)	7164(1)	25(1)
C(11A)	3850(1)	694(1)	1592(1)	24(1)
C(12A)	4512(1)	1064(1)	2522(1)	21(1)
C(1A)	9744(1)	655(1)	6231(1)	22(1)

Table A.2.3:Bond lengths [Å] for HL3.

Bond	Length(Å)	Bond	Length(Å)
N(2B)-C(5B)	1.2775(13)	C(10B)-H(10B)	0.9500
N(2B)-C(6B)	1.4674(13)	C(1B)-H(1B)	0.9500
N(1B)-C(1B)	1.3627(14)	C(8B)-C(9B)	1.3894(16)
N(1B)-C(4B)	1.3780(13)	C(8B)-H(8B)	0.9500
N(1B)-H(102)	0.903(14)	C(9B)-H(9B)	0.9500
N(2A)-C(5A)	1.2768(14)	C(10A)-C(9A)	1.3865(16)
N(2A)-C(6A)	1.4699(13)	C(10A)-C(11A)	1.3874(16)
N(1A)-C(1A)	1.3658(14)	C(10A)-H(10A)	0.9500
N(1A)-C(4A)	1.3758(13)	C(9A)-C(8A)	1.3907(15)
N(1A)-H(101)	0.908(14)	C(9A)-H(9A)	0.9500
C(2B)-C(1B)	1.3721(16)	C(8A)-C(7A)	1.3913(15)
C(2B)-C(3B)	1.4098(16)	C(8A)-H(8A)	0.9500
C(2B)-H(2B)	0.9500	C(7A)-C(12A)	1.3929(15)
C(3B)-C(4B)	1.3828(15)	C(7A)-C(6A)	1.5142(14)
C(3B)-H(3B)	0.9500	C(6A)-H(6A1)	0.9900
C(4B)-C(5B)	1.4411(15)	C(6A)-H(6A2)	0.9900
C(5B)-H(5B)	0.9500	C(5A)-C(4A)	1.4433(15)
C(6B)-C(7B)	1.5146(14)	C(5A)-H(5A)	0.9500
C(6B)-H(6B1)	0.9900	C(4A)-C(3A)	1.3839(15)
C(6B)-H(6B2)	0.9900	C(3A)-C(2A)	1.4144(16)
C(7B)-C(8B)	1.3912(14)	C(3A)-H(3A)	0.9500
C(7B)-C(12B)	1.3921(15)	C(2A)-C(1A)	1.3709(16)
C(12B)-C(11B)	1.3905(16)	C(2A)-H(2A)	0.9500
C(12B)-H(12B)	0.9500	C(11A)-C(12A)	1.3903(16)
C(11B)-C(10B)	1.3910(16)	C(11A)-H(11A)	0.9500
C(11B)-H(11B)	0.9500	C(12A)-H(12A)	0.9500
C(10B)-C(9B)	1.3854(17)	C(1A)-H(1A)	0.9500

Table A.2.4:Bond angles [°] for HL3.

Bond	Angle (°)	Bond	Angle (°)
C(5B)-N(2B)-C(6B)	115.72(9)	C(7B)-C(8B)-H(8B)	119.5
C(1B)-N(1B)-C(4B)	109.16(9)	C(10B)-C(9B)-C(8B)	120.04(10)
C(1B)-N(1B)-H(102)	124.4(9)	C(10B)-C(9B)-H(9B)	120.0
C(4B)-N(1B)-H(102)	125.5(9)	C(8B)-C(9B)-H(9B)	120.0
C(5A)-N(2A)-C(6A)	116.08(9)	C(9A)-C(10A)-C(11A)	119.20(10)
C(1A)-N(1A)-C(4A)	109.20(9)	C(9A)-C(10A)-H(10A)	120.4
C(1A)-N(1A)-H(101)	123.6(9)	C(11A)-C(10A)-H(10A)	120.4
C(4A)-N(1A)-H(101)	125.8(9)	C(10A)-C(9A)-C(8A)	120.20(10)
C(1B)-C(2B)-C(3B)	107.33(10)	C(10A)-C(9A)-H(9A)	119.9
C(1B)-C(2B)-H(2B)	126.3	C(8A)-C(9A)-H(9A)	119.9
C(3B)-C(2B)-H(2B)	126.3	C(9A)-C(8A)-C(7A)	121.01(10)
C(4B)-C(3B)-C(2B)	107.47(10)	C(9A)-C(8A)-H(8A)	119.5
C(4B)-C(3B)-H(3B)	126.3	C(7A)-C(8A)-H(8A)	119.5
C(2B)-C(3B)-H(3B)	126.3	C(8A)-C(7A)-C(12A)	118.42(10)
N(1B)-C(4B)-C(3B)	107.48(9)	C(8A)-C(7A)-C(6A)	120.31(10)
N(1B)-C(4B)-C(5B)	124.27(9)	C(12A)-C(7A)-C(6A)	121.27(9)
C(3B)-C(4B)-C(5B)	128.23(10)	N(2A)-C(6A)-C(7A)	112.30(9)
N(2B)-C(5B)-C(4B)	123.72(10)	N(2A)-C(6A)-H(6A1)	109.1
N(2B)-C(5B)-H(5B)	118.1	C(7A)-C(6A)-H(6A1)	109.1
C(4B)-C(5B)-H(5B)	118.1	N(2A)-C(6A)-H(6A2)	109.1
N(2B)-C(6B)-C(7B)	112.48(9)	C(7A)-C(6A)-H(6A2)	109.1
N(2B)-C(6B)-H(6B1)	109.1	H(6A1)-C(6A)-H(6A2)	107.9
C(7B)-C(6B)-H(6B1)	109.1	N(2A)-C(5A)-C(4A)	123.69(10)
N(2B)-C(6B)-H(6B2)	109.1	N(2A)-C(5A)-H(5A)	118.2
C(7B)-C(6B)-H(6B2)	109.1	C(4A)-C(5A)-H(5A)	118.2
H(6B1)-C(6B)-H(6B2)	107.8	N(1A)-C(4A)-C(3A)	107.46(9)
C(8B)-C(7B)-C(12B)	118.75(10)	N(1A)-C(4A)-C(5A)	124.29(9)
C(8B)-C(7B)-C(6B)	119.73(9)	C(3A)-C(4A)-C(5A)	128.25(10)
C(12B)-C(7B)-C(6B)	121.52(9)	C(4A)-C(3A)-C(2A)	107.56(10)
C(11B)-C(12B)-C(7B)	120.41(10)	C(4A)-C(3A)-H(3A)	126.2
C(11B)-C(12B)-H(12B)	119.8	C(2A)-C(3A)-H(3A)	126.2
C(7B)-C(12B)-H(12B)	119.8	C(1A)-C(2A)-C(3A)	107.08(10)
C(12B)-C(11B)-C(10B)	120.39(10)	C(1A)-C(2A)-H(2A)	126.5
C(12B)-C(11B)-H(11B)	119.8	C(3A)-C(2A)-H(2A)	126.5
C(10B)-C(11B)-H(11B)	119.8	C(10A)-C(11A)-C(12A)	120.56(10)

C(9B)-C(10B)-C(11B)	119.46(10)	C(10A)-C(11A)-H(11A)	119.7
C(9B)-C(10B)-H(10B)	120.3	C(12A)-C(11A)-H(11A)	119.7
C(11B)-C(10B)-H(10B)	120.3	C(11A)-C(12A)-C(7A)	120.60(10)
N(1B)-C(1B)-C(2B)	108.55(10)	C(11A)-C(12A)-H(12A)	119.7
N(1B)-C(1B)-H(1B)	125.7	C(7A)-C(12A)-H(12A)	119.7
C(2B)-C(1B)-H(1B)	125.7	N(1A)-C(1A)-C(2A)	108.69(10)
C(9B)-C(8B)-C(7B)	120.96(10)	N(1A)-C(1A)-H(1A)	125.7
C(9B)-C(8B)-H(8B)	119.5	C(2A)-C(1A)-H(1A)	125.7

Table A.2.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for HL3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(2B)	16(1)	21(1)	20(1)	1(1)	0(1)	2(1)
N(1B)	20(1)	20(1)	17(1)	0(1)	3(1)	1(1)
N(2A)	16(1)	22(1)	19(1)	-2(1)	0(1)	0(1)
N(1A)	19(1)	20(1)	17(1)	-1(1)	2(1)	-1(1)
C(2B)	26(1)	31(1)	21(1)	-7(1)	2(1)	-2(1)
C(3B)	23(1)	27(1)	21(1)	-2(1)	6(1)	1(1)
C(4B)	18(1)	19(1)	19(1)	2(1)	3(1)	4(1)
C(5B)	16(1)	19(1)	21(1)	3(1)	4(1)	4(1)
C(6B)	18(1)	21(1)	22(1)	0(1)	1(1)	-1(1)
C(7B)	13(1)	21(1)	21(1)	-1(1)	3(1)	-2(1)
C(12B)	18(1)	22(1)	23(1)	-5(1)	1(1)	0(1)
C(11B)	22(1)	20(1)	35(1)	0(1)	0(1)	1(1)
C(10B)	20(1)	30(1)	26(1)	6(1)	-2(1)	-1(1)
C(1B)	22(1)	24(1)	23(1)	-2(1)	1(1)	-3(1)
C(8B)	19(1)	21(1)	25(1)	-4(1)	2(1)	-2(1)
C(9B)	22(1)	32(1)	21(1)	-5(1)	0(1)	-2(1)
C(10A)	18(1)	29(1)	24(1)	-3(1)	-1(1)	1(1)
C(9A)	21(1)	28(1)	20(1)	5(1)	1(1)	3(1)
C(8A)	19(1)	19(1)	25(1)	4(1)	3(1)	1(1)
C(7A)	13(1)	21(1)	21(1)	0(1)	3(1)	3(1)
C(6A)	19(1)	21(1)	23(1)	-1(1)	1(1)	3(1)
C(5A)	17(1)	19(1)	21(1)	-3(1)	4(1)	-2(1)
C(4A)	19(1)	18(1)	20(1)	-2(1)	3(1)	-3(1)
C(3A)	24(1)	27(1)	22(1)	2(1)	7(1)	-1(1)
C(2A)	29(1)	26(1)	21(1)	5(1)	2(1)	1(1)
C(11A)	19(1)	21(1)	32(1)	3(1)	1(1)	-3(1)
C(12A)	17(1)	24(1)	23(1)	6(1)	2(1)	1(1)
C(1A)	22(1)	21(1)	22(1)	0(1)	1(1)	2(1)

A.3: Crystallographic Data Tables for HL4

Table A.3.1: Crystal data and structure refinement for HL4.

Identification code	HL4	
Empirical formula	$C_{16}H_{14}N_2$	
Formula weight	234.29	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 5.3017(3) Å	α= 104.896(3)°.
	b = 8.8579(5) Å	β= 99.212(2)°.
	c = 13.9265(8) Å	γ = 96.675(2)°.
Volume	615.33(6) $Å^3$	
Z	2	
Density (calculated)	1.265 Mg/m^3	
Absorption coefficient	0.075 mm^{-1}	
F(000)	248	
Crystal size	0.40 x 0.35 x 0.30 mm^3	
Theta range for data collection	1.54 to 26.07°.	
Index ranges	-6<=h<=2, -10<=k<=10, -17<=l<=17	
Reflections collected	9163	
Independent reflections	2395 [R(int) = 0.0221]	
Completeness to theta = 26.07°	98.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9777 and 0.9705	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2395 / 0 / 167	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.1052	
R indices (all data)	R1 = 0.0399, wR2 = 0.1066	
Largest diff. peak and hole	0.199 and -0.292 $e.Å^{-3}$	

Table A.3.2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for HL4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
N(1)	2847(2)	9052(1)	3474(1)	16(1)
N(2)	2287(2)	8662(1)	5460(1)	16(1)
C(1)	2457(2)	8911(1)	2462(1)	18(1)
C(4)	785(2)	8167(1)	3669(1)	16(1)
C(5)	546(2)	8036(1)	4661(1)	16(1)
C(6)	1684(2)	8419(1)	6404(1)	17(1)
C(7)	3433(2)	7408(1)	6833(1)	15(1)
C(12)	3630(2)	7414(1)	7872(1)	15(1)
C(13)	2218(2)	8322(1)	8534(1)	19(1)
C(14)	2459(2)	8287(2)	9523(1)	23(1)
C(15)	4125(3)	7362(2)	9911(1)	24(1)
C(2)	147(2)	7923(1)	1994(1)	19(1)
C(16)	5504(2)	6467(1)	9294(1)	21(1)
C(11)	5305(2)	6470(1)	8266(1)	16(1)
C(10)	6727(2)	5548(1)	7628(1)	19(1)
C(9)	6482(2)	5546(1)	6638(1)	19(1)
C(8)	4825(2)	6478(1)	6241(1)	17(1)
C(3)	-925(2)	7454(1)	2757(1)	18(1)

Table A.3.3: Bond lengths [Å] for HL4.

Bond	**Length(Å)**	**Bond**	**Length(Å)**
N(1)-C(1)	1.3625(14)	C(13)-C(14)	1.3715(16)
N(1)-C(4)	1.3746(15)	C(13)-H(13)	0.9500
N(1)-H(101)	0.927(17)	C(14)-C(15)	1.4095(18)
N(2)-C(5)	1.2777(15)	C(14)-H(14)	0.9500
N(2)-C(6)	1.4626(13)	C(15)-C(16)	1.3739(17)
C(1)-C(2)	1.3756(17)	C(15)-H(15)	0.9500
C(1)-H(1)	0.9500	C(2)-C(3)	1.4095(16)
C(4)-C(3)	1.3859(16)	C(2)-H(2)	0.9500
C(4)-C(5)	1.4398(15)	C(16)-C(11)	1.4182(16)
C(5)-H(5)	0.9500	C(16)-H(16)	0.9500
C(6)-C(7)	1.5203(15)	C(11)-C(10)	1.4178(16)
C(6)-H(6A)	0.9900	C(10)-C(9)	1.3632(16)
C(6)-H(6B)	0.9900	C(10)-H(10)	0.9500
C(7)-C(8)	1.3751(16)	C(9)-C(8)	1.4168(16)
C(7)-C(12)	1.4323(15)	C(9)-H(9)	0.9500
C(12)-C(13)	1.4267(16)	C(8)-H(8)	0.9500
C(12)-C(11)	1.4290(16)	C(3)-H(3)	0.9500

Table A.3.3: Bond lengths [Å] for HL4.

Bond	**Angle (°)**	**Bond**	**Angle (°)**
C(1)-N(1)-C(4)	108.92(10)	C(13)-C(14)-C(15)	120.70(11)
C(1)-N(1)-H(101)	122.9(10)	C(13)-C(14)-H(14)	119.6
C(4)-N(1)-H(101)	128.1(10)	C(15)-C(14)-H(14)	119.6
C(5)-N(2)-C(6)	116.31(10)	C(16)-C(15)-C(14)	120.02(11)
N(1)-C(1)-C(2)	108.82(10)	C(16)-C(15)-H(15)	120.0
N(1)-C(1)-H(1)	125.6	C(14)-C(15)-H(15)	120.0
C(2)-C(1)-H(1)	125.6	C(1)-C(2)-C(3)	107.11(10)
N(1)-C(4)-C(3)	107.81(10)	C(1)-C(2)-H(2)	126.4
N(1)-C(4)-C(5)	124.20(10)	C(3)-C(2)-H(2)	126.4
C(3)-C(4)-C(5)	127.99(11)	C(15)-C(16)-C(11)	120.97(11)
N(2)-C(5)-C(4)	124.10(10)	C(15)-C(16)-H(16)	119.5
N(2)-C(5)-H(5)	118.0	C(11)-C(16)-H(16)	119.5
C(4)-C(5)-H(5)	118.0	C(10)-C(11)-C(16)	121.07(11)
N(2)-C(6)-C(7)	112.31(9)	C(10)-C(11)-C(12)	119.79(10)
N(2)-C(6)-H(6A)	109.1	C(16)-C(11)-C(12)	119.14(10)
C(7)-C(6)-H(6A)	109.1	C(9)-C(10)-C(11)	120.28(11)
N(2)-C(6)-H(6B)	109.1	C(9)-C(10)-H(10)	119.9
C(7)-C(6)-H(6B)	109.1	C(11)-C(10)-H(10)	119.9
H(6A)-C(6)-H(6B)	107.9	C(10)-C(9)-C(8)	120.32(10)
C(8)-C(7)-C(12)	119.23(10)	C(10)-C(9)-H(9)	119.8
C(8)-C(7)-C(6)	121.18(10)	C(8)-C(9)-H(9)	119.8
C(12)-C(7)-C(6)	119.59(10)	C(7)-C(8)-C(9)	121.53(10)
C(13)-C(12)-C(11)	118.35(10)	C(7)-C(8)-H(8)	119.2
C(13)-C(12)-C(7)	122.82(10)	C(9)-C(8)-H(8)	119.2
C(11)-C(12)-C(7)	118.82(10)	C(4)-C(3)-C(2)	107.34(10)
C(14)-C(13)-C(12)	120.81(11)	C(4)-C(3)-H(3)	126.3
C(14)-C(13)-H(13)	119.6	C(2)-C(3)-H(3)	126.3

Table A.3.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for HL4. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2 [h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	16(1)	18(1)	13(1)	5(1)	2(1)	2(1)
N(2)	17(1)	17(1)	16(1)	7(1)	4(1)	5(1)
C(1)	21(1)	20(1)	15(1)	6(1)	5(1)	6(1)
C(4)	16(1)	14(1)	17(1)	5(1)	3(1)	5(1)
C(5)	16(1)	15(1)	20(1)	7(1)	5(1)	4(1)
C(6)	17(1)	20(1)	15(1)	7(1)	5(1)	4(1)
C(7)	15(1)	13(1)	16(1)	4(1)	2(1)	-1(1)
C(12)	15(1)	14(1)	16(1)	4(1)	3(1)	-1(1)
C(13)	20(1)	20(1)	18(1)	7(1)	5(1)	6(1)
C(14)	26(1)	26(1)	19(1)	6(1)	9(1)	8(1)
C(15)	32(1)	28(1)	14(1)	8(1)	5(1)	6(1)
C(2)	23(1)	19(1)	13(1)	3(1)	1(1)	7(1)
C(16)	23(1)	21(1)	20(1)	9(1)	1(1)	4(1)
C(11)	17(1)	14(1)	18(1)	5(1)	2(1)	-1(1)
C(10)	19(1)	15(1)	23(1)	7(1)	3(1)	4(1)
C(9)	21(1)	15(1)	22(1)	3(1)	7(1)	5(1)
C(8)	20(1)	17(1)	15(1)	4(1)	4(1)	1(1)
C(3)	17(1)	16(1)	19(1)	3(1)	1(1)	3(1)

A.4: Crystallographic Data Tables for HL5

Table A.4.1: Crystal data and structure refinement for HL5.

Identification code	HL5	
Empirical formula	$C_{13}\ H_{14}\ N_2$	
Formula weight	198.26	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 7.0928(5) Å	α= 90°.
	b = 16.0355(12) Å	β= 96.261(3)°.
	c = 9.2398(7) Å	γ = 90°.
Volume	1044.64(13) $Å^3$	
Z	4	
Density (calculated)	1.261 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	424	
Crystal size	0.35 x 0.20 x 0.03 mm^3	
Theta range for data collection	2.54 to 26.20°.	
Index ranges	-8<=h<=6, -16<=k<=19, -10<=l<=11	
Reflections collected	10042	
Independent reflections	2078 [R(int) = 0.0233]	
Completeness to theta = 26.20°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9977 and 0.9740	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2078 / 0 / 140	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0940	
R indices (all data)	R1 = 0.0427, wR2 = 0.0980	
Largest diff. peak and hole	0.230 and -0.274 $e.Å^{-3}$	

Table A.4.2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for HL5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	**x**	**y**	**z**	**U(eq)**
N(2)	8863(2)	4973(1)	1960(1)	15(1)
N(1)	11771(2)	6021(1)	791(1)	15(1)
C(11)	1479(2)	2987(1)	3672(2)	18(1)
C(10)	1450(2)	3171(1)	2203(1)	17(1)
C(9)	2725(2)	3738(1)	1727(1)	16(1)
C(8)	4050(2)	4140(1)	2714(1)	13(1)
C(7)	5476(2)	4737(1)	2196(1)	15(1)
C(6)	7523(2)	4492(1)	2723(1)	16(1)
C(5)	9897(2)	5490(1)	2730(1)	15(1)
C(4)	11297(2)	6026(1)	2195(1)	15(1)
C(3)	12380(2)	6629(1)	2956(1)	17(1)
C(2)	13540(2)	6998(1)	1987(2)	19(1)
C(1)	13133(2)	6608(1)	667(1)	17(1)
C(12)	2787(2)	3385(1)	4667(1)	18(1)
C(13)	4048(2)	3959(1)	4192(1)	15(1)

Table A.4.3: Bond lengths [Å] for HL5.

Bond	**Length(Å)**	**Bond**	**Length(Å)**
N(2)-C(5)	1.2717(17)	C(7)-H(7A)	0.9900
N(2)-C(6)	1.4636(16)	C(7)-H(7B)	0.9900
N(1)-C(1)	1.3620(16)	C(6)-H(6A)	0.9900
N(1)-C(4)	1.3747(16)	C(6)-H(6B)	0.9900
N(1)-H(101)	0.914(17)	C(5)-C(4)	1.4407(18)
C(11)-C(10)	1.3867(19)	C(5)-H(5)	0.9500
C(11)-C(12)	1.3882(19)	C(4)-C(3)	1.3794(18)
C(11)-H(11)	0.9500	C(3)-C(2)	1.4111(19)
C(10)-C(9)	1.3880(19)	C(3)-H(3)	0.9500
C(10)-H(10)	0.9500	C(2)-C(1)	1.3737(19)
C(9)-C(8)	1.3931(18)	C(2)-H(2)	0.9500
C(9)-H(9)	0.9500	C(1)-H(1)	0.9500
C(8)-C(13)	1.3973(17)	C(12)-C(13)	1.3868(18)
C(8)-C(7)	1.5084(17)	C(12)-H(12)	0.9500
C(7)-C(6)	1.5315(17)	C(13)-H(13)	0.9500

Table A.4.4: Bond angles [°] for HL5.

Bond	Angle (°)	Bond	Angle (°)
C(5)-N(2)-C(6)	116.08(11)	N(2)-C(6)-H(6B)	109.5
C(1)-N(1)-C(4)	108.95(11)	C(7)-C(6)-H(6B)	109.5
C(1)-N(1)-H(101)	124.4(11)	H(6A)-C(6)-H(6B)	108.1
C(4)-N(1)-H(101)	126.5(11)	N(2)-C(5)-C(4)	124.99(12)
C(10)-C(11)-C(12)	119.27(12)	N(2)-C(5)-H(5)	117.5
C(10)-C(11)-H(11)	120.4	C(4)-C(5)-H(5)	117.5
C(12)-C(11)-H(11)	120.4	N(1)-C(4)-C(3)	107.75(11)
C(11)-C(10)-C(9)	120.53(12)	N(1)-C(4)-C(5)	124.72(11)
C(11)-C(10)-H(10)	119.7	C(3)-C(4)-C(5)	127.52(12)
C(9)-C(10)-H(10)	119.7	C(4)-C(3)-C(2)	107.56(12)
C(10)-C(9)-C(8)	120.83(12)	C(4)-C(3)-H(3)	126.2
C(10)-C(9)-H(9)	119.6	C(2)-C(3)-H(3)	126.2
C(8)-C(9)-H(9)	119.6	C(1)-C(2)-C(3)	106.93(11)
C(9)-C(8)-C(13)	118.09(12)	C(1)-C(2)-H(2)	126.5
C(9)-C(8)-C(7)	120.92(11)	C(3)-C(2)-H(2)	126.5
C(13)-C(8)-C(7)	120.98(11)	N(1)-C(1)-C(2)	108.80(12)
C(8)-C(7)-C(6)	112.42(10)	N(1)-C(1)-H(1)	125.6
C(8)-C(7)-H(7A)	109.1	C(2)-C(1)-H(1)	125.6
C(6)-C(7)-H(7A)	109.1	C(13)-C(12)-C(11)	120.15(12)
C(8)-C(7)-H(7B)	109.1	C(13)-C(12)-H(12)	119.9
C(6)-C(7)-H(7B)	109.1	C(11)-C(12)-H(12)	119.9
H(7A)-C(7)-H(7B)	107.9	C(12)-C(13)-C(8)	121.12(12)
N(2)-C(6)-C(7)	110.71(10)	C(12)-C(13)-H(13)	119.4
N(2)-C(6)-H(6A)	109.5	C(8)-C(13)-H(13)	119.4
C(7)-C(6)-H(6A)	109.5		

Table A.4.5: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for HL5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(2)	13(1)	17(1)	16(1)	1(1)	2(1)	1(1)
N(1)	15(1)	15(1)	16(1)	-1(1)	1(1)	-1(1)
C(11)	15(1)	17(1)	23(1)	1(1)	5(1)	-1(1)
C(10)	13(1)	17(1)	21(1)	-4(1)	0(1)	1(1)
C(9)	14(1)	19(1)	14(1)	0(1)	1(1)	4(1)
C(8)	12(1)	12(1)	17(1)	0(1)	3(1)	4(1)
C(7)	14(1)	15(1)	15(1)	2(1)	1(1)	1(1)
C(6)	13(1)	19(1)	16(1)	3(1)	2(1)	-1(1)
C(5)	14(1)	18(1)	14(1)	1(1)	2(1)	4(1)
C(4)	14(1)	15(1)	15(1)	0(1)	1(1)	4(1)
C(3)	16(1)	16(1)	18(1)	-2(1)	-1(1)	4(1)
C(2)	15(1)	13(1)	26(1)	-1(1)	-1(1)	-1(1)
C(1)	15(1)	15(1)	22(1)	3(1)	4(1)	0(1)
C(12)	19(1)	20(1)	15(1)	2(1)	4(1)	1(1)
C(13)	15(1)	16(1)	15(1)	-2(1)	1(1)	1(1)

checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) aupropyl_f

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: aupropyl_f

```
Bond precision:      C-C = 0.0097 A              Wavelength=0.71073
Cell:          a=19.6184(9)   b=7.3679(4)    c=7.2571(3)
               alpha=90       beta=90         gamma=90
Temperature: 100 K
                    Calculated                    Reported
Volume              1048.99(9)                    1048.99(9)
Space group         P c a 21                      P ca21
Hall group          P 2c -2ac                     P 2c -2ac
Moiety formula      C8 H11 Au Cl2 N2              C8 H11 Au Cl2 N2
Sum formula         C8 H11 Au Cl2 N2              C8 H11 Au Cl2 N2
Mr                  403.06                        403.05
Dx,g cm-3           2.552                         2.552
Z                   4                             4
Mu (mm-1)           14.488                        14.488
F000                744.0                         744.0
F000'               737.96
h,k,lmax            24,9,9                        24,9,8
Nref                2141[ 1162]                   2051
Tmin,Tmax           0.043,0.647                   0.046,0.670
Tmin'               0.000
Correction method= MULTI-SCAN
Data completeness= 1.77/0.96   Theta(max)= 26.420
R(reflections)= 0.0213( 1968)     wR2(reflections)= 0.0566( 2051)
S = 0.752             Npar= 119
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 0.752
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 9.66 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0097 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 10 Report

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....
1 Note
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by .....
0.0026 Check

Alert level G

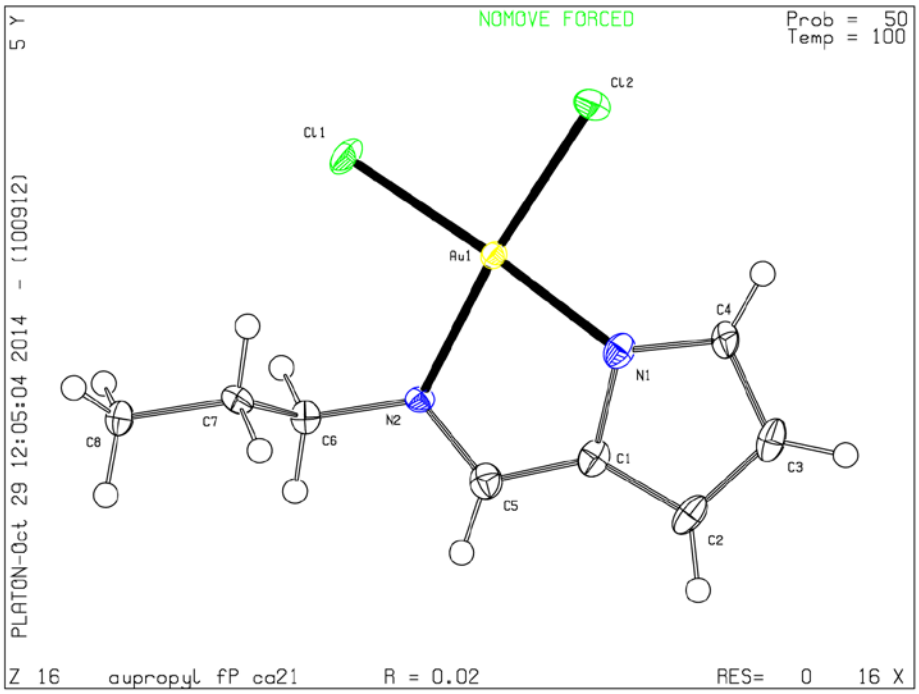
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF
Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually
Large. 15.77 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .
mixed
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
7 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by
SHELXL 2014 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock aupropyl_f - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) aupropyl_f

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: aupropyl_f

Bond precision: C-C = 0.0097 A Wavelength=0.71073
Cell: a=19.6184(9) b=7.3679(4) c=7.2571(3)
alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1048.99(9)	1048.99(9)
Space group	P c a 21	P ca21
Hall group	P 2c -2ac	P 2c -2ac
Moiety formula	C8 H11 Au Cl2 N2	C8 H11 Au Cl2 N2
Sum formula	C8 H11 Au Cl2 N2	C8 H11 Au Cl2 N2
Mr	403.06	403.05
Dx,g cm-3	2.552	2.552
Z	4	4
Mu (mm-1)	14.488	14.488
F000	744.0	744.0
F000'	737.96	
h,k,lmax	24,9,9	24,9,8
Nref	2141[1162]	2051
Tmin,Tmax	0.043,0.647	0.046,0.670
Tmin'	0.000	

Correction method= MULTI-SCAN
Data completeness= 1.77/0.96 Theta(max)= 26.420
R(reflections)= 0.0213(1968) wR2(reflections)= 0.0566(2051)
S = 0.752 Npar= 119

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 0.752
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 9.66 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0097 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 10 Report

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....
1 Note
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by .....
0.0026 Check

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF
Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually
Large. 15.77 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .
mixed
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
7 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by
SHELXL 2014 Note

---

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6 **ALERT level G** = General information/check it is not something unexpected

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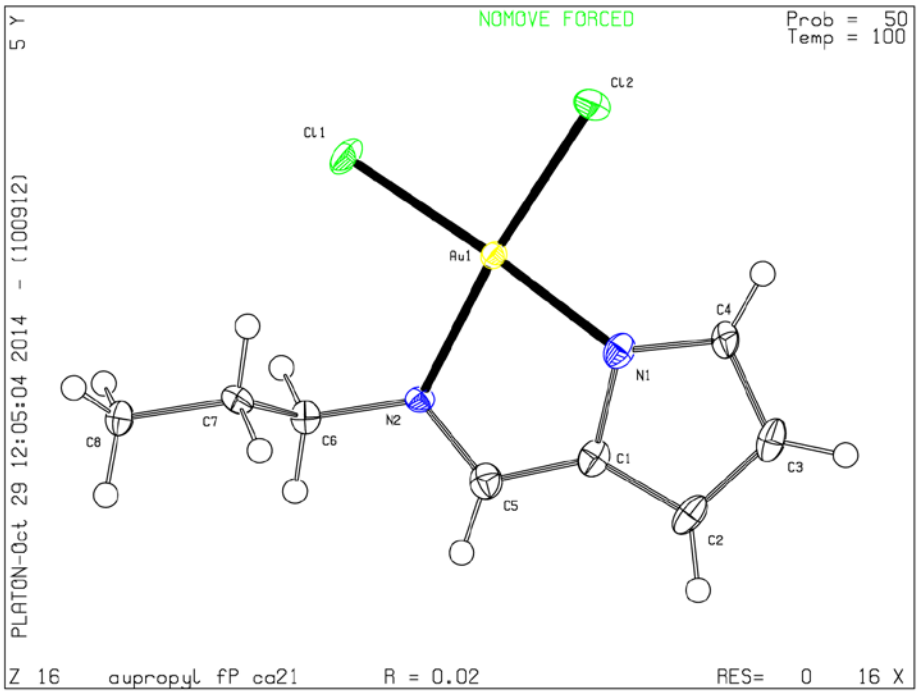
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock aupropyl_f - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_auaniline

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_auaniline

Bond precision: C-C = 0.0054 A Wavelength=0.71073
Cell: a=18.4739(10) b=4.1151(2) c=15.1775(8)
alpha=90 beta=99.534(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1137.89(10)	1137.89(10)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H9 Au Cl2 N2	C11 H9 Au Cl2 N2
Sum formula	C11 H9 Au Cl2 N2	C11 H9 Au Cl2 N2
Mr	437.07	437.07
Dx,g cm-3	2.551	2.551
Z	4	4
Mu (mm-1)	13.368	13.368
F000	808.0	808.0
F000'	801.92	
h,k,lmax	22,5,18	22,5,18
Nref	2247	2214
Tmin,Tmax	0.288,0.586	0.046,0.617
Tmin'	0.000	

Correction method= MULTI-SCAN
Data completeness= 0.985 Theta(max)= 26.070
R(reflections)= 0.0171(2086) wR2(reflections)= 0.0411(2214)
S = 1.055 Npar= 145

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.054
Additional refinement cycles may be required.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 12 Report

Alert level G

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....
1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
22 Note

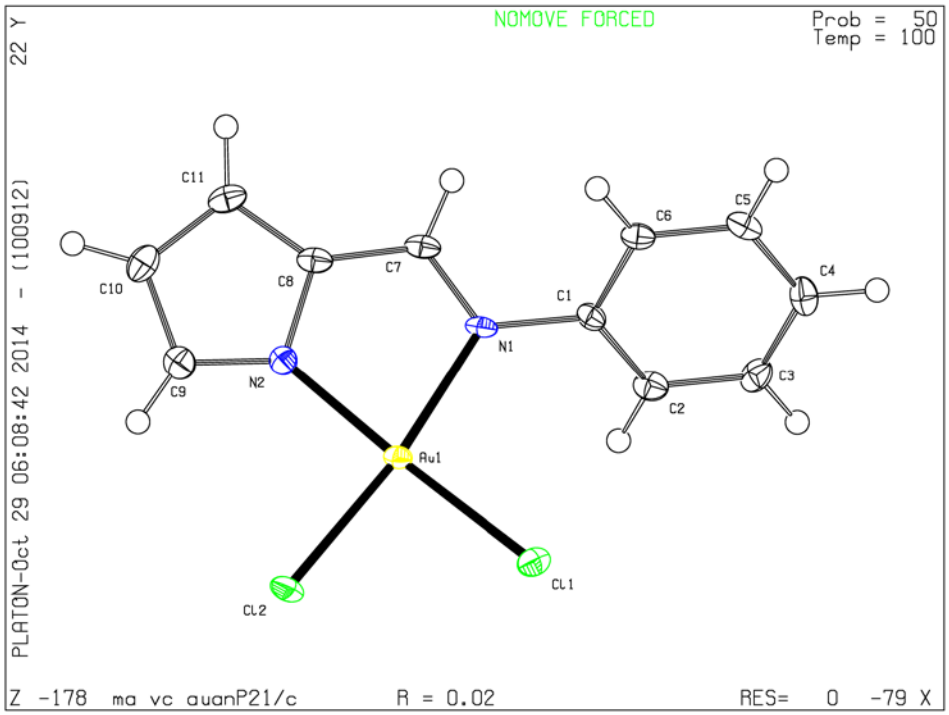
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_auaniline - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_auaniline

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_auaniline

Bond precision: C-C = 0.0054 A Wavelength=0.71073
Cell: a=18.4739(10) b=4.1151(2) c=15.1775(8)
alpha=90 beta=99.534(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1137.89(10)	1137.89(10)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C11 H9 Au Cl2 N2	C11 H9 Au Cl2 N2
Sum formula	C11 H9 Au Cl2 N2	C11 H9 Au Cl2 N2
Mr	437.07	437.07
Dx,g cm-3	2.551	2.551
Z	4	4
Mu (mm-1)	13.368	13.368
F000	808.0	808.0
F000'	801.92	
h,k,lmax	22,5,18	22,5,18
Nref	2247	2214
Tmin,Tmax	0.288,0.586	0.046,0.617
Tmin'	0.000	

Correction method= MULTI-SCAN
Data completeness= 0.985 Theta(max)= 26.070
R(reflections)= 0.0171(2086) wR2(reflections)= 0.0411(2214)
S = 1.055 Npar= 145

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.054
Additional refinement cycles may be required.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 12 Report

Alert level G

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....
1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
22 Note

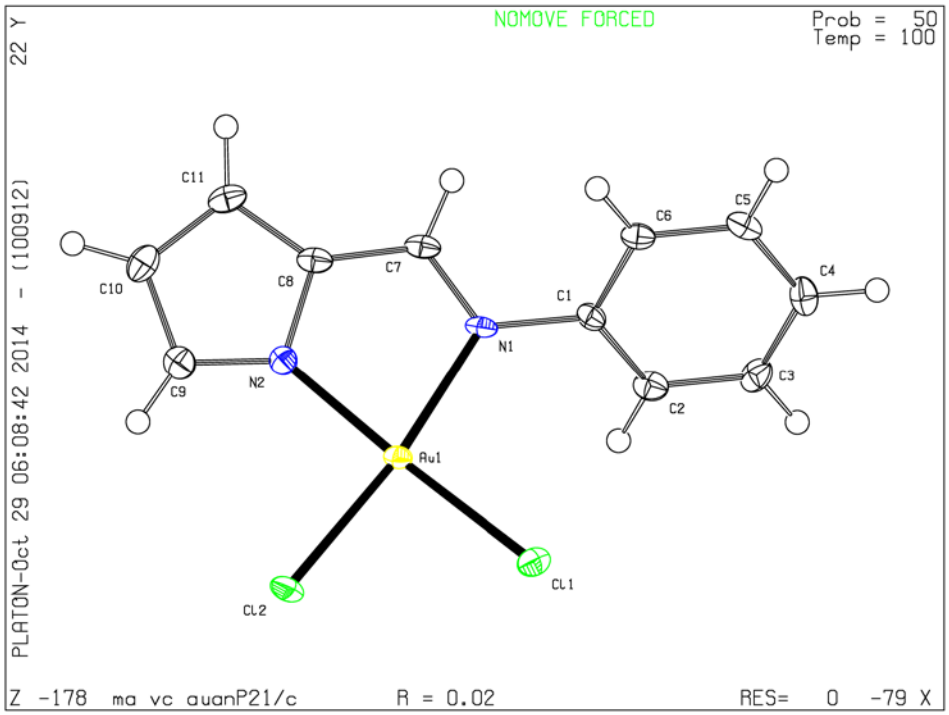
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_auaniline - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_aubenzyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_aubenzyl

```
Bond precision:      C-C = 0.0196 A              Wavelength=0.71073
Cell:          a=7.096(5)     b=4.557(5)     c=19.792(5)
               alpha=90       beta=99.298(5) gamma=90
Temperature: 100 K
                    Calculated                    Reported
Volume              631.6(8)                      631.6(8)
Space group         P 21                          P21
Hall group          P 2yb                         P 2yb
Moiety formula      C12 H11 Au Cl2 N2             C12 H11 Au Cl2 N2
Sum formula         C12 H11 Au Cl2 N2             C12 H11 Au Cl2 N2
Mr                  451.10                        451.09
Dx,g cm-3           2.372                         2.372
Z                   2                             2
Mu (mm-1)           12.046                        12.046
F000                420.0                         420.0
F000'               416.95
h,k,lmax            8,5,24                        8,5,24
Nref                2628[ 1484]                   2029
Tmin,Tmax           0.327,0.618                   0.052,0.644
Tmin'               0.001
Correction method= MULTI-SCAN
Data completeness= 1.37/0.77   Theta(max)= 26.510
R(reflections)= 0.0348( 1946)     wR2(reflections)= 0.0792( 2029)
S = 1.204             Npar= 154
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Residual Density 2.43A From C10 -3.92 eA-3

Alert level B

PLAT213_ALERT_2_B Atom N2 has ADP max/min Ratio ..... 4.2 oblate
PLAT213_ALERT_2_B Atom C9 has ADP max/min Ratio ..... 4.2 prolat
PLAT924_ALERT_1_B The Reported and Calculated Rho(min) Differ by . 2.27 eA-3

PLAT971_ALERT_2_B Check Calcd Residual Density 0.79A From Au1
3.43 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density 0.92A From Au1
3.32 eA-3

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .....
9.46 Note
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio .....
3.5 oblate
PLAT213_ALERT_2_C Atom C10 has ADP max/min Ratio .....
3.1 prolat
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....
0.0196 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=
0.600 17 Report
PLAT915_ALERT_3_C Low Friedel Pair Coverage 50
%
PLAT971_ALERT_2_C Check Calcd Residual Density 1.76A From C10
2.24 eA-3
And 4 other PLAT971 Alerts
More ...

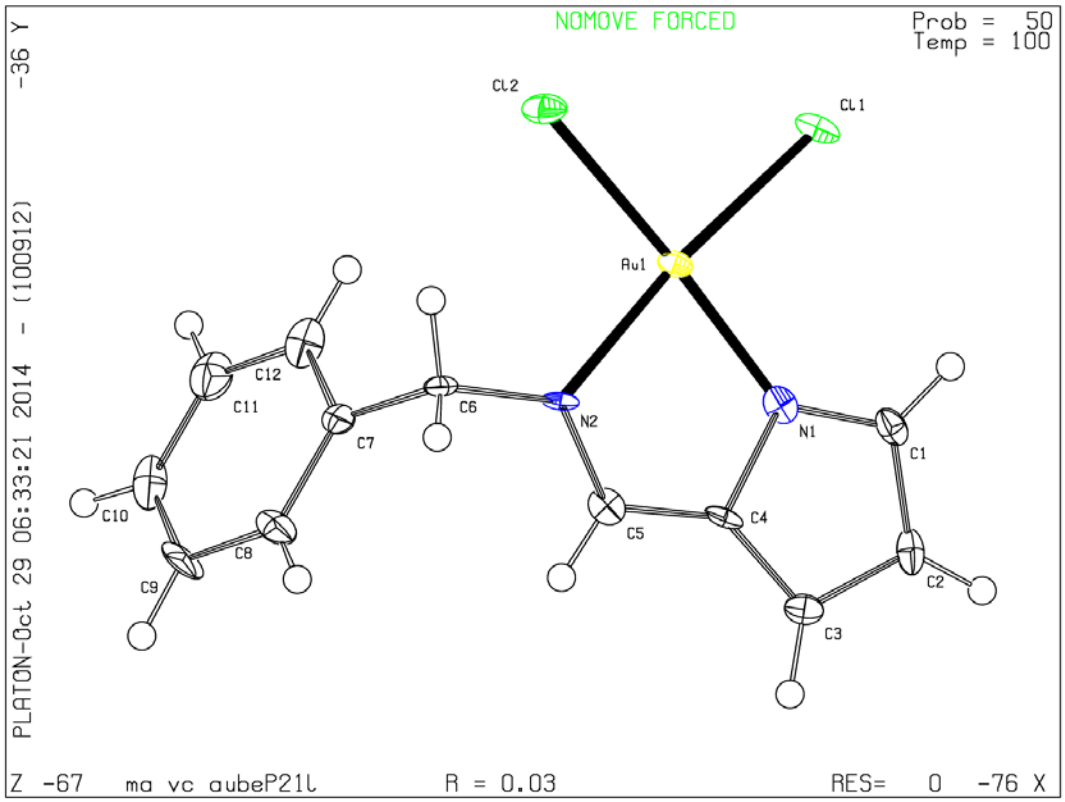
Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero .....
0.049
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually
Large. 10.69 Why ?
PLAT153_ALERT_1_G The su's on the Cell Axes are Equal .....
0.00500 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....
7 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
7 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by
SHELXL 2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....
1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
10 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
9 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock ma_vc_aubenzyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_aubenzyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_aubenzyl

Bond precision: C-C = 0.0196 A Wavelength=0.71073
Cell: a=7.096(5) b=4.557(5) c=19.792(5)
alpha=90 beta=99.298(5) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	631.6(8)	631.6(8)
Space group	P 21	P21
Hall group	P 2yb	P 2yb
Moiety formula	C12 H11 Au Cl2 N2	C12 H11 Au Cl2 N2
Sum formula	C12 H11 Au Cl2 N2	C12 H11 Au Cl2 N2
Mr	451.10	451.09
Dx,g cm-3	2.372	2.372
Z	2	2
Mu (mm-1)	12.046	12.046
F000	420.0	420.0
F000'	416.95	
h,k,lmax	8,5,24	8,5,24
Nref	2628[1484]	2029
Tmin,Tmax	0.327,0.618	0.052,0.644
Tmin'	0.001	

Correction method= MULTI-SCAN
Data completeness= 1.37/0.77 Theta(max)= 26.510
R(reflections)= 0.0348(1946) wR2(reflections)= 0.0792(2029)
S = 1.204 Npar= 154

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT972_ALERT_2_A Check Calcd Residual Density 2.43A From C10 -3.92 eA-3

Alert level B

PLAT213_ALERT_2_B Atom N2 has ADP max/min Ratio ..... 4.2 oblate
PLAT213_ALERT_2_B Atom C9 has ADP max/min Ratio ..... 4.2 prolat
PLAT924_ALERT_1_B The Reported and Calculated Rho(min) Differ by . 2.27 eA-3

PLAT971_ALERT_2_B Check Calcd Residual Density 0.79A From Au1
3.43 eA-3
PLAT971_ALERT_2_B Check Calcd Residual Density 0.92A From Au1
3.32 eA-3

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .....
9.46 Note
PLAT213_ALERT_2_C Atom C5 has ADP max/min Ratio .....
3.5 oblate
PLAT213_ALERT_2_C Atom C10 has ADP max/min Ratio .....
3.1 prolat
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....
0.0196 Ang.
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=
0.600 17 Report
PLAT915_ALERT_3_C Low Friedel Pair Coverage 50
%
PLAT971_ALERT_2_C Check Calcd Residual Density 1.76A From C10
2.24 eA-3
And 4 other PLAT971 Alerts
More ...

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 2*sigma from Zero .....
0.049
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually
Large. 10.69 Why ?
PLAT153_ALERT_1_G The su's on the Cell Axes are Equal .....
0.00500 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....
7 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....
7 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by
SHELXL 2014 Note
PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) .....
1 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
10 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain
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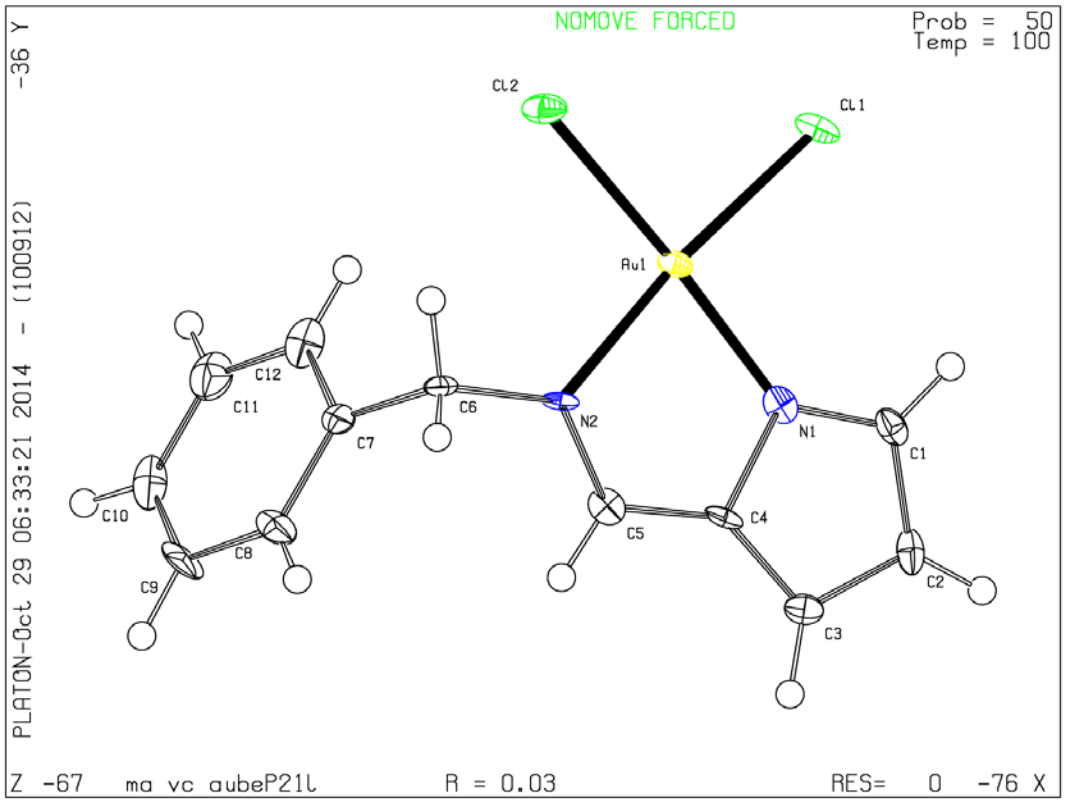
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Datablock ma_vc_aubenzyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_aumenapth

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_aumenapth

Bond precision: C-C = 0.0064 A Wavelength=0.71073
Cell: a=4.8648(3) b=13.9634(8) c=21.7386(13)
alpha=90 beta=90.050(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1476.68(15)	1476.68(15)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H13 Au Cl2 N2	C16 H13 Au Cl2 N2
Sum formula	C16 H13 Au Cl2 N2	C16 H13 Au Cl2 N2
Mr	501.15	501.15
Dx,g cm-3	2.254	2.254
Z	4	4
Mu (mm-1)	10.317	10.317
F000	944.0	944.0
F000'	937.85	
h,k,lmax	6,17,26	5,17,26
Nref	2919	2100
Tmin,Tmax	0.235,0.486	0.090,0.532
Tmin'	0.009	

Correction method= MULTI-SCAN
Data completeness= 0.719 Theta(max)= 26.120
R(reflections)= 0.0188(1880) wR2(reflections)= 0.0457(2100)
S = 1.042 Npar= 190

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.718 Note

Alert level B

PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L= 0.600 753 Report

Alert level C

SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.061
Additional refinement cycles may be required.
PLAT080_ALERT_2_C Maximum Shift/Error 0.06
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....
1 Note

Alert level G

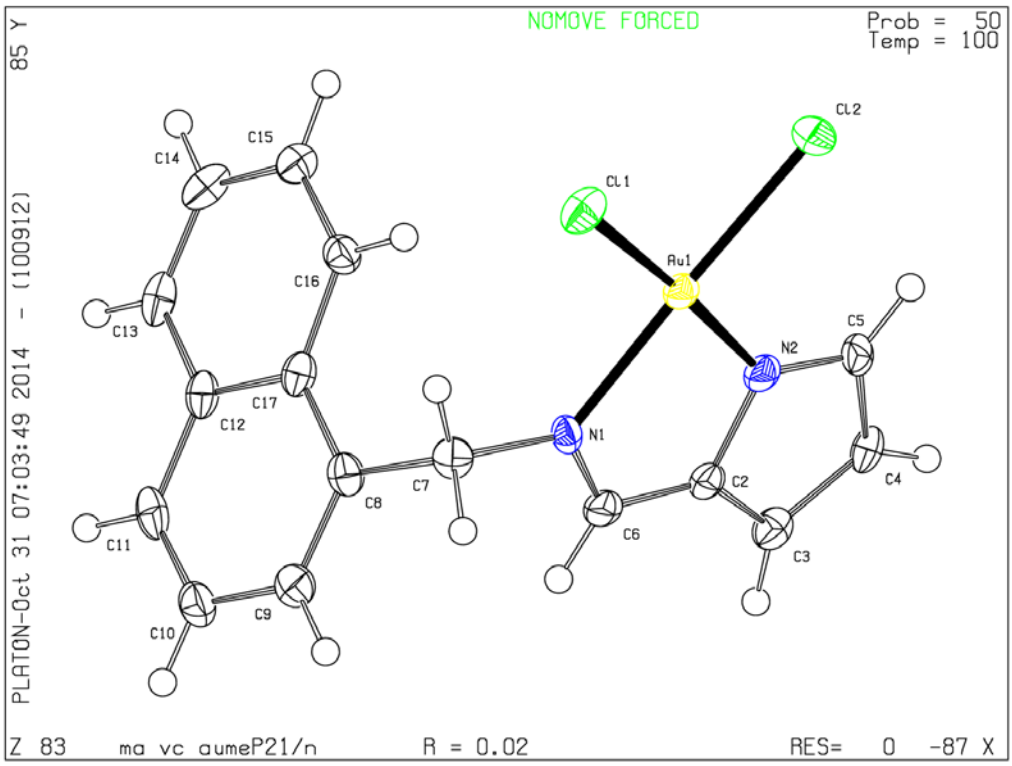
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
63 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_aumenapth - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_aumenapth

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_aumenapth

Bond precision: C-C = 0.0064 A Wavelength=0.71073
Cell: a=4.8648(3) b=13.9634(8) c=21.7386(13)
alpha=90 beta=90.050(1) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1476.68(15)	1476.68(15)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H13 Au Cl2 N2	C16 H13 Au Cl2 N2
Sum formula	C16 H13 Au Cl2 N2	C16 H13 Au Cl2 N2
Mr	501.15	501.15
Dx,g cm-3	2.254	2.254
Z	4	4
Mu (mm-1)	10.317	10.317
F000	944.0	944.0
F000'	937.85	
h,k,lmax	6,17,26	5,17,26
Nref	2919	2100
Tmin,Tmax	0.235,0.486	0.090,0.532
Tmin'	0.009	

Correction method= MULTI-SCAN
Data completeness= 0.719 Theta(max)= 26.120
R(reflections)= 0.0188(1880) wR2(reflections)= 0.0457(2100)
S = 1.042 Npar= 190

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low ..... 0.718 Note

Alert level B

PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L= 0.600 753 Report

Alert level C

SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.061
Additional refinement cycles may be required.
PLAT080_ALERT_2_C Maximum Shift/Error 0.06
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....
1 Note

Alert level G

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
63 Note

1 **ALERT level A** = Most likely a serious problem - resolve or explain
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3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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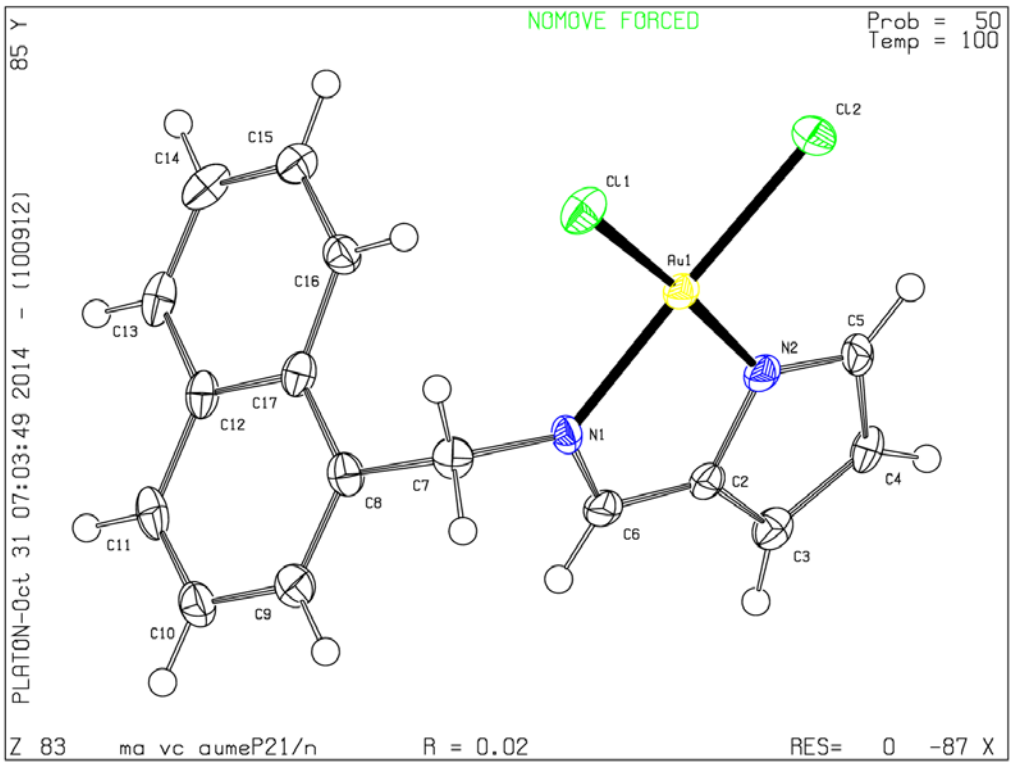
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_aumenapth - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_auphet

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_auphet

Bond precision: C-C = 0.0217 A Wavelength=0.71073
Cell: a=19.0672(14) b=7.2240(4) c=20.2020(14)
alpha=90 beta=92.602(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2779.8(3)	2779.8(3)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C13 H13 Au Cl2 N2	C13 H13 Au Cl2 N2
Sum formula	C13 H13 Au Cl2 N2	C13 H13 Au Cl2 N2
Mr	465.12	465.12
Dx,g cm-3	2.223	2.223
Z	8	8
Mu (mm-1)	10.951	10.951
F000	1744.0	1744.0
F000'	1731.75	
h,k,lmax	25,9,26	25,9,26
Nref	6891	6757
Tmin,Tmax	0.079,0.193	0.058,0.290
Tmin'	0.001	

Correction method= MULTI-SCAN
Data completeness= 0.981 Theta(max)= 28.270
R(reflections)= 0.0656(6094) wR2(reflections)= 0.1788(6757)
S = 1.141 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0217 Ang.
PLAT930_ALERT_2_B Check Twin Law (1 0 1)[1 0 1] Estimated BASF 0.17

Alert level C

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
_refine_diff_density_max given = 6.974
Test value = 5.925
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....
2.13 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density
6.97 eA-3
PLAT213_ALERT_2_C Atom C24 has ADP max/min Ratio 3.2
prolat
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 4.552
Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.074
Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600
85 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.
293.08 Why ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints 6
Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..
! Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..
! Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL
2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
52 Note
PLAT931_ALERT_5_G Found Twin Law (1 0 1)[ ] Estimated BASF
0.17 Check

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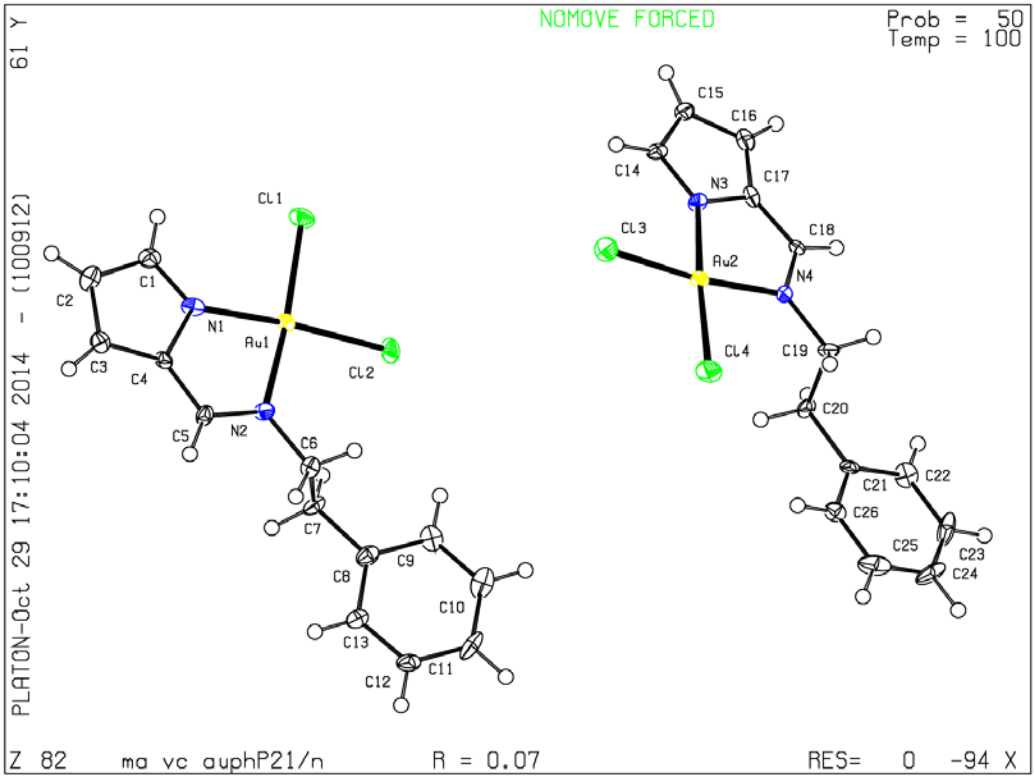
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
8 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_auphet - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_auphet

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No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_auphet

Bond precision: C-C = 0.0217 A Wavelength=0.71073
Cell: a=19.0672(14) b=7.2240(4) c=20.2020(14)
alpha=90 beta=92.602(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2779.8(3)	2779.8(3)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C13 H13 Au Cl2 N2	C13 H13 Au Cl2 N2
Sum formula	C13 H13 Au Cl2 N2	C13 H13 Au Cl2 N2
Mr	465.12	465.12
Dx,g cm-3	2.223	2.223
Z	8	8
Mu (mm-1)	10.951	10.951
F000	1744.0	1744.0
F000'	1731.75	
h,k,lmax	25,9,26	25,9,26
Nref	6891	6757
Tmin,Tmax	0.079,0.193	0.058,0.290
Tmin'	0.001	

Correction method= MULTI-SCAN
Data completeness= 0.981 Theta(max)= 28.270
R(reflections)= 0.0656(6094) wR2(reflections)= 0.1788(6757)
S = 1.141 Npar= 325

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds .....
0.0217 Ang.
PLAT930_ALERT_2_B Check Twin Law (1 0 1)[1 0 1] Estimated BASF
0.17

Alert level C

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
_refine_diff_density_max given = 6.974
Test value = 5.925
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....
2.13 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density
6.97 eA-3
PLAT213_ALERT_2_C Atom C24 has ADP max/min Ratio 3.2
prolat
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 4.552
Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.074
Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600
85 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...
1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.
293.08 Why ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints 6
Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..
! Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..
! Info
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL
2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600
52 Note
PLAT931_ALERT_5_G Found Twin Law (1 0 1)[ ] Estimated BASF
0.17 Check

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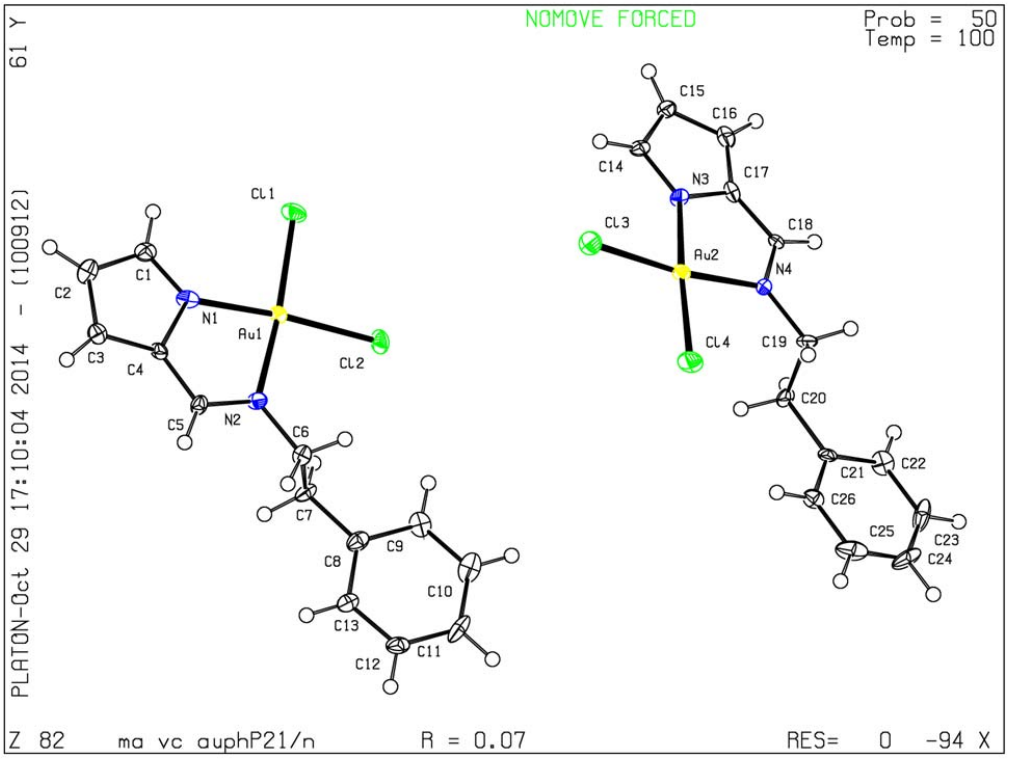
1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_auphet - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_anilinel

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: HL2

```
Bond precision:      C-C = 0.0019 A              Wavelength=0.71073
Cell:          a=9.4092(8)    b=18.1595(16)  c=21.2310(18)
               alpha=90       beta=90        gamma=90
Temperature: 296 K
                    Calculated                    Reported
Volume              3627.7(5)                     3627.7(5)
Space group         P b c a                       P bca
Hall group          -P 2ac 2ab                    -P 2ac 2ab
Moiety formula      C11 H10 N2                    C11 H10 N2
Sum formula         C11 H10 N2                    C11 H10 N2
Mr                  170.21                        170.21
Dx,g cm-3           1.247                         1.247
Z                   16                            16
Mu (mm-1)           0.076                         0.076
F000                1440.0                        1440.0
F000'               1440.45
h,k,lmax            11,22,26                      11,22,26
Nref                3572                          3555
Tmin,Tmax           0.962,0.977                   0.962,0.991
Tmin'               0.958
Correction method= MULTI-SCAN
Data completeness= 0.995        Theta(max)= 26.000
R(reflections)= 0.0361( 3121)      wR2(reflections)= 0.0922( 3555)
S = 1.044              Npar= Npar = 243
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 9 Why ?

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) ..... 2 Why ?
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7 Note

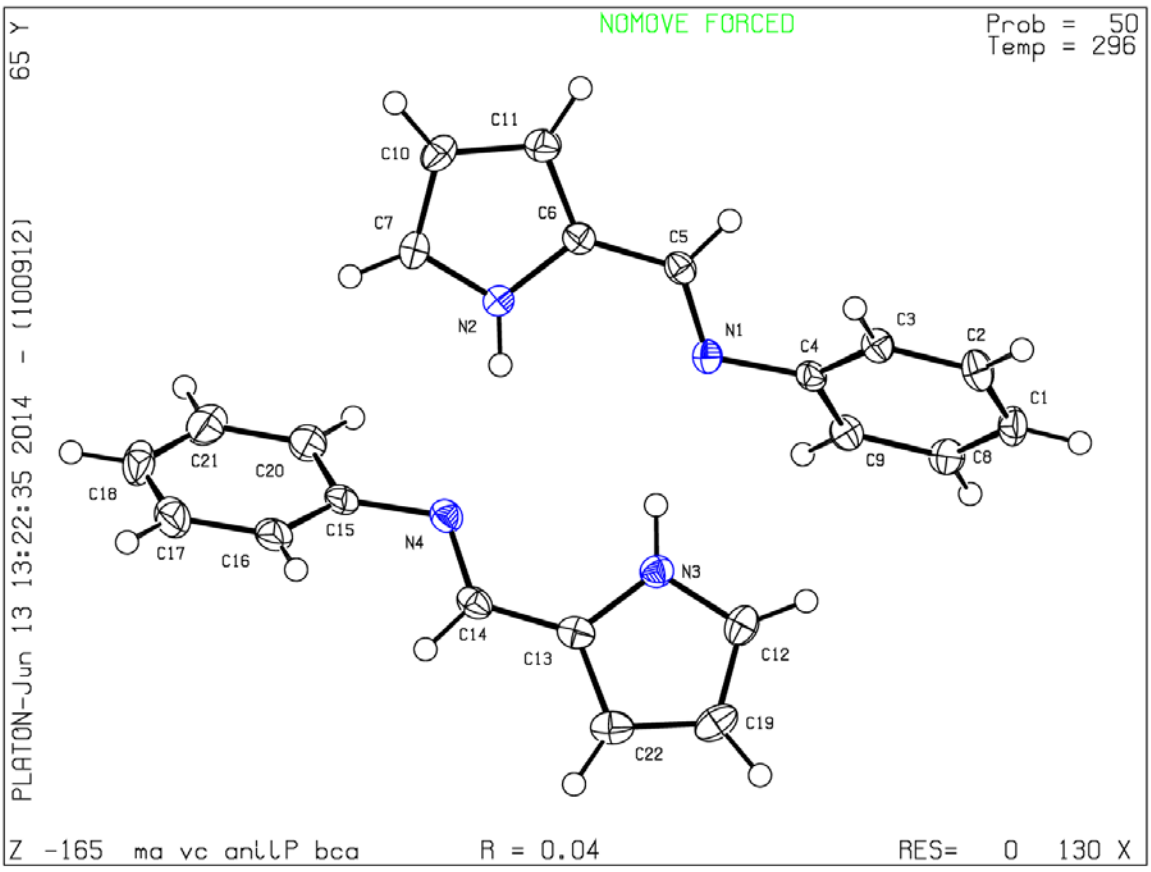
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

Datablock ma_vc_anilinel - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_anilinel

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: HL2

```
Bond precision:      C-C = 0.0019 A              Wavelength=0.71073
Cell:          a=9.4092(8)    b=18.1595(16)  c=21.2310(18)
               alpha=90       beta=90        gamma=90
Temperature: 296 K
                    Calculated                    Reported
Volume              3627.7(5)                     3627.7(5)
Space group         P b c a                       P bca
Hall group          -P 2ac 2ab                    -P 2ac 2ab
Moiety formula      C11 H10 N2                    C11 H10 N2
Sum formula         C11 H10 N2                    C11 H10 N2
Mr                  170.21                        170.21
Dx,g cm-3           1.247                         1.247
Z                   16                            16
Mu (mm-1)           0.076                         0.076
F000                1440.0                        1440.0
F000'               1440.45
h,k,lmax            11,22,26                      11,22,26
Nref                3572                          3555
Tmin,Tmax           0.962,0.977                   0.962,0.991
Tmin'               0.958
Correction method= MULTI-SCAN
Data completeness= 0.995        Theta(max)= 26.000
R(reflections)= 0.0361( 3121)      wR2(reflections)= 0.0922( 3555)
S = 1.044              Npar= Npar = 243
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 9 Why ?

Alert level G

PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) ..... 2 Why ?
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7 Note

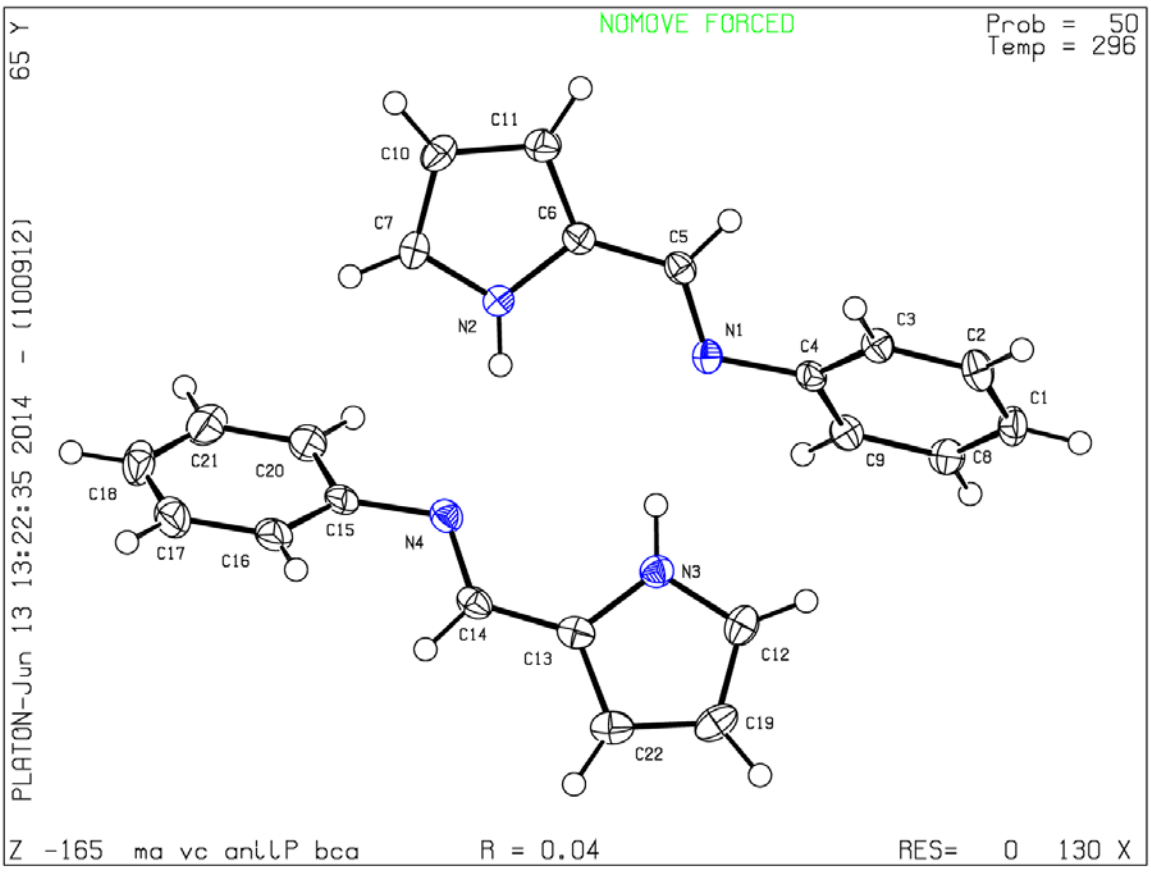
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

2 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 05/02/2014; check.def file version of 05/02/2014

Datablock ma_vc_anilinel - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_benzyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_benzyl

Bond precision: C-C = 0.0016 A Wavelength=0.71073
Cell: a=9.8555(5) b=17.3532(9) c=11.7790(6)
alpha=90 beta=94.184(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2009.13(18)	2009.13(18)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C12 H12 N2	C12 H12 N2
Sum formula	C12 H12 N2	C12 H12 N2
Mr	184.24	184.24
Dx,g cm-3	1.218	1.218
Z	8	8
Mu (mm-1)	0.074	0.074
F000	784.0	784.0
F000'	784.25	
h,k,lmax	12,21,14	12,21,14
Nref	4139	4118
Tmin,Tmax	0.961,0.978	0.957,0.978
Tmin'	0.957	

Correction method= MULTI-SCAN
Data completeness= 0.995 Theta(max)= 26.430
R(reflections)= 0.0357(3683) wR2(reflections)= 0.1016(4118)
S = 1.038 Npar= 261

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 1 Note

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C12 H12 N2
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12 Note

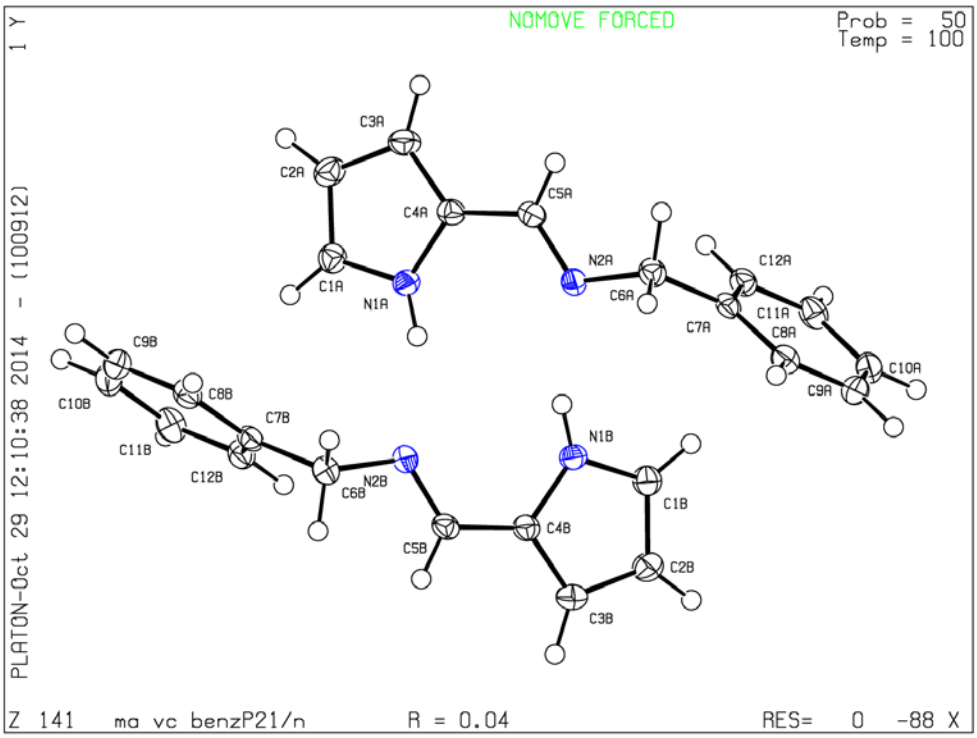
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_benzyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_benzyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_benzyl

Bond precision: C-C = 0.0016 A Wavelength=0.71073
Cell: a=9.8555(5) b=17.3532(9) c=11.7790(6)
alpha=90 beta=94.184(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2009.13(18)	2009.13(18)
Space group	P 21/n	P21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C12 H12 N2	C12 H12 N2
Sum formula	C12 H12 N2	C12 H12 N2
Mr	184.24	184.24
Dx,g cm-3	1.218	1.218
Z	8	8
Mu (mm-1)	0.074	0.074
F000	784.0	784.0
F000'	784.25	
h,k,lmax	12,21,14	12,21,14
Nref	4139	4118
Tmin,Tmax	0.961,0.978	0.957,0.978
Tmin'	0.957	

Correction method= MULTI-SCAN
Data completeness= 0.995 Theta(max)= 26.430
R(reflections)= 0.0357(3683) wR2(reflections)= 0.1016(4118)
S = 1.038 Npar= 261

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 7 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 1 Note

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 4 Note

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C12 H12 N2
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12 Note

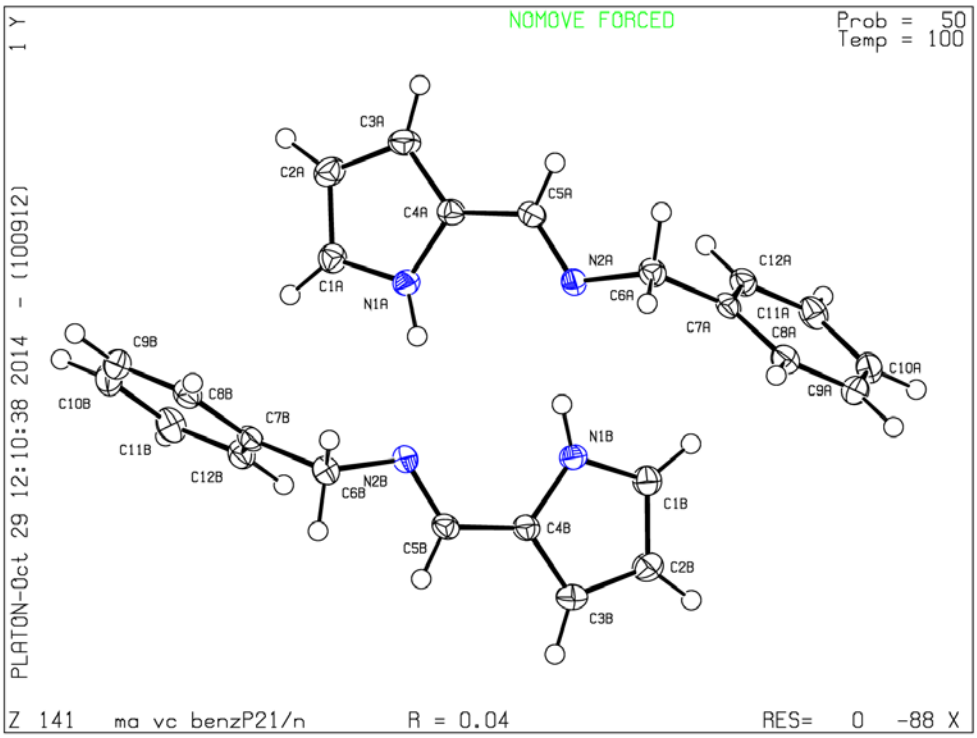
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_benzyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_menaphthyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_menaphthyl

Bond precision: C-C = 0.0016 A Wavelength=0.71073
Cell: a=5.3017(3) b=8.8579(5) c=13.9265(8)
alpha=104.896(3) beta=99.212(2) gamma=96.675(2)
Temperature: 100 K

	Calculated	Reported
Volume	615.34(6)	615.33(6)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C16 H14 N2	C16 H14 N2
Sum formula	C16 H14 N2	C16 H14 N2
Mr	234.29	234.29
Dx,g cm-3	1.265	1.265
Z	2	2
Mu (mm-1)	0.075	0.075
F000	248.0	248.0
F000'	248.08	
h,k,lmax	6,10,17	6,10,17
Nref	2437	2395
Tmin,Tmax	0.970,0.978	0.970,0.978
Tmin'	0.970	

Correction method= MULTI-SCAN
Data completeness= 0.983 Theta(max)= 26.070
R(reflections)= 0.0383(2258) wR2(reflections)= 0.1066(2395)
S = 1.079 Npar= 167

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 40 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note

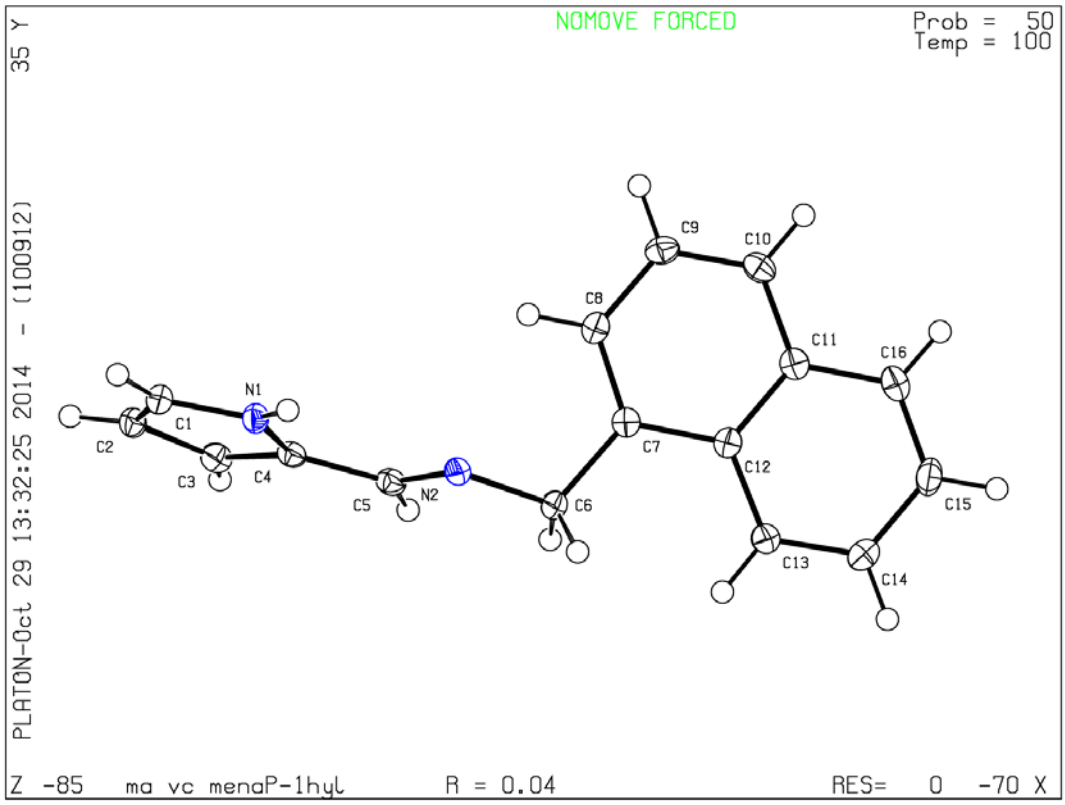
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_menaphthyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_menaphthyl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_menaphthyl

Bond precision: C-C = 0.0016 A Wavelength=0.71073
Cell: a=5.3017(3) b=8.8579(5) c=13.9265(8)
alpha=104.896(3) beta=99.212(2) gamma=96.675(2)
Temperature: 100 K

	Calculated	Reported
Volume	615.34(6)	615.33(6)
Space group	P -1	P-1
Hall group	-P 1	-P 1
Moiety formula	C16 H14 N2	C16 H14 N2
Sum formula	C16 H14 N2	C16 H14 N2
Mr	234.29	234.29
Dx,g cm-3	1.265	1.265
Z	2	2
Mu (mm-1)	0.075	0.075
F000	248.0	248.0
F000'	248.08	
h,k,lmax	6,10,17	6,10,17
Nref	2437	2395
Tmin,Tmax	0.970,0.978	0.970,0.978
Tmin'	0.970	

Correction method= MULTI-SCAN
Data completeness= 0.983 Theta(max)= 26.070
R(reflections)= 0.0383(2258) wR2(reflections)= 0.1066(2395)
S = 1.079 Npar= 167

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 40 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4 Note

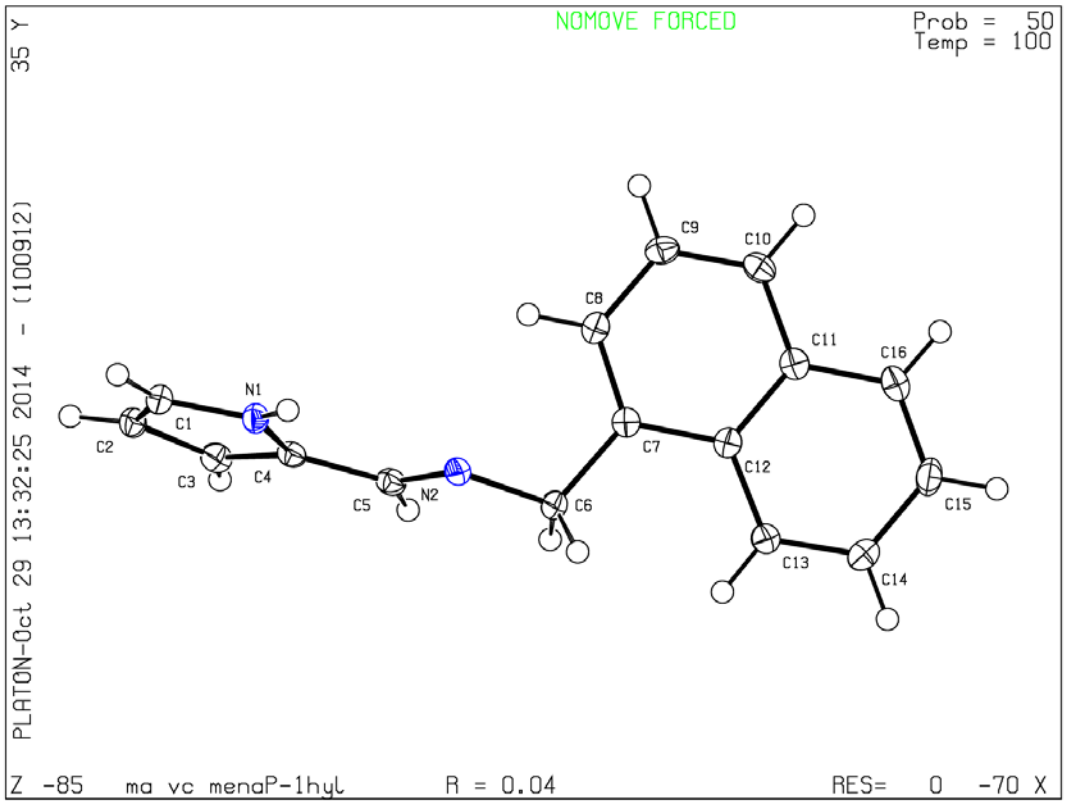
---

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_menaphthyl - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_phet

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_phet

Bond precision: C-C = 0.0018 A Wavelength=0.71073
Cell: a=7.0928(5) b=16.0355(12) c=9.2398(7)
alpha=90 beta=96.261(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1044.64(13)	1044.64(13)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H14 N2	C13 H14 N2
Sum formula	C13 H14 N2	C13 H14 N2
Mr	198.26	198.26
Dx,g cm-3	1.261	1.261
Z	4	4
Mu (mm-1)	0.076	0.076
F000	424.0	424.0
F000'	424.13	
h,k,lmax	8,19,11	8,19,11
Nref	2093	2078
Tmin,Tmax	0.982,0.998	0.974,0.998
Tmin'	0.974	

Correction method= MULTI-SCAN
Data completeness= 0.993 Theta(max)= 26.200
R(reflections)= 0.0373(1834) wR2(reflections)= 0.0980(2078)
S = 1.062 Npar= 140

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report

Alert level G

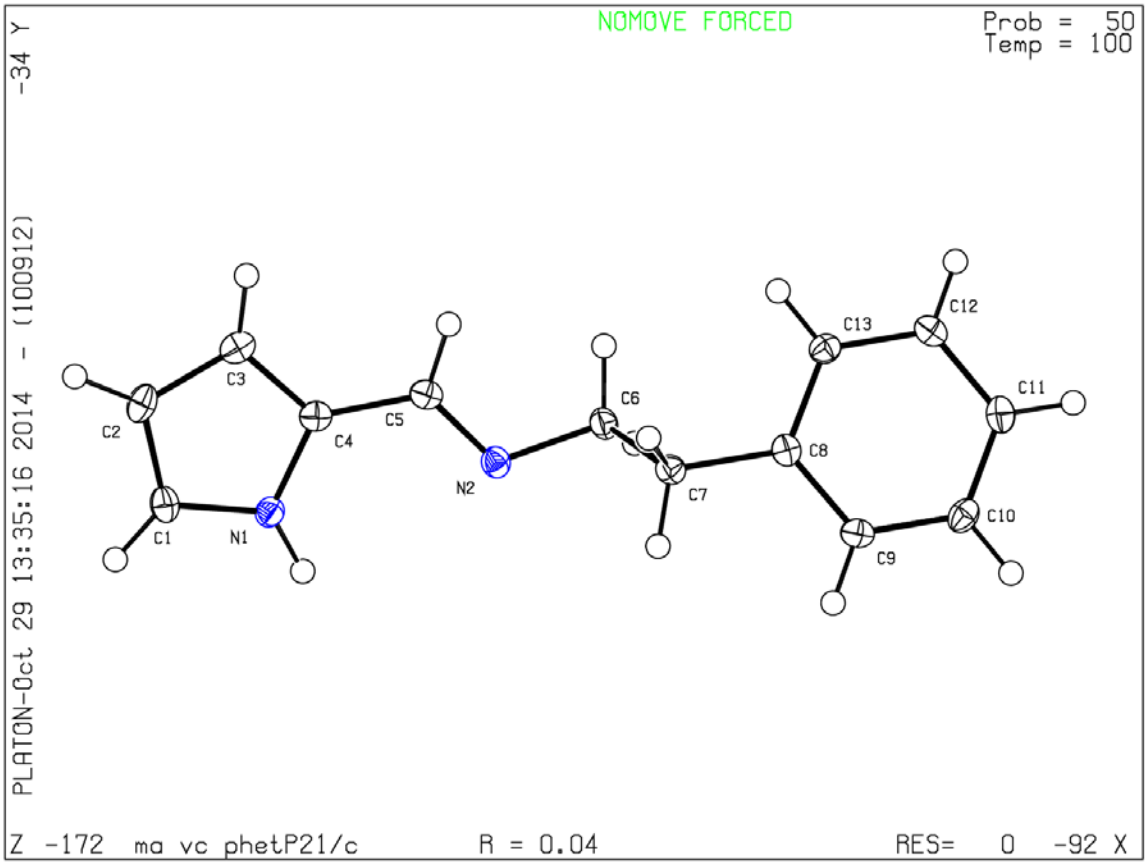
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
3 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_phet - ellipsoid plot



checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) ma_vc_phet

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Structure factor report

Datablock: ma_vc_phet

Bond precision: C-C = 0.0018 A Wavelength=0.71073
Cell: a=7.0928(5) b=16.0355(12) c=9.2398(7)
alpha=90 beta=96.261(3) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1044.64(13)	1044.64(13)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C13 H14 N2	C13 H14 N2
Sum formula	C13 H14 N2	C13 H14 N2
Mr	198.26	198.26
Dx,g cm-3	1.261	1.261
Z	4	4
Mu (mm-1)	0.076	0.076
F000	424.0	424.0
F000'	424.13	
h,k,lmax	8,19,11	8,19,11
Nref	2093	2078
Tmin,Tmax	0.982,0.998	0.974,0.998
Tmin'	0.974	

Correction method= MULTI-SCAN
Data completeness= 0.993 Theta(max)= 26.200
R(reflections)= 0.0373(1834) wR2(reflections)= 0.0980(2078)
S = 1.062 Npar= 140

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report

Alert level G

PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
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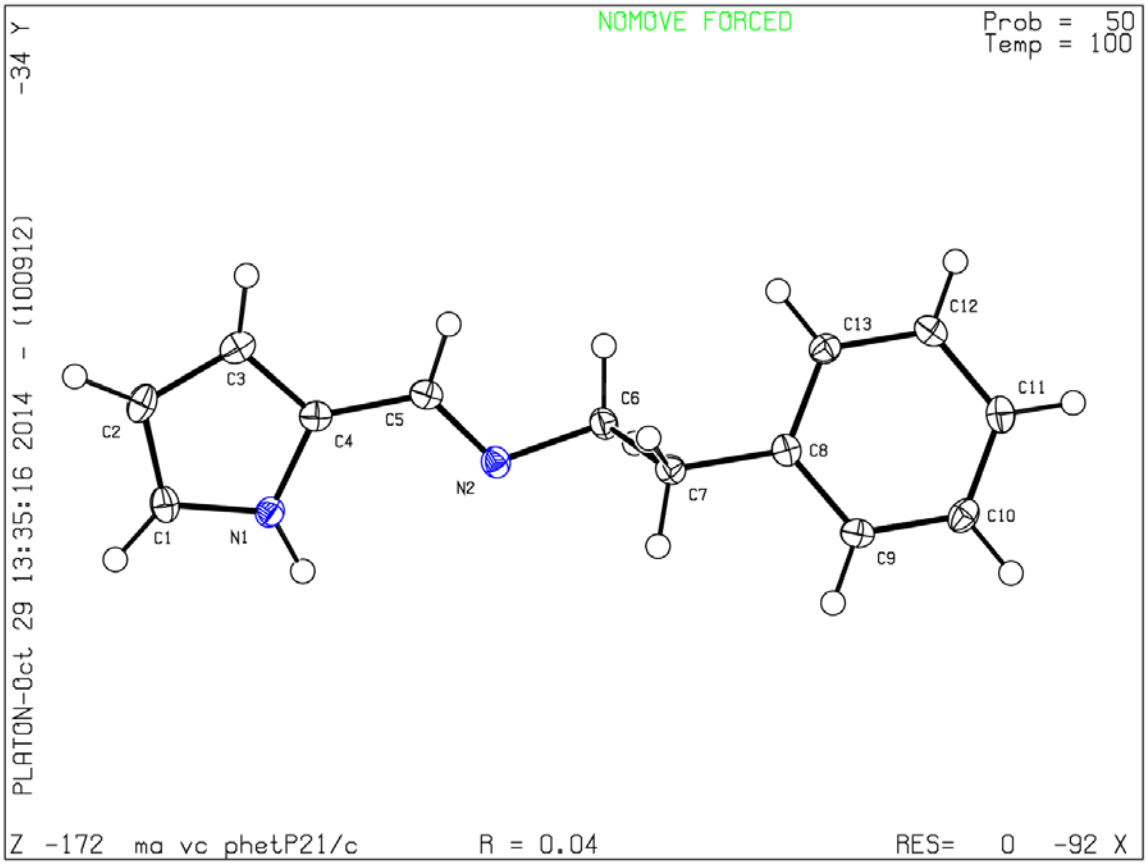
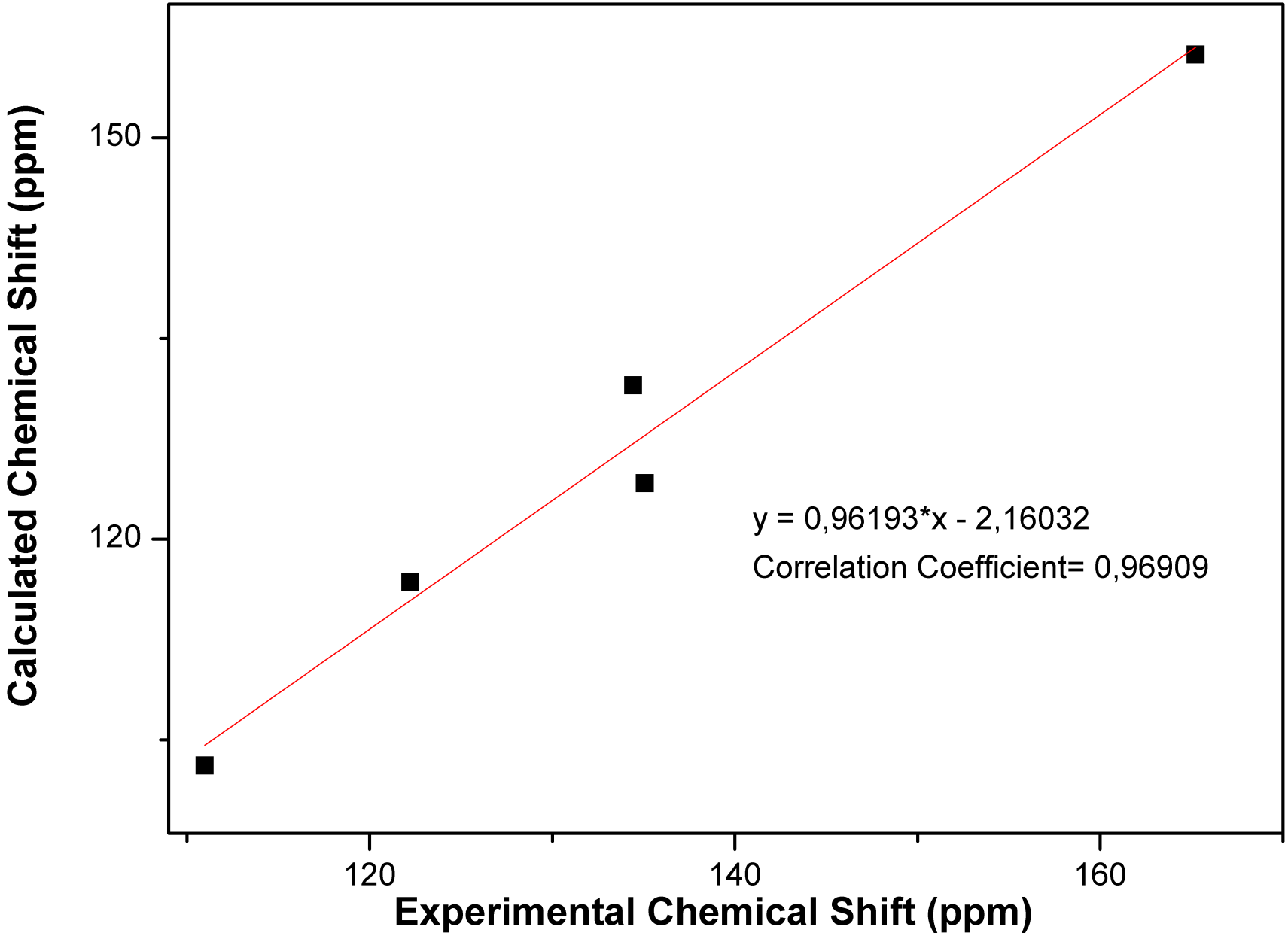
1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

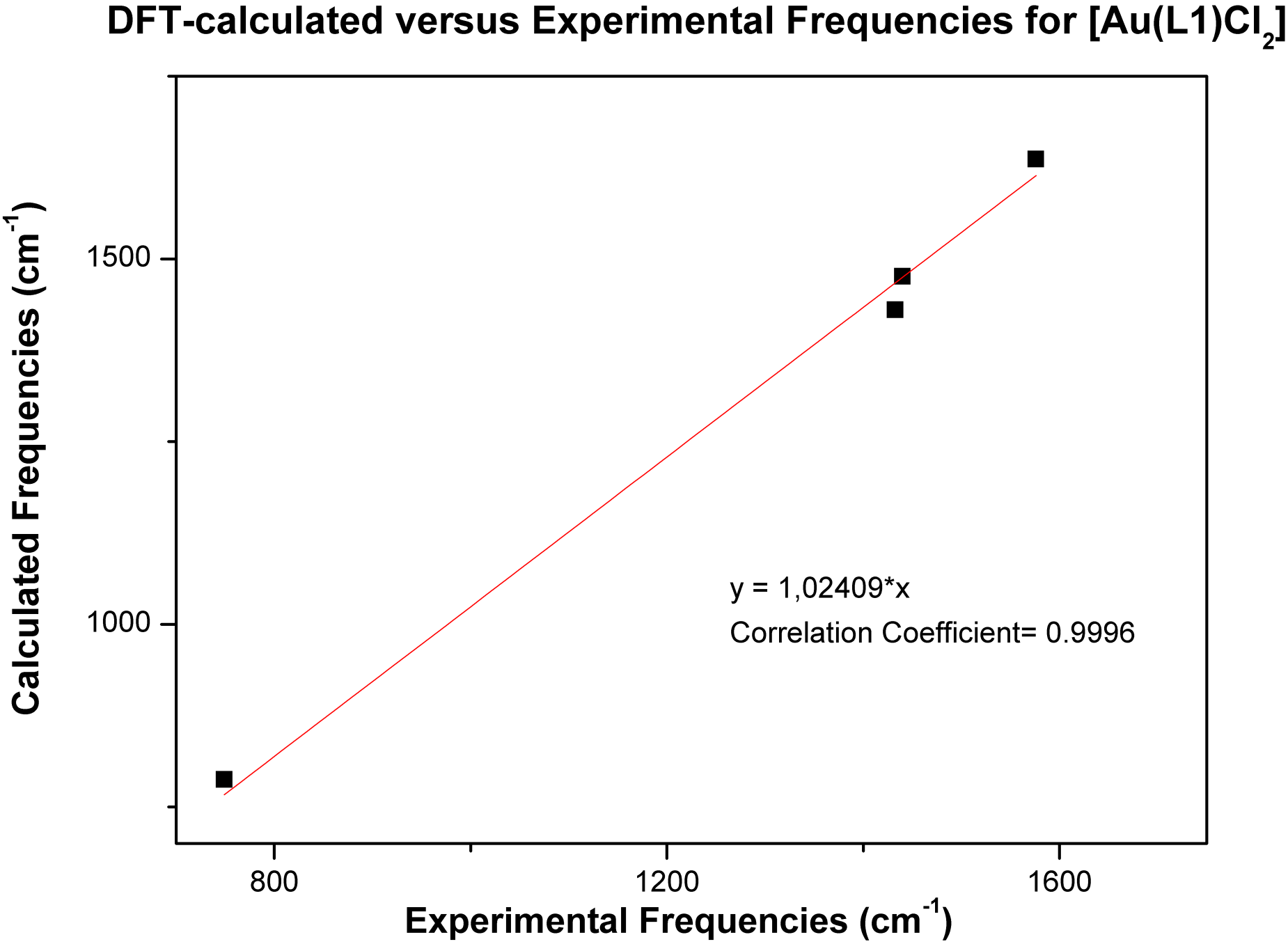
PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock ma_vc_phet - ellipsoid plot

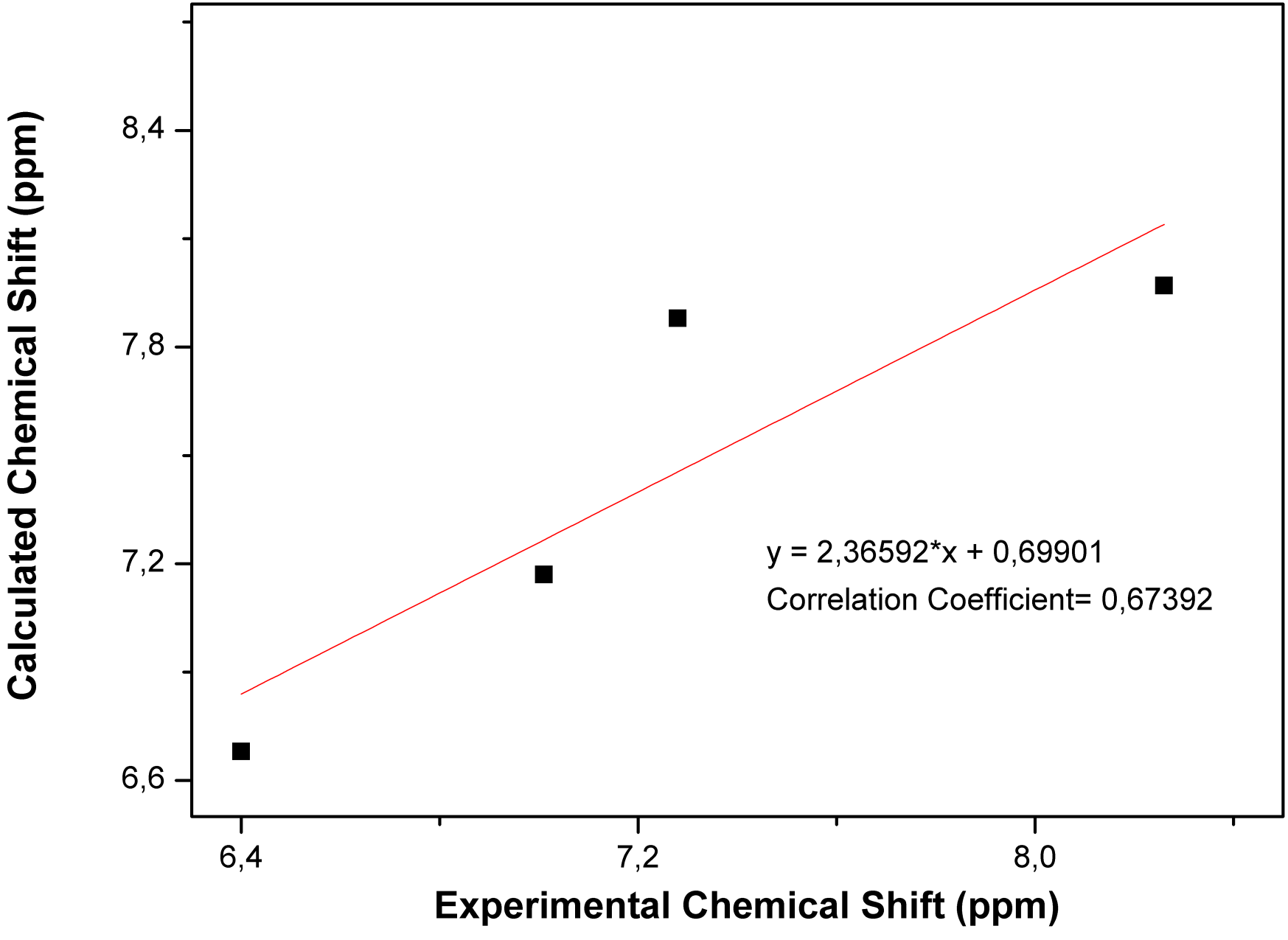


DFT-Calculated versus Experimental ^{13}C NMR Chemical Shifts for $[Au(L1)Cl_2]$

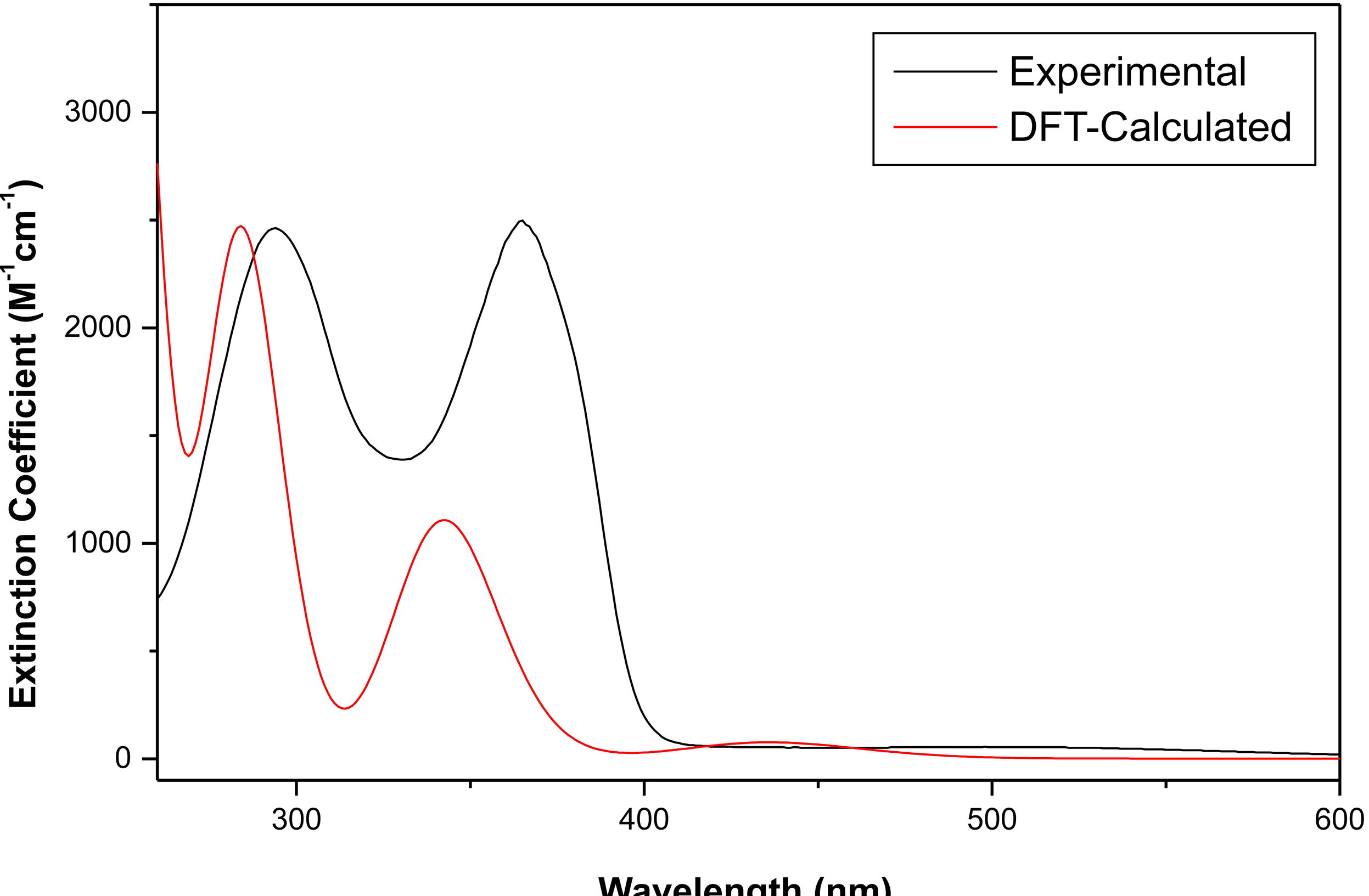


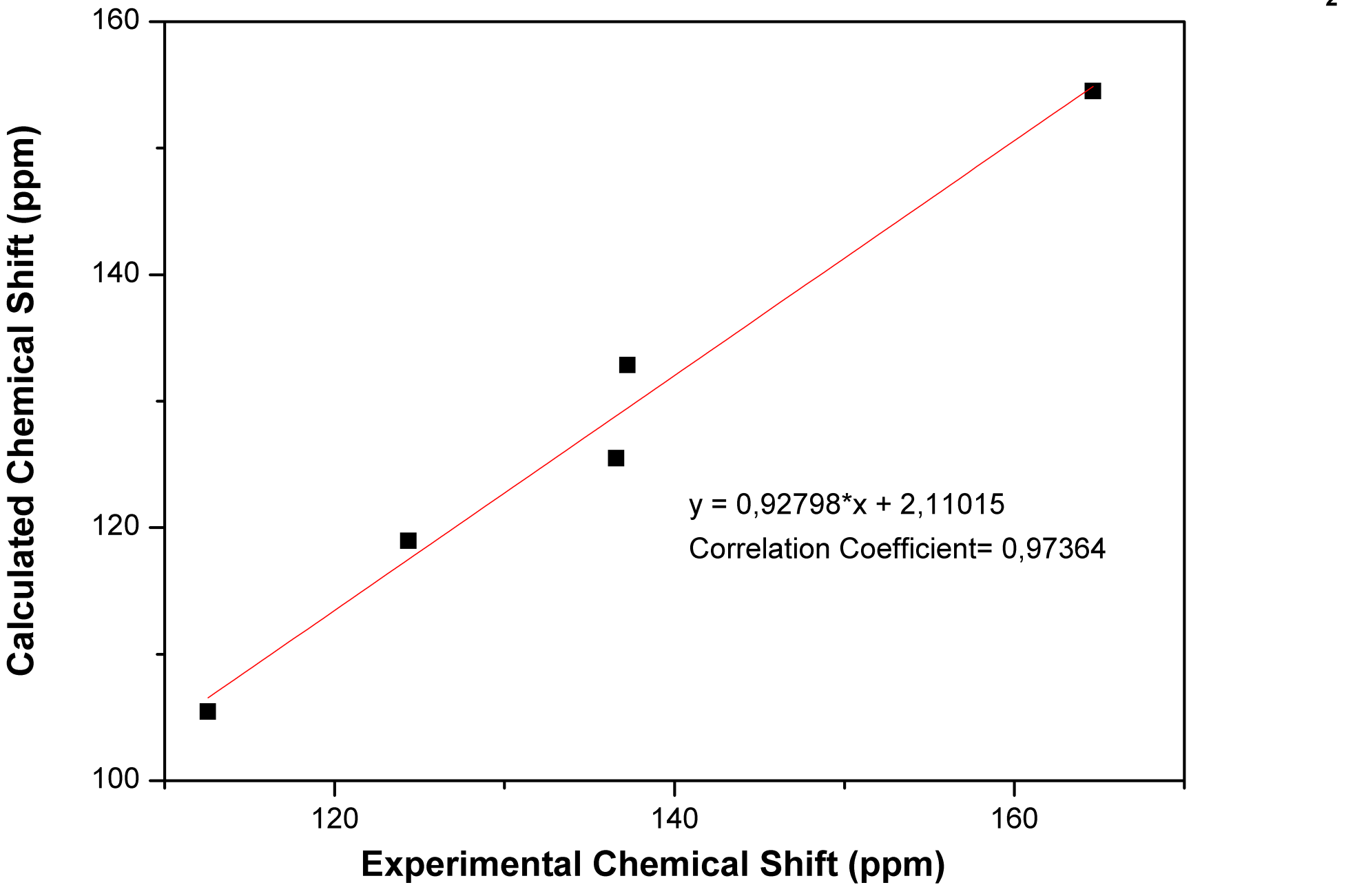

DFT-calculated versus Experimental Frequencies for [Au(L1)Cl2]
Calculated Frequencies (cm-1)
1500
1000
800
1200
1600
Experimental Frequencies (cm-1)
y = 1,02409*x
Correlation Coefficient= 0.9996

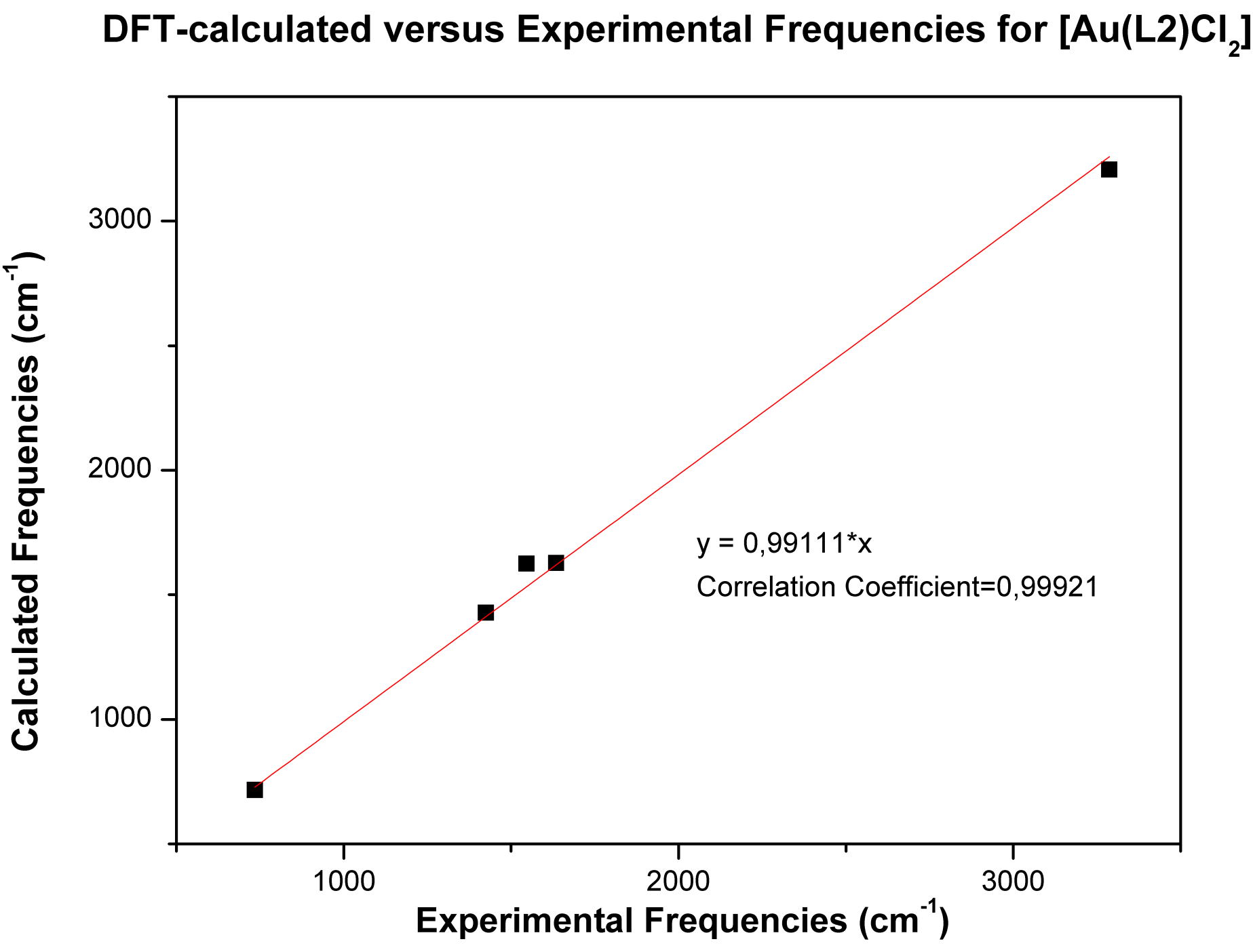
DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for $[Au(L1)Cl_2]$



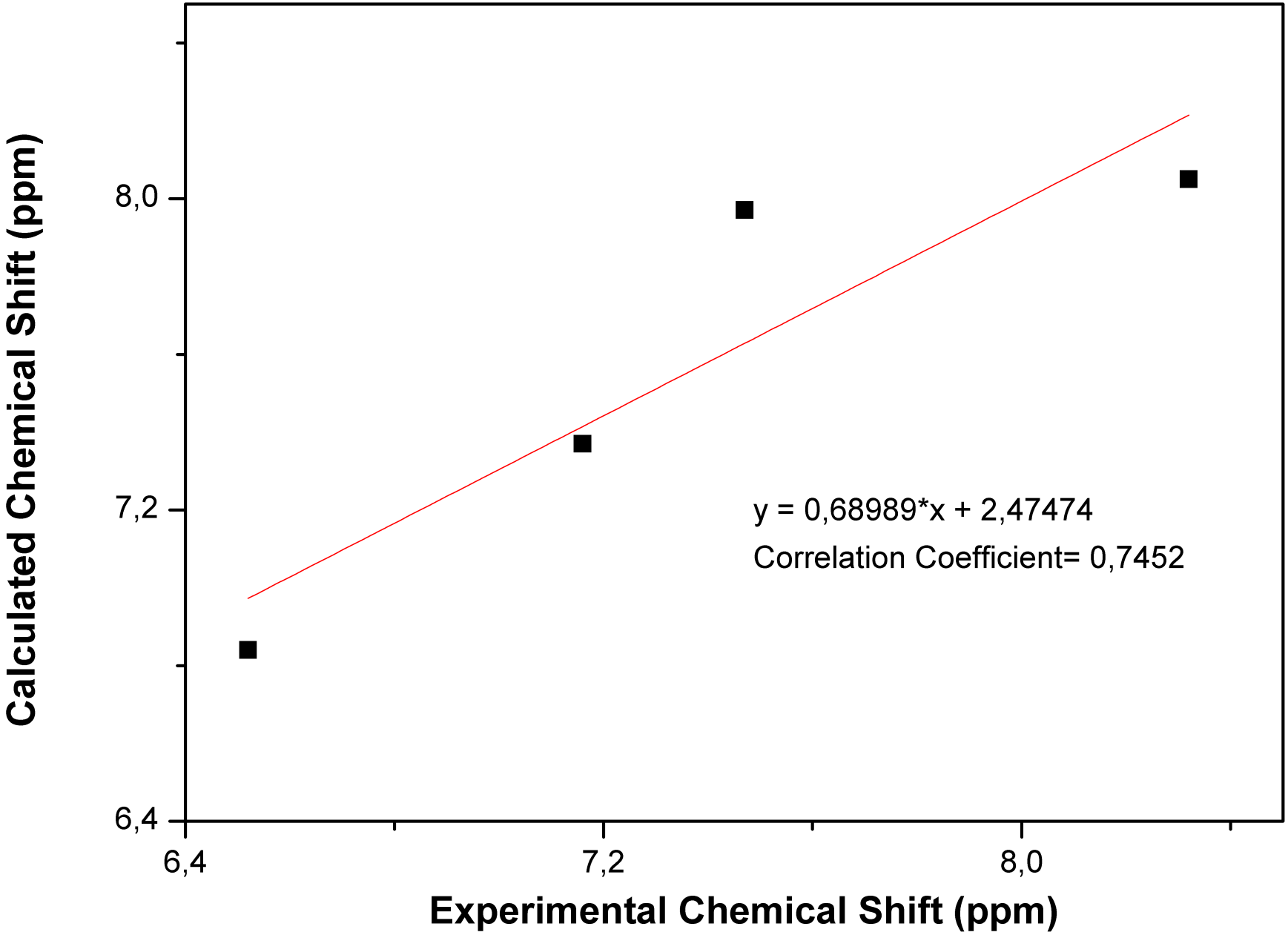
Superposition of Experimental and DFT-calculated UV/vis Spectra for $[Au(L1)Cl_2]$



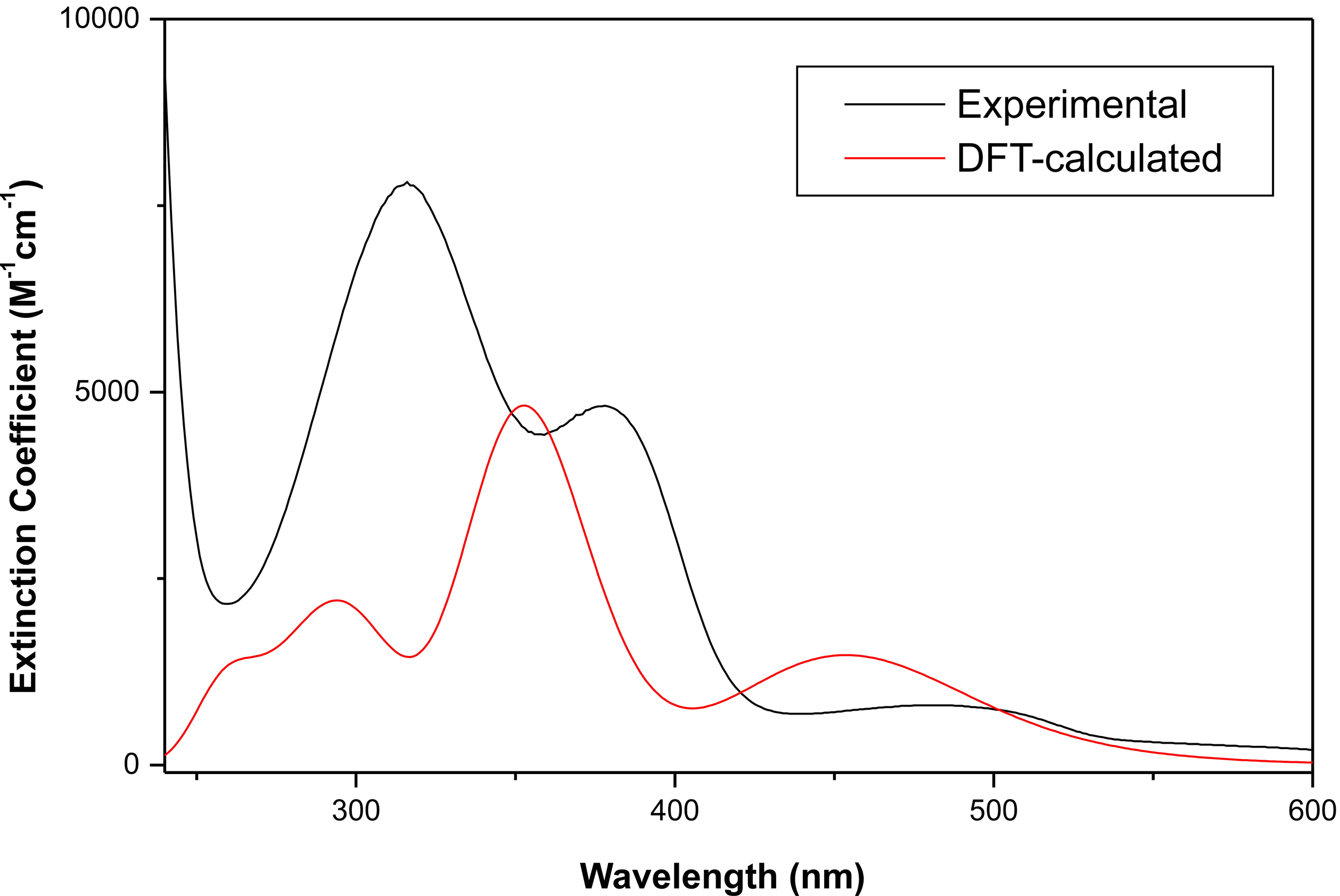

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for [Au(L2)Cl2]
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
160
140
120
100
120
140
160
y = 0,92798*x + 2,11015
Correlation Coefficient= 0,97364

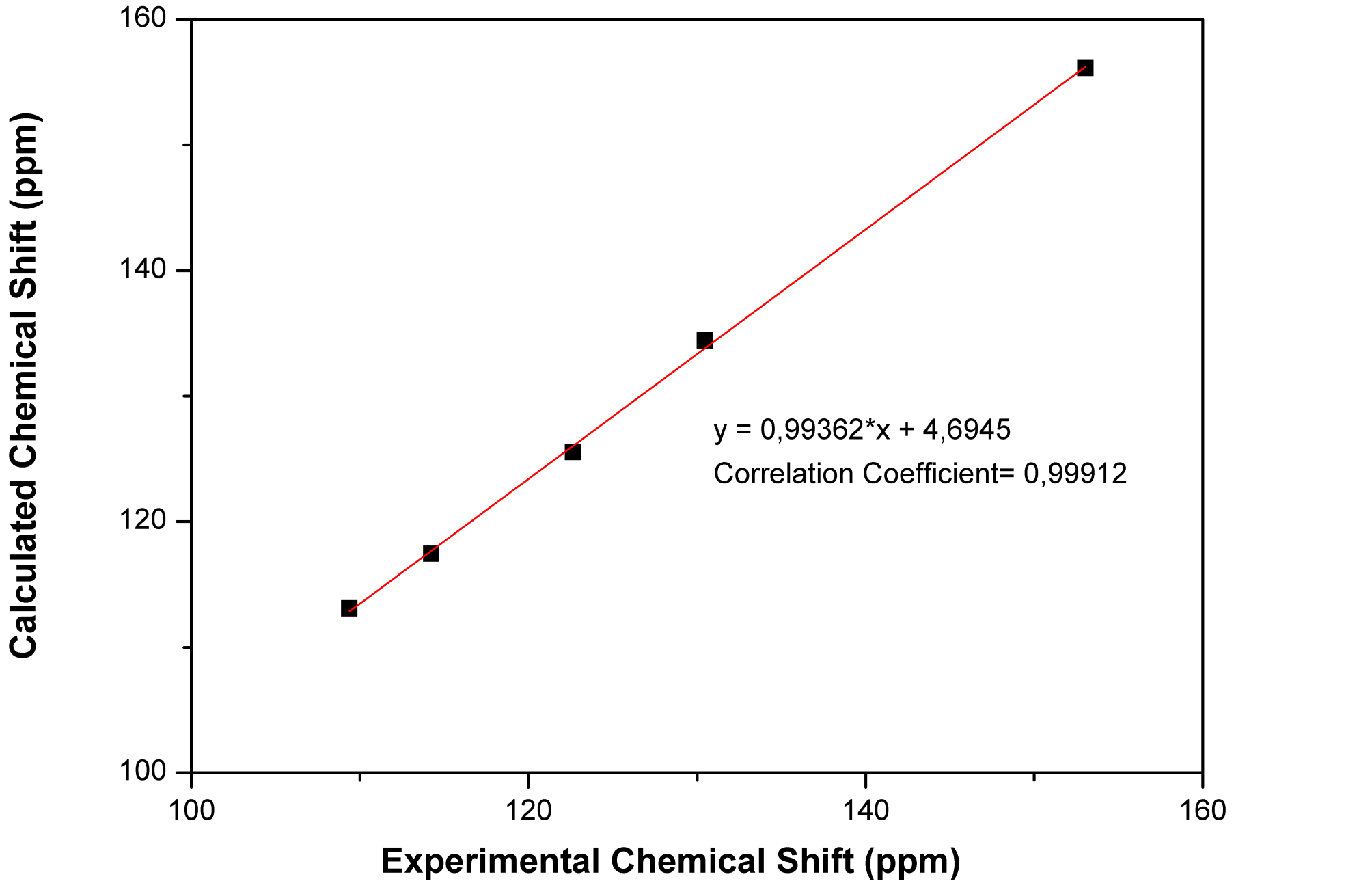

DFT-calculated versus Experimental Frequencies for [Au(L2)Cl2]
Calculated Frequencies (cm-1)
3000
2000
1000
y = 0,99111*x
Correlation Coefficient=0,99921
1000
2000
3000
Experimental Frequencies (cm-1)

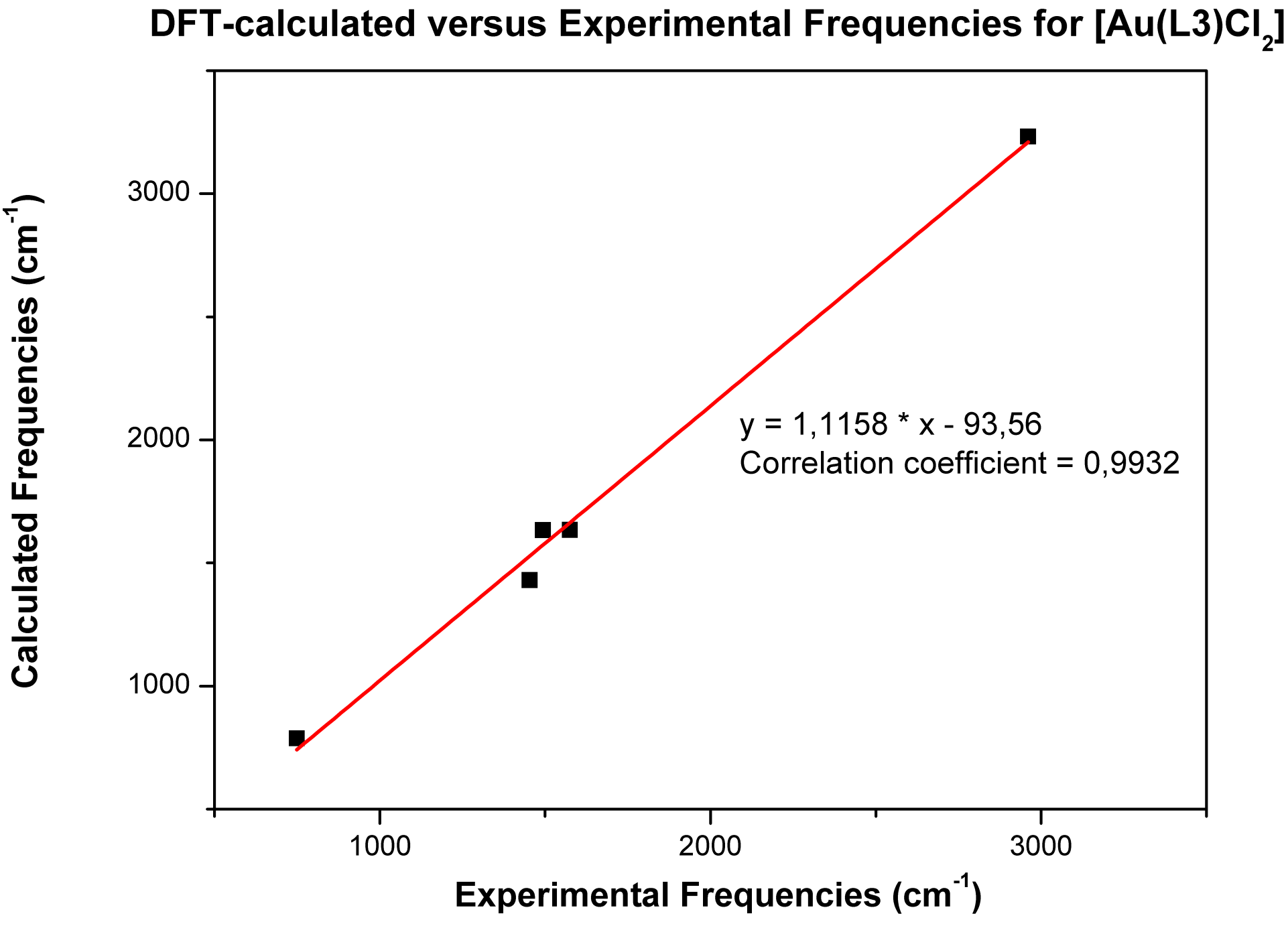
DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for $[Au(L2)Cl_2]$



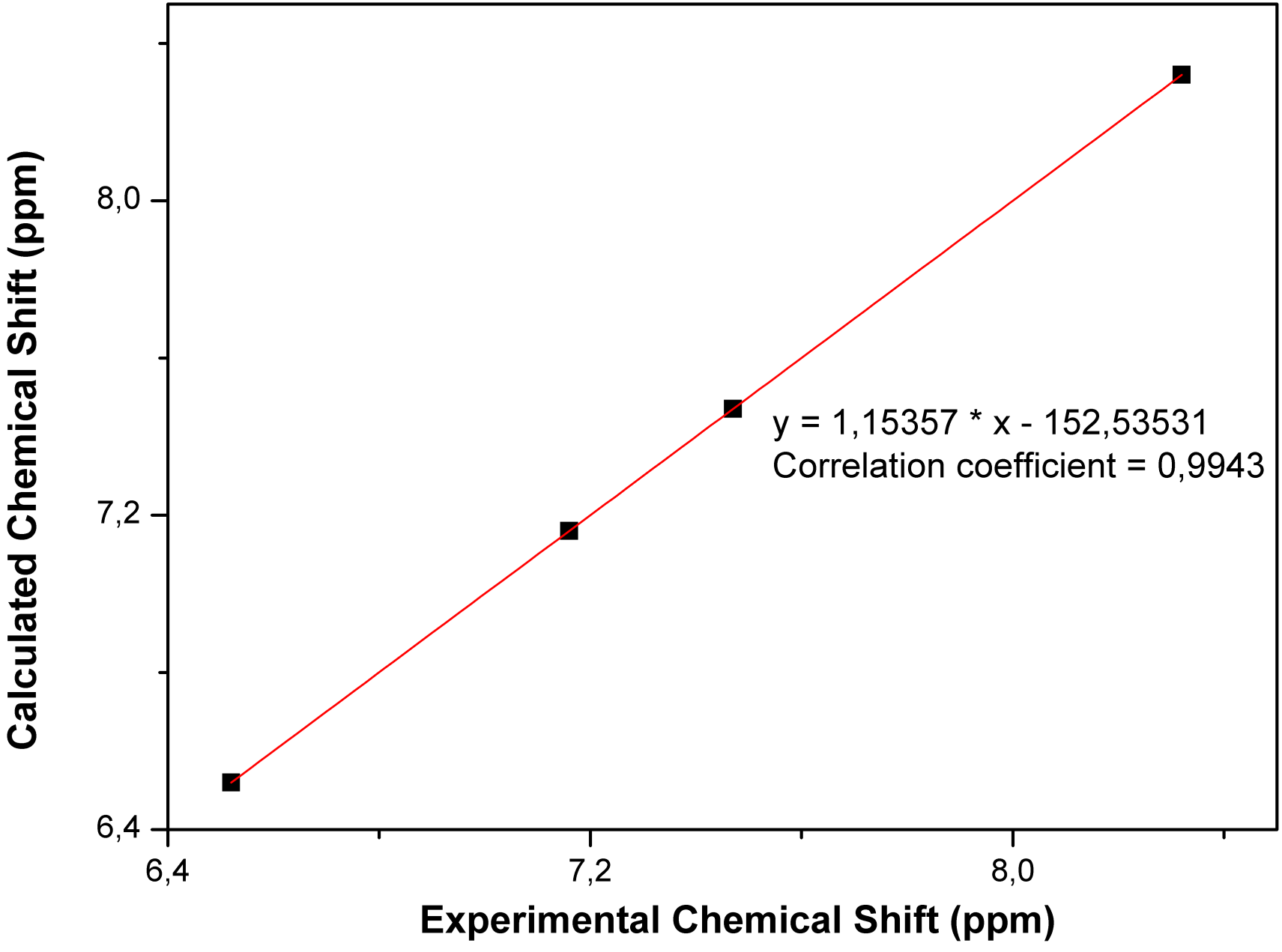
Superposition of Experimental and DFT-calculated UV/vis Spectra for $[Au(L2)Cl_2]$

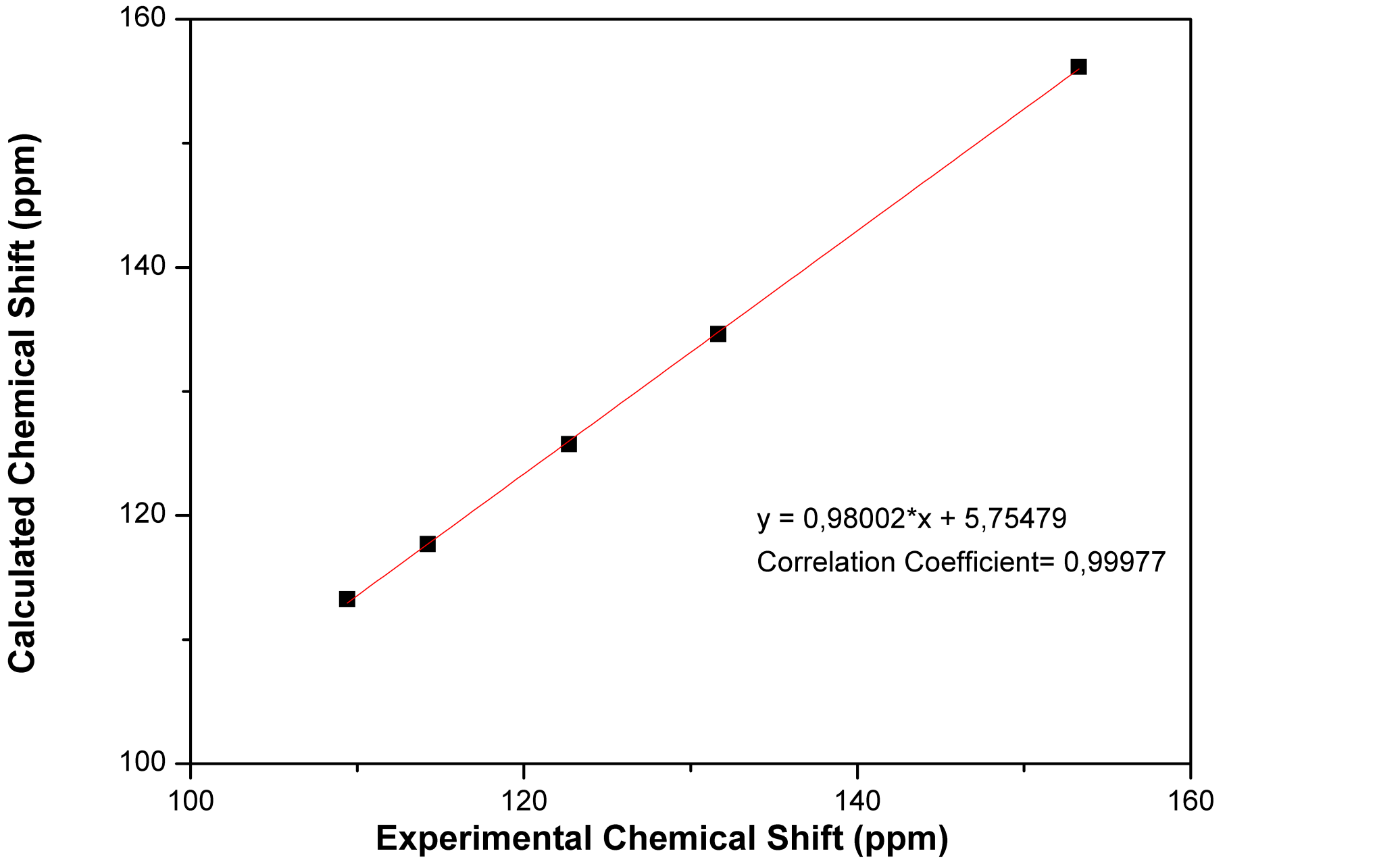


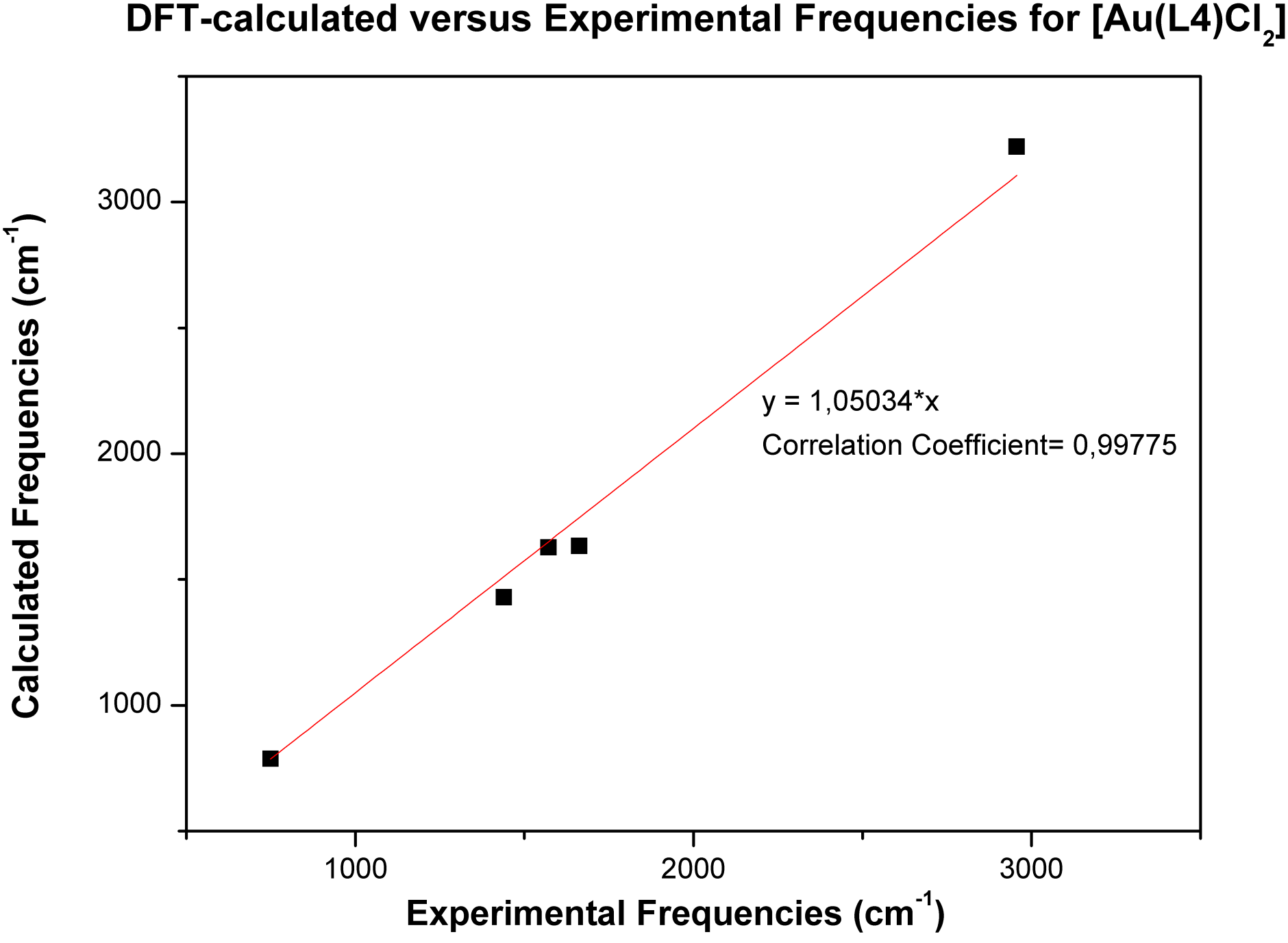

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for [Au(L3)Cl2]
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
160
140
120
100
100
120
140
160
y = 0,99362*x + 4,6945
Correlation Coefficient= 0,99912


DFT-calculated versus Experimental Frequencies for [Au(L3)Cl2]
Calculated Frequencies (cm-1)
Experimental Frequencies (cm-1)
3000
2000
1000
1000
2000
3000
y = 1,1158 * x - 93,56
Correlation coefficient = 0,9932

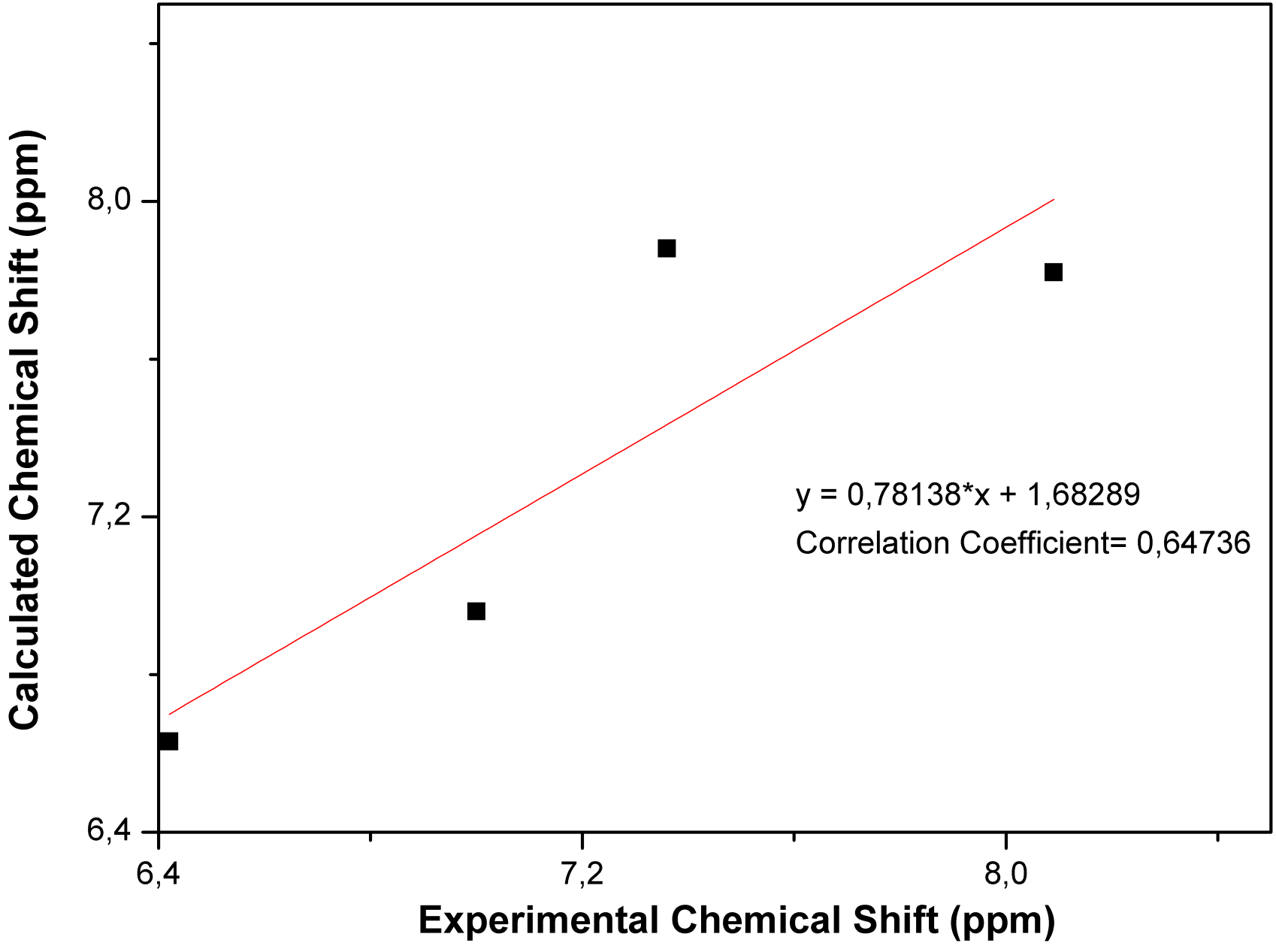
DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for $[Au(L3)Cl_2]$

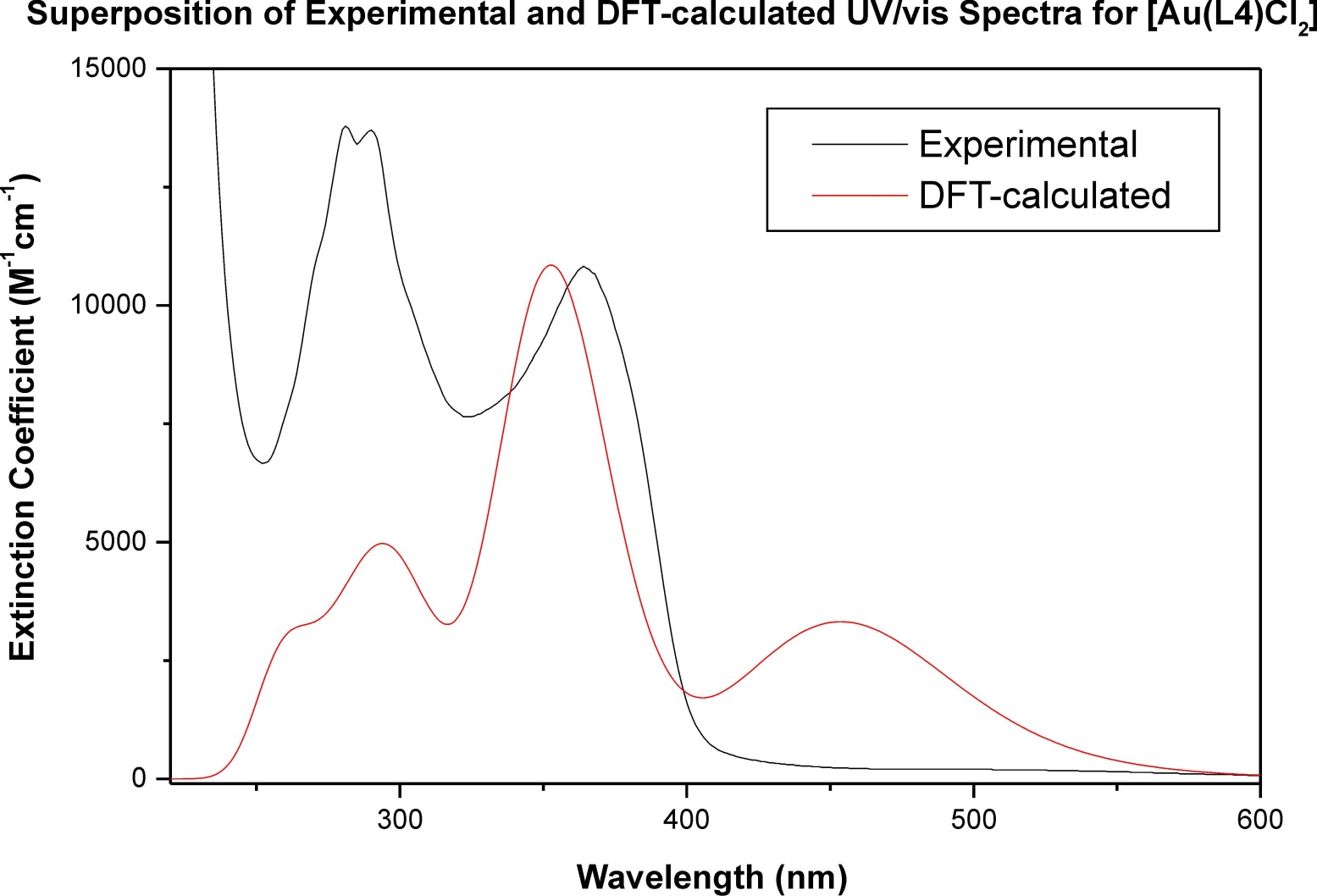


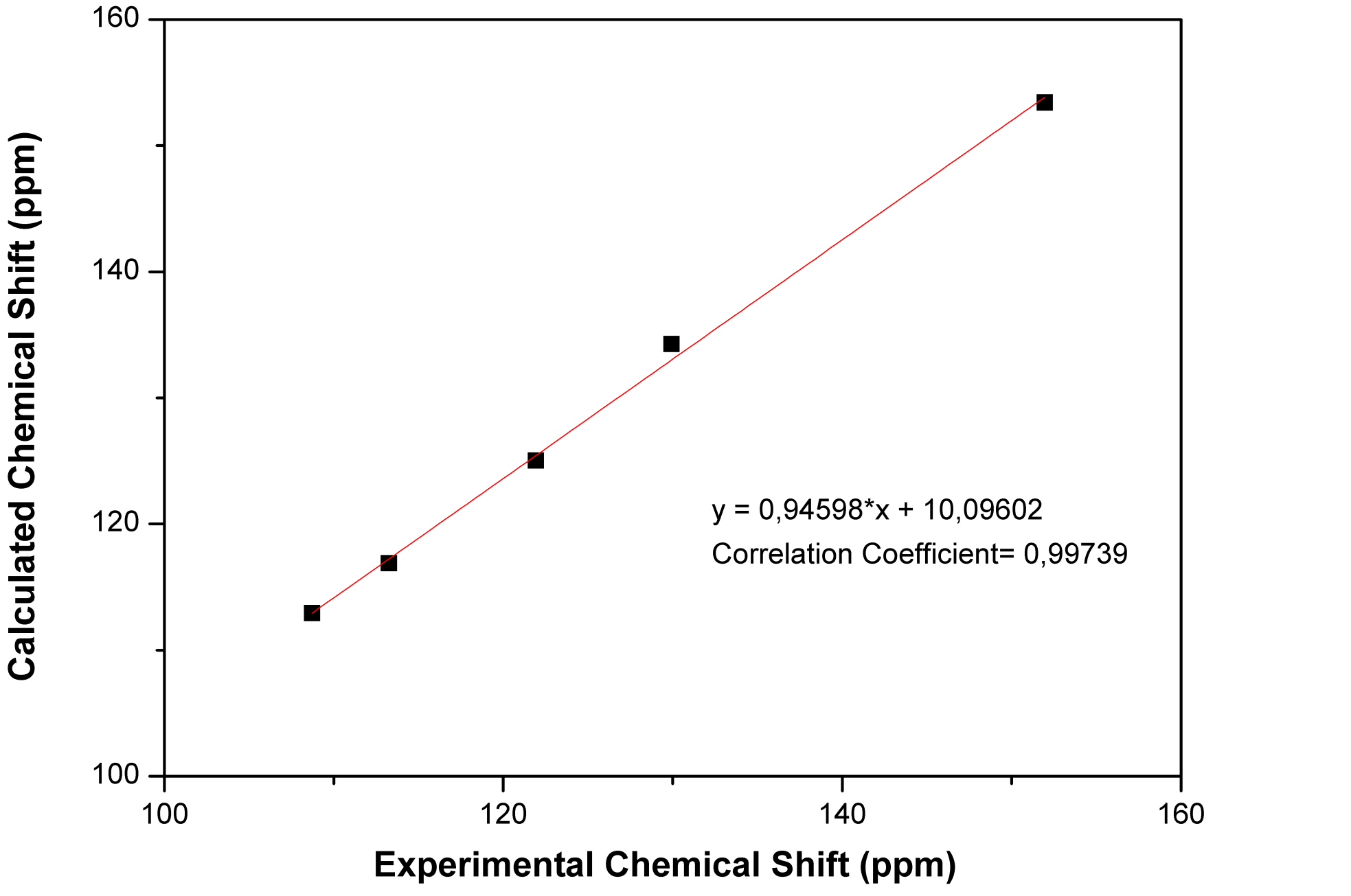

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for [Au(L4)Cl2]
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
160
140
120
100
100
120
140
160
y = 0,98002*x + 5,75479
Correlation Coefficient= 0,99977


DFT-calculated versus Experimental Frequencies for [Au(L4)Cl2]
Calculated Frequencies (cm-1)
Experimental Frequencies (cm-1)
3000
2000
1000
1000
2000
3000
y = 1,05034*x
Correlation Coefficient= 0,99775

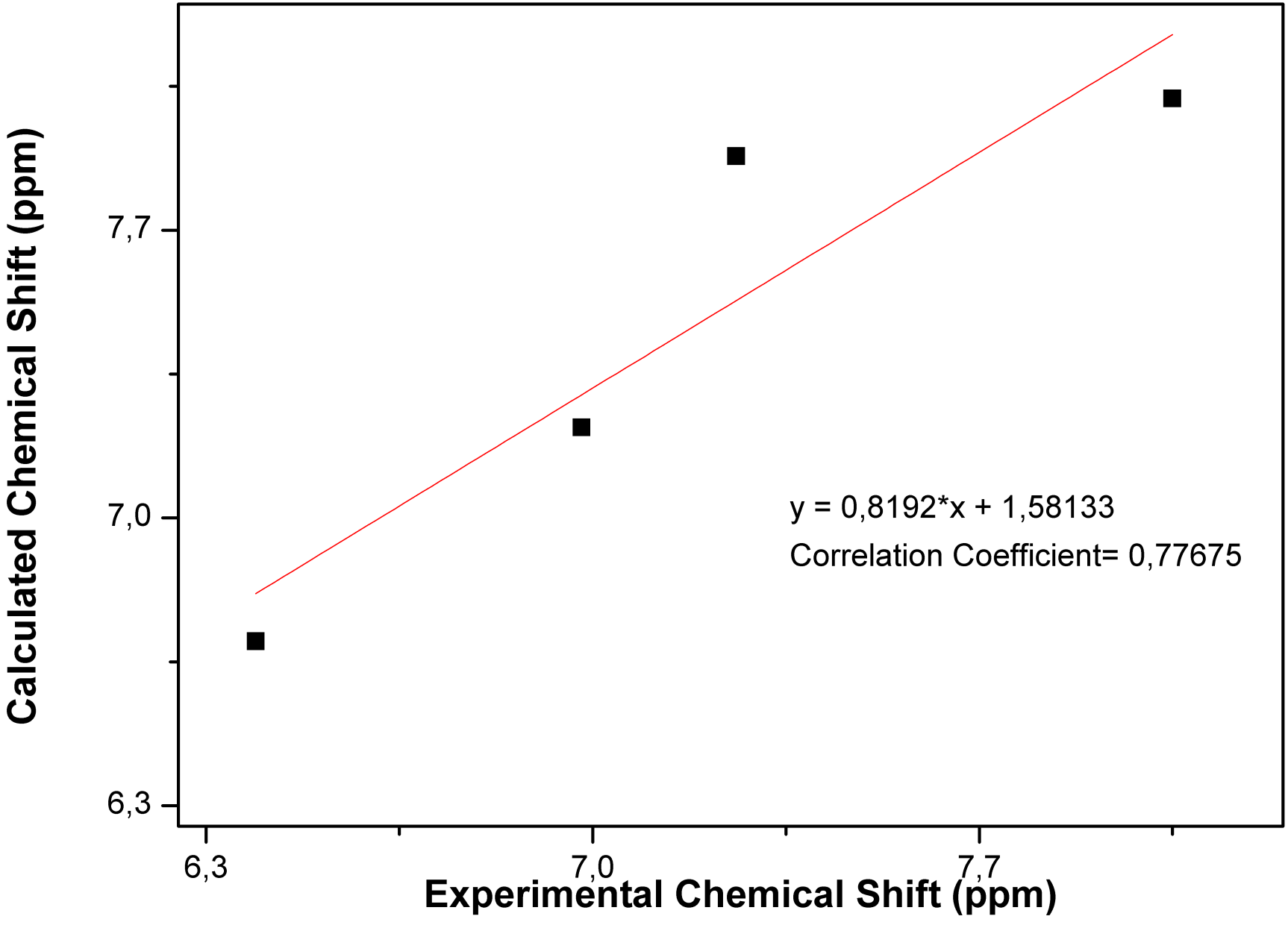
DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for $[Au(L4)Cl_2]$

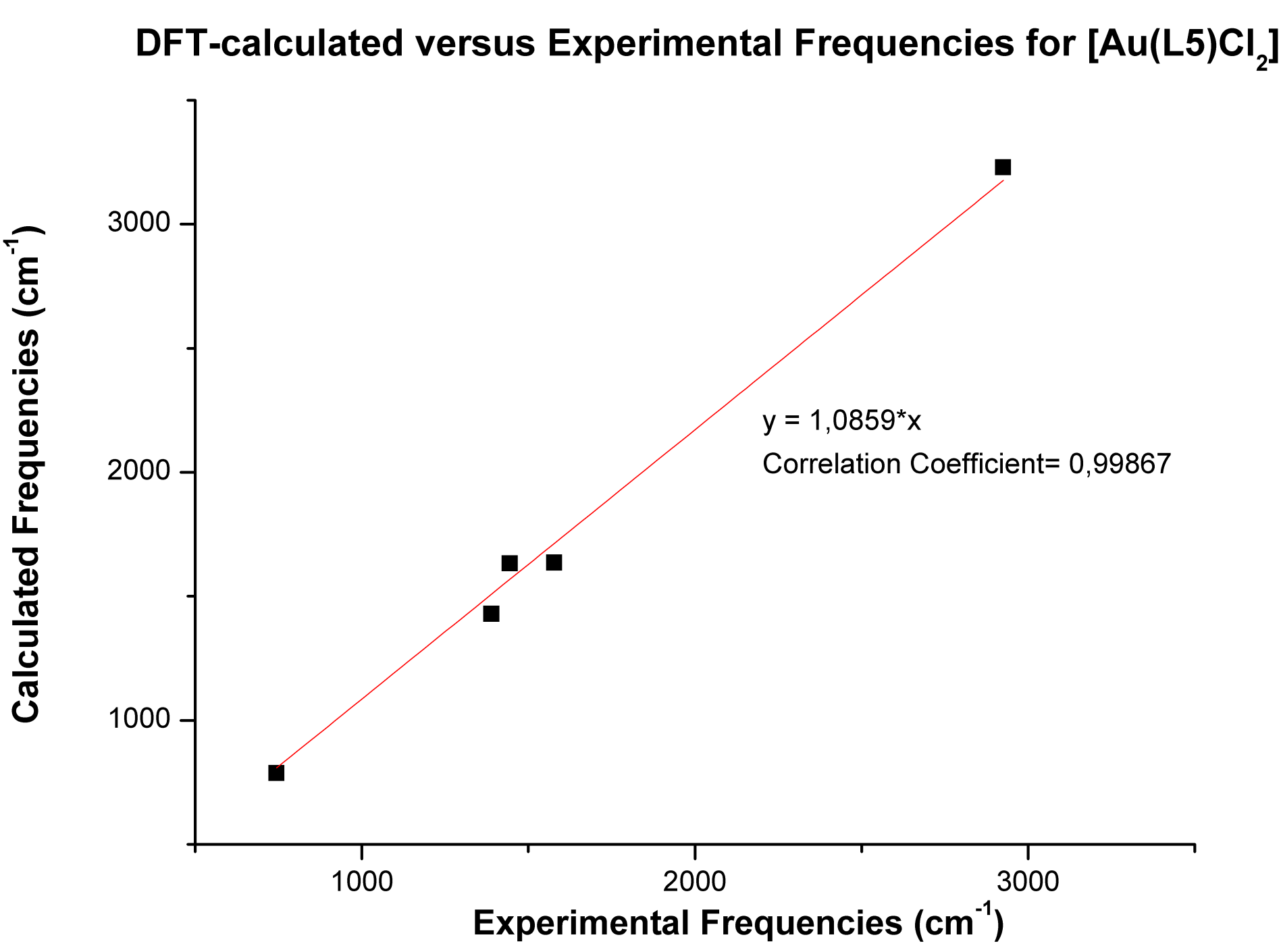



Superposition of Experimental and DFT-calculated UV/vis Spectra for [Au(L4)Cl2]
Experimental
DFT-calculated
Extinction Coefficient (M-1cm-1)
Wavelength (nm)
15000
10000
5000
0
300
400
500
600

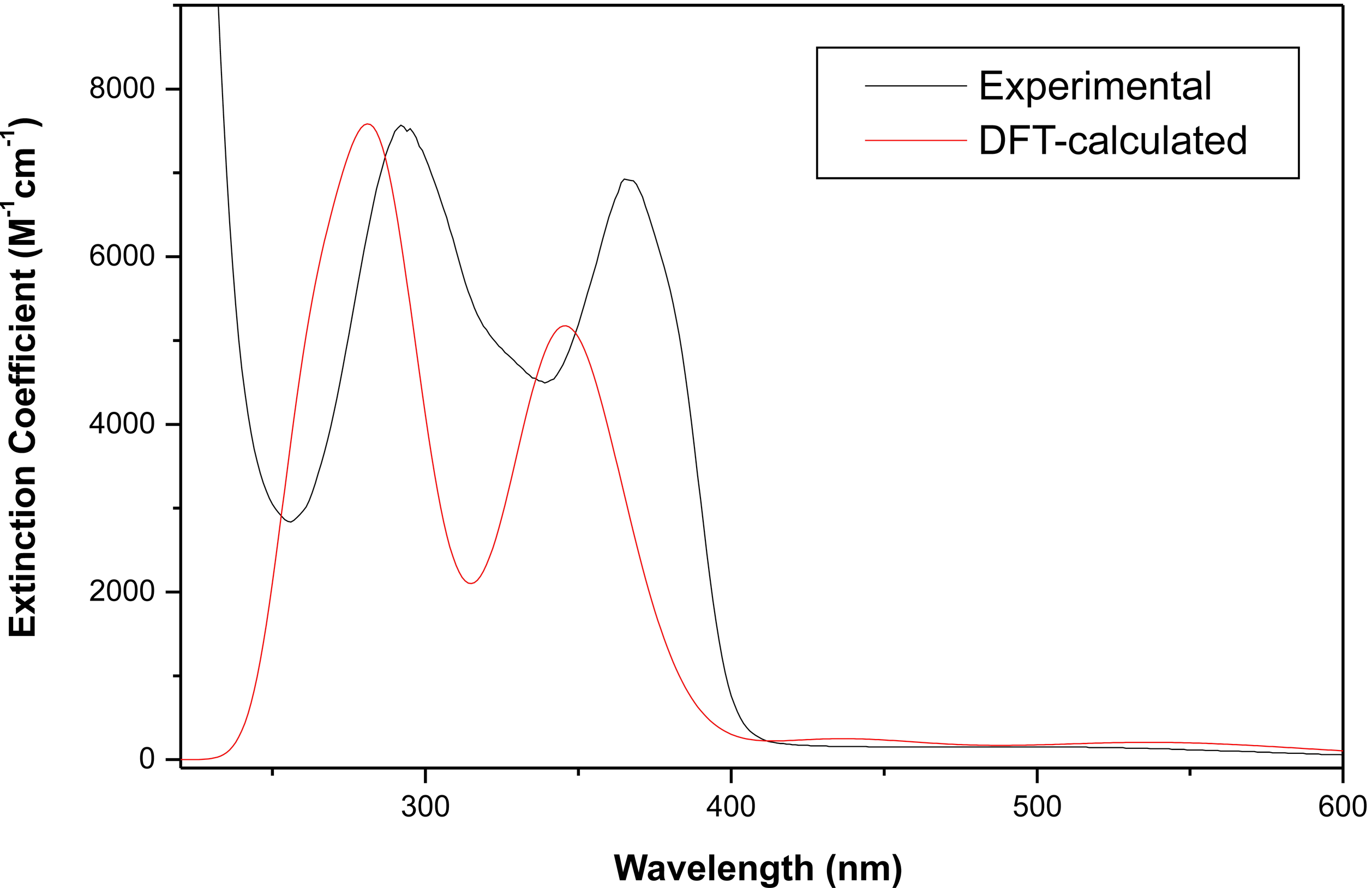

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for [Au(L5)Cl2]
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
160
140
120
100
100
120
140
160
y = 0,94598*x + 10,09602
Correlation Coefficient= 0,99739

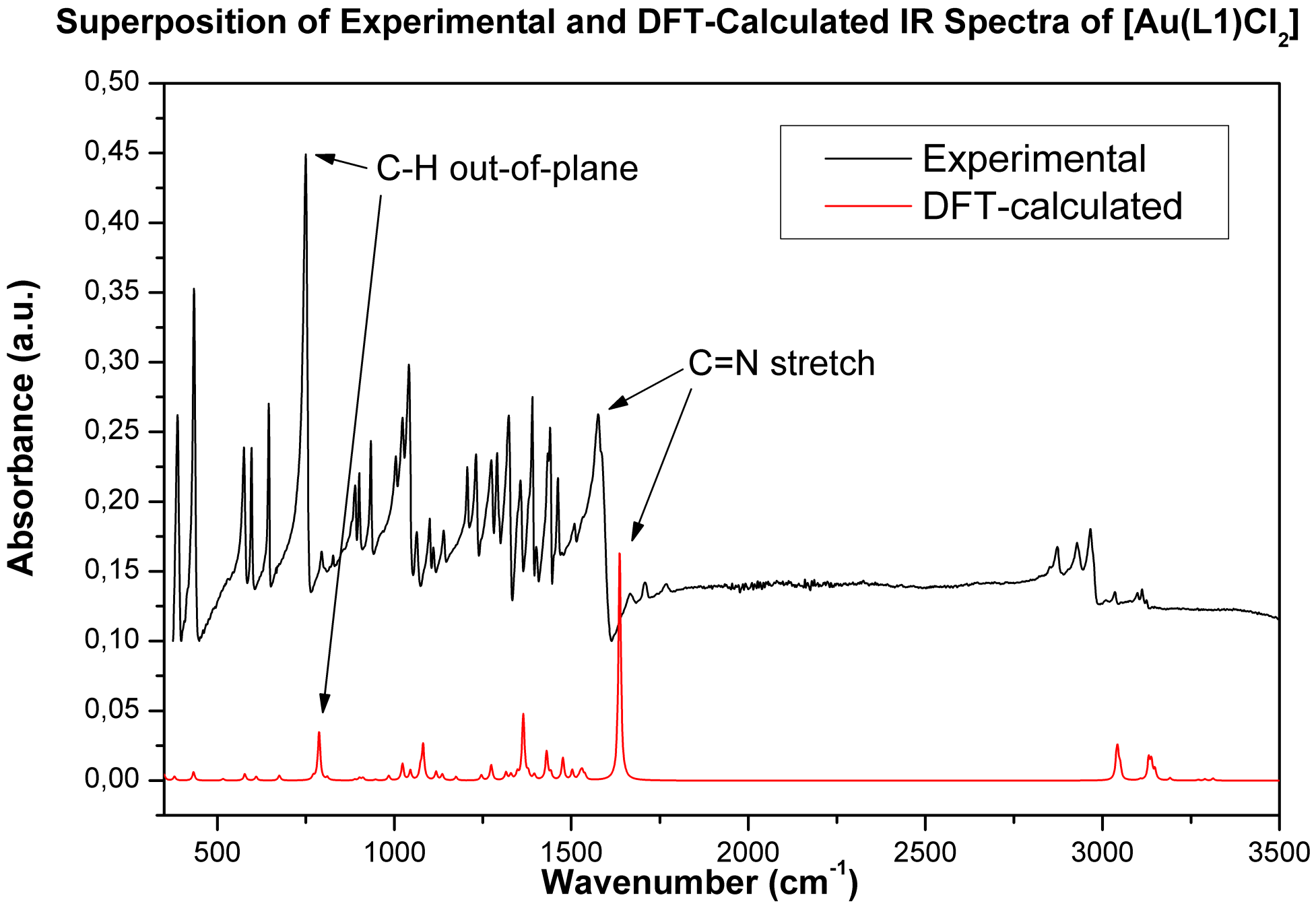
DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for $[Au(L5)Cl_2]$

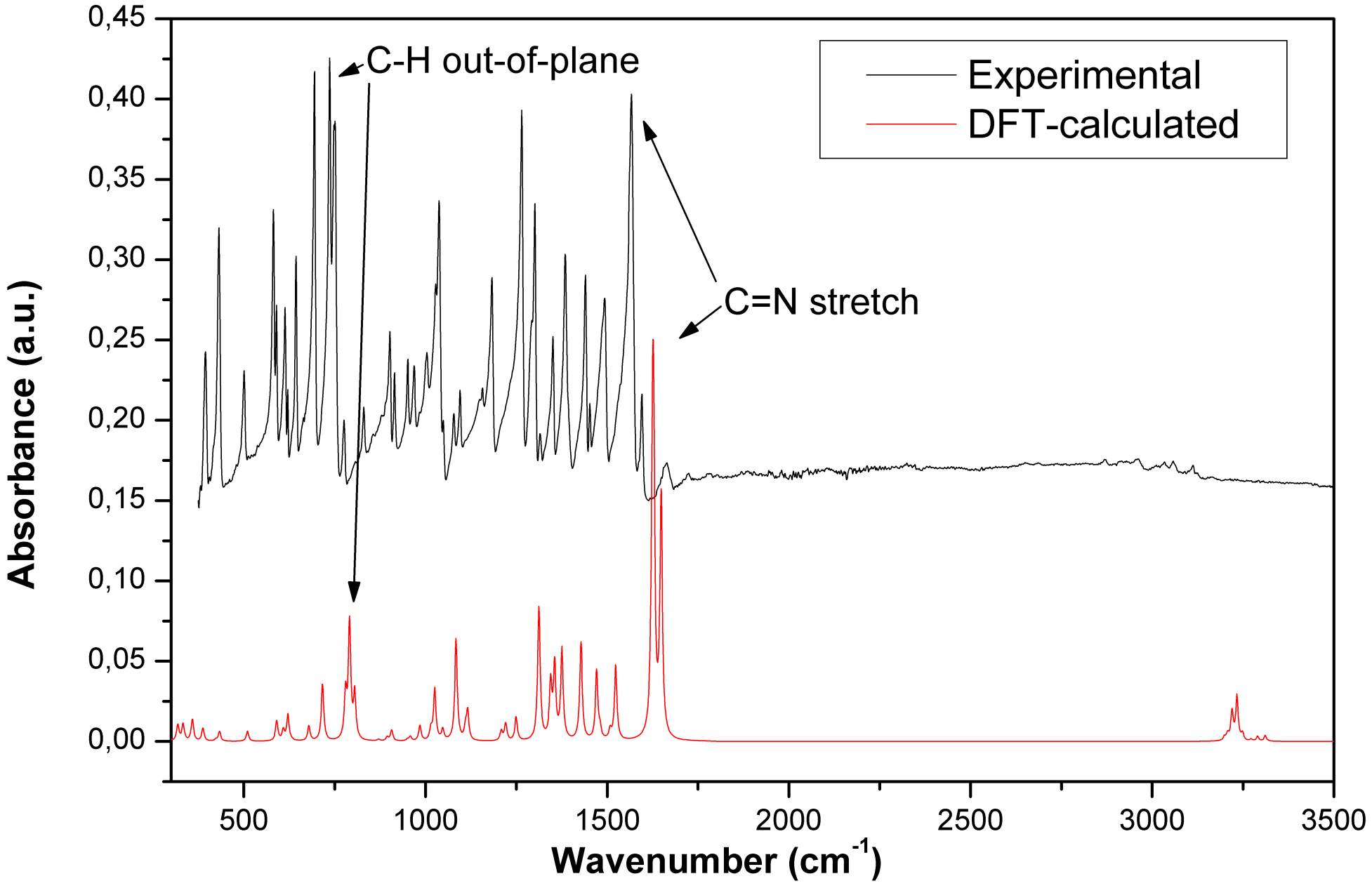


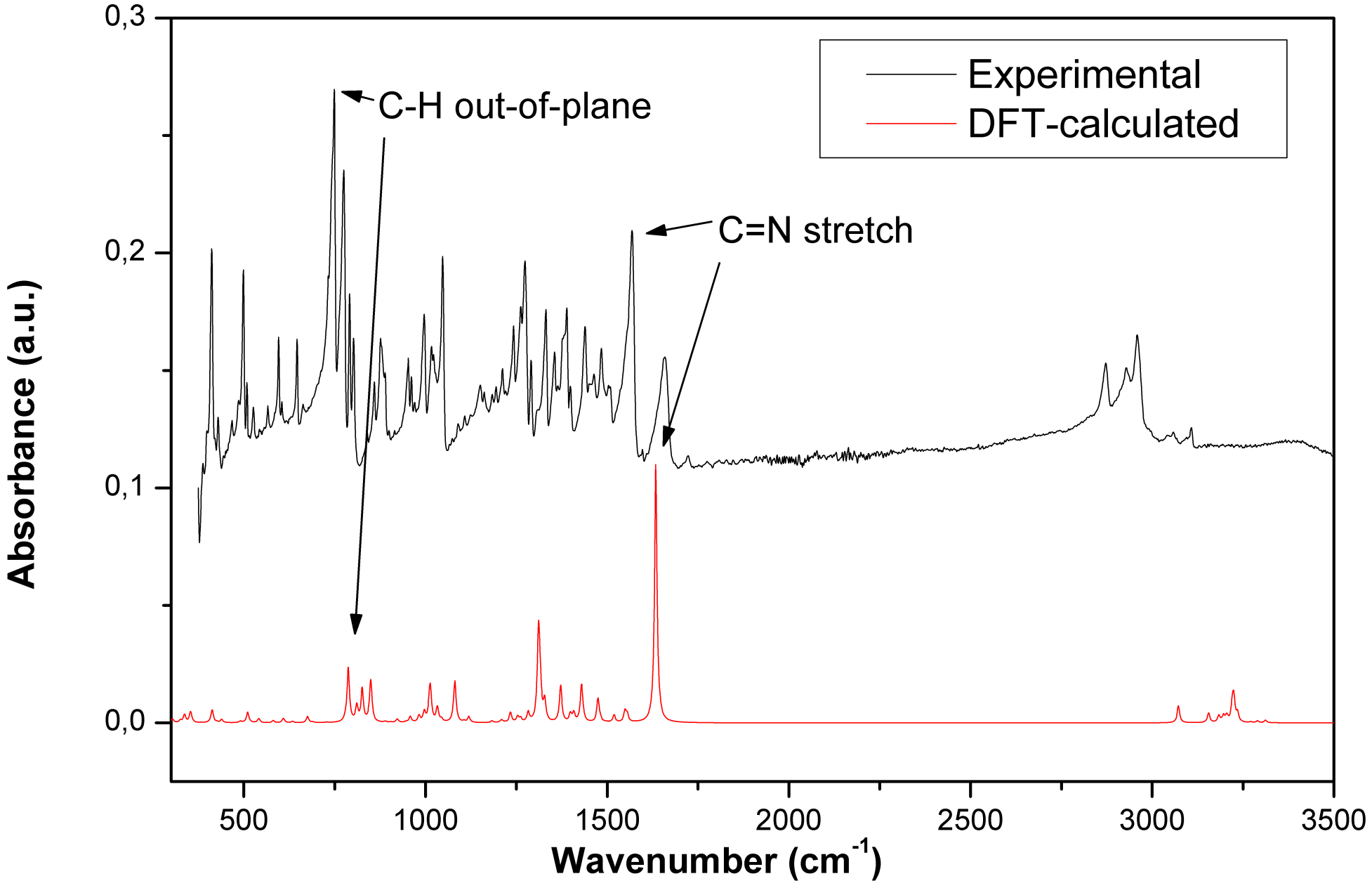

DFT-calculated versus Experimental Frequencies for [Au(L5)Cl2]
Calculated Frequencies (cm-1)
3000
2000
1000
y = 1,0859*x
Correlation Coefficient= 0,99867
1000
2000
3000
Experimental Frequencies (cm-1)

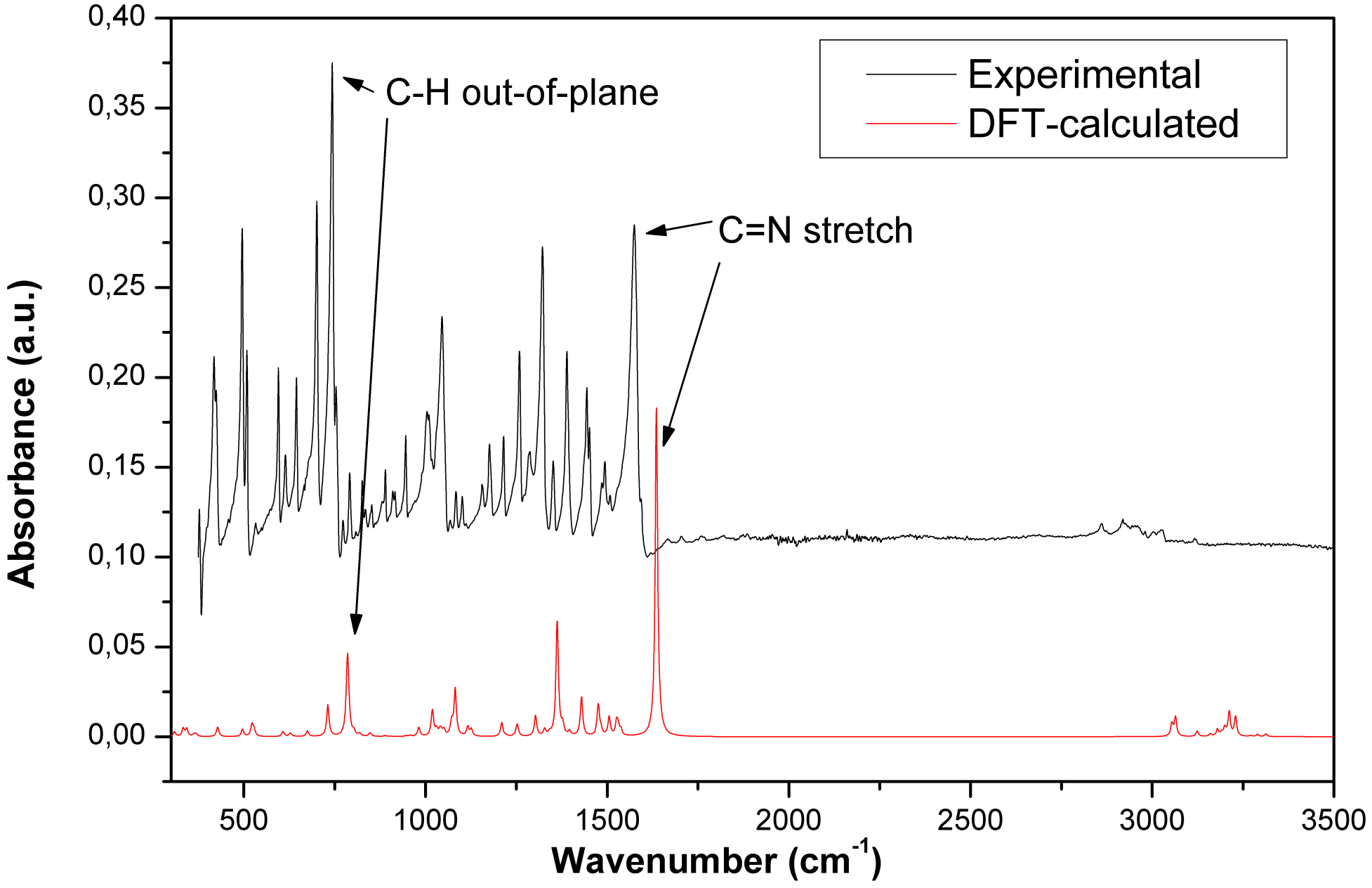
Superposition of Experimental and DFT-calculated UV/vis Spectra for $[Au(L5)Cl_2]$

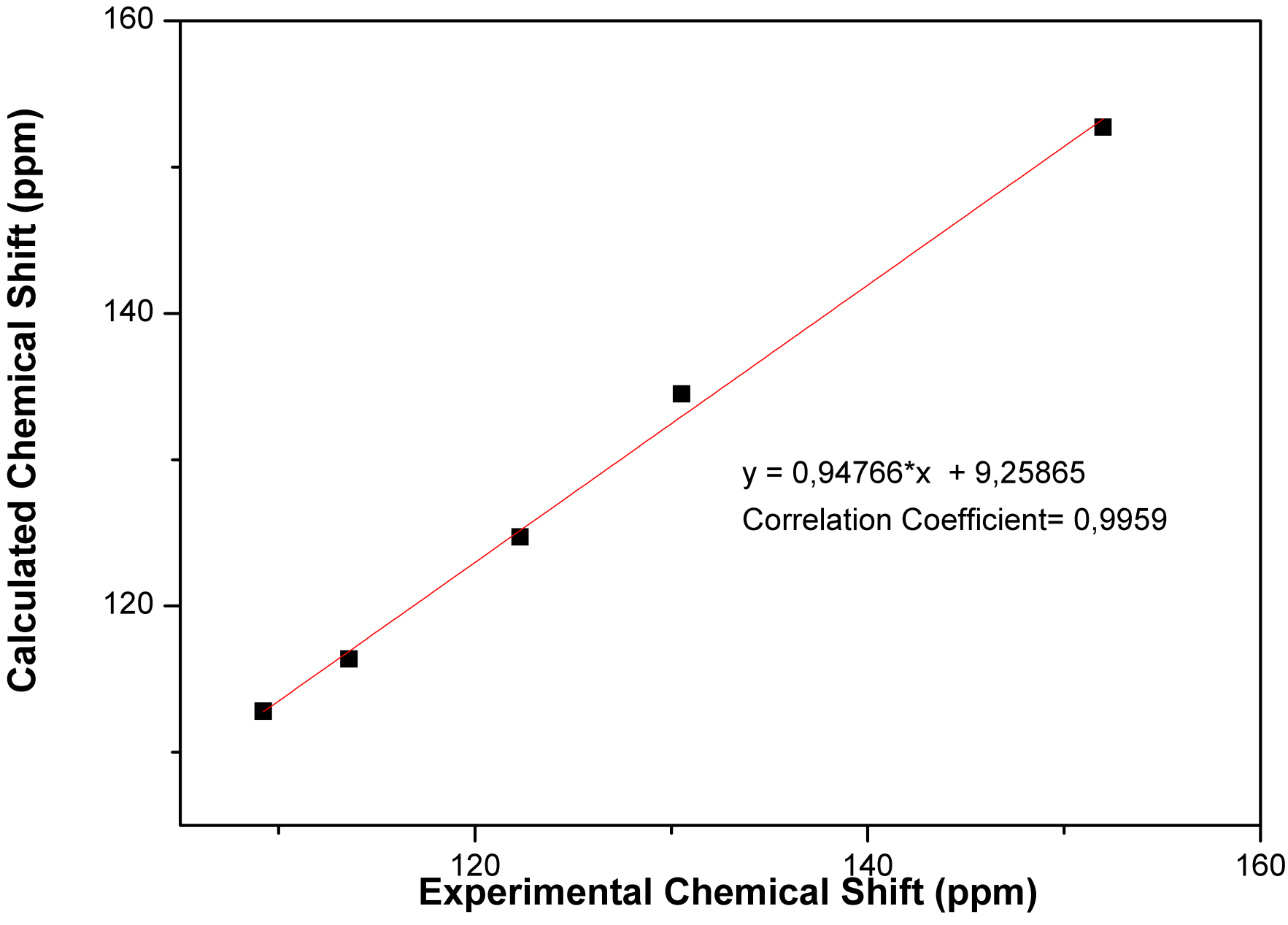


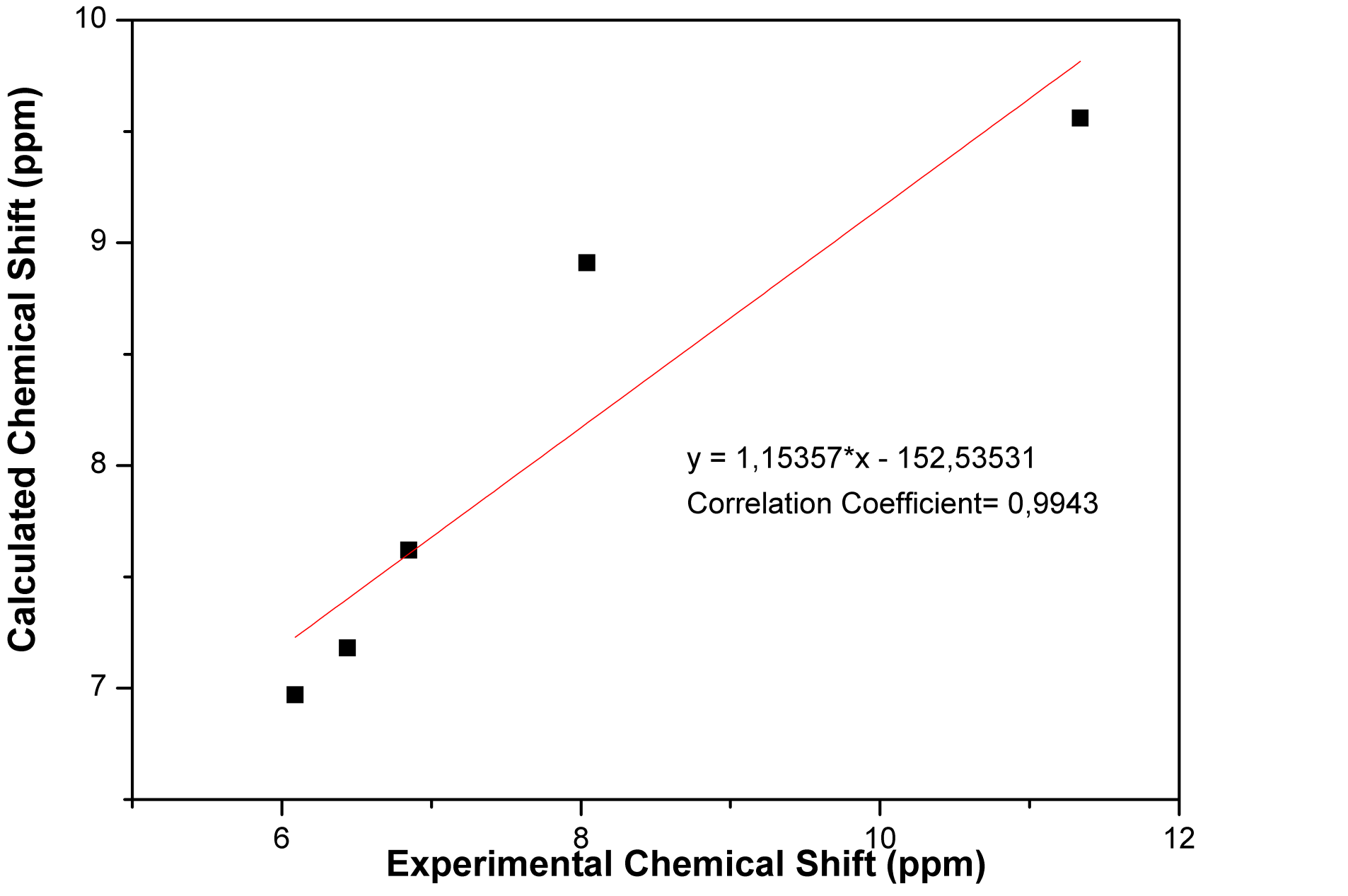

Superposition of Experimental and DFT-Calculated IR Spectra of [Au(L1)Cl2]
Absorbance (a.u.)
0,50
0,45
0,40
0,35
0,30
0,25
0,20
0,15
0,10
0,05
0,00
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)
C-H out-of-plane
C=N stretch
Experimental
DFT-calculated

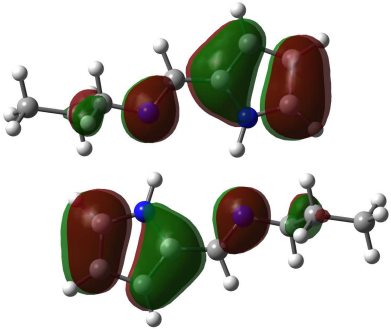

Superposition of Experimental and DFT-Calculated IR Spectra of [Au(L2)Cl2]
C-H out-of-plane
C=N stretch
Experimental
DFT-calculated
Absorbance (a.u.)
Wavenumber (cm-1)
0,45
0,40
0,35
0,30
0,25
0,20
0,15
0,10
0,05
0,00
500
1000
1500
2000
2500
3000
3500


Superposition of Experimental and DFT-Calculated IR Spectra of [Au(L4)Cl2]
Experimental
DFT-calculated
C-H out-of-plane
C=N stretch
Absorbance (a.u.)
0,3
0,2
0,1
0,0
500
1000
1500
2000
2500
3000
3500
Wavenumber (cm-1)

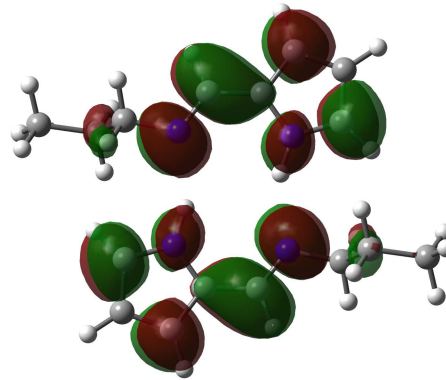

Superposition of Experimental and DFT-Calculated IR Spectra of [Au(L5)Cl2]
Experimental
DFT-calculated
C-H out-of-plane
C=N stretch
Absorbance (a.u.)
Wavenumber (cm-1)
0,40
0,35
0,30
0,25
0,20
0,15
0,10
0,05
0,00
500
1000
1500
2000
2500
3000
3500


DFT-Calculated versus Experimental 13C NMR Chemical Shifts for HL1
Calculated Chemical Shift (ppm)
160
140
120
120
140
160
Experimental Chemical Shift (ppm)
y = 0,94766*x + 9,25865
Correlation Coefficient= 0,9959

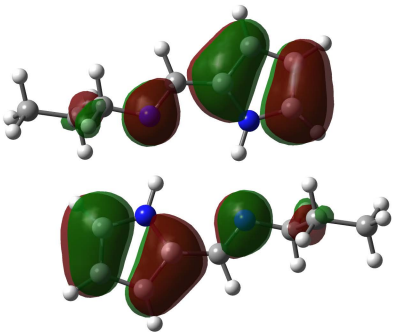

DFT-Calculated versus Experimental 1H NMR Chemical Shifts for HL1
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
10
9
8
7
6
8
10
12
y = 1,15357*x - 152,53531
Correlation Coefficient= 0,9943



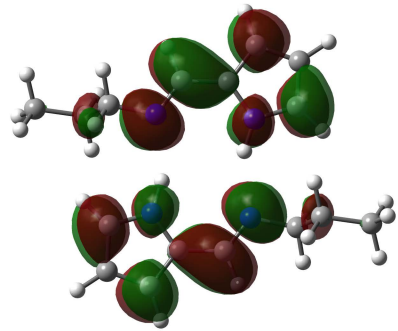
HOMO:Orbital 82



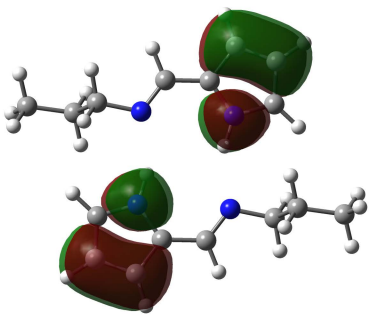
LUMO: Orbital 83



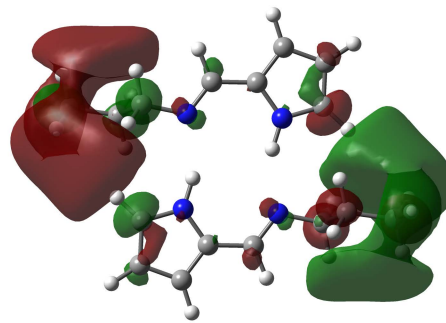
HOMO-1: Orbital 81



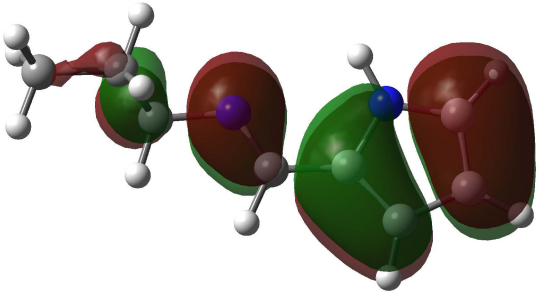
LUMO+1: Orbital 84



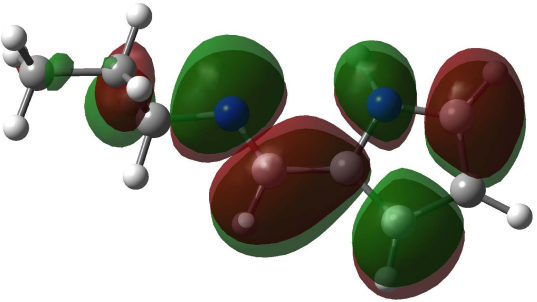
HOMO-2: Orbital 80



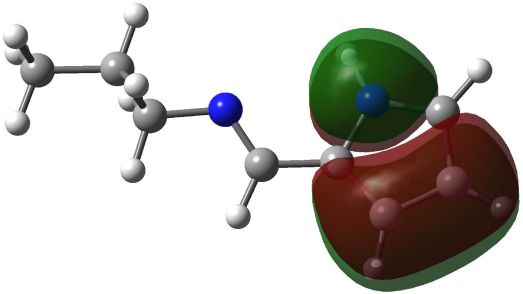
LUMO+2: Orbital 85



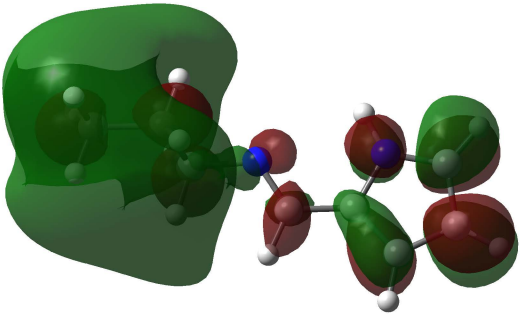
HOMO:Orbital 37



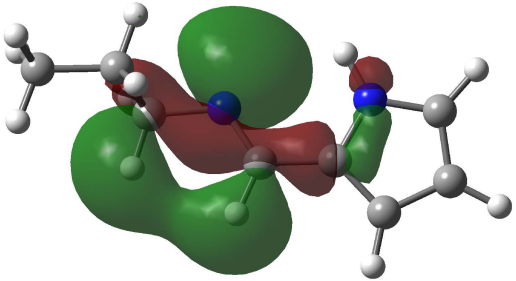
LUMO: Orbital 38



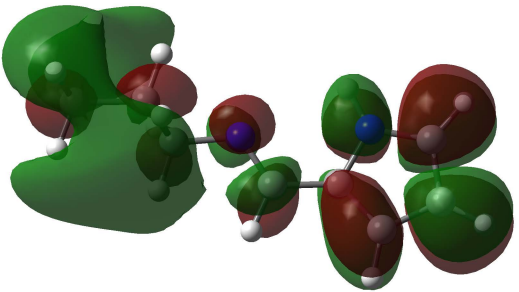
HOMO-1: Orbital 36



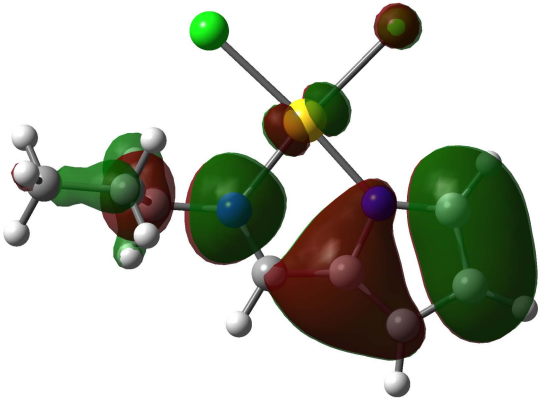
LUMO+1: Orbital 39



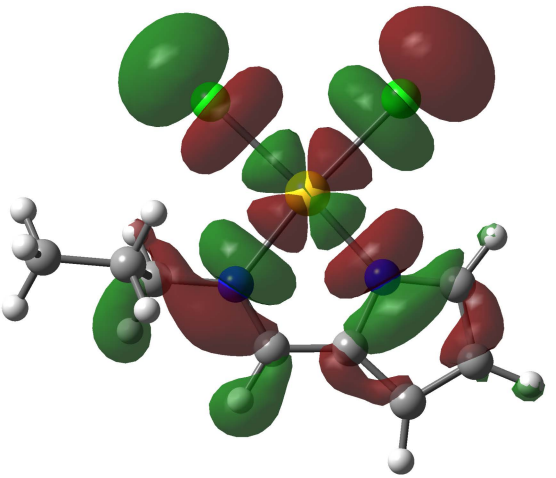
HOMO: Orbital 35



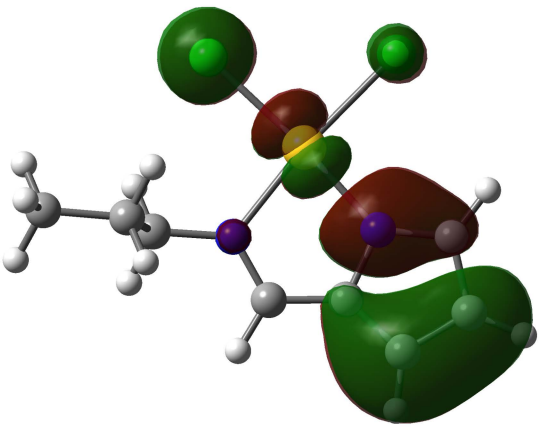
LUMO+2: Orbital 40



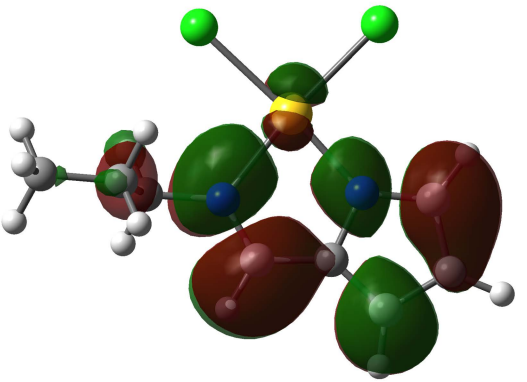
HOMO: Orbital 53



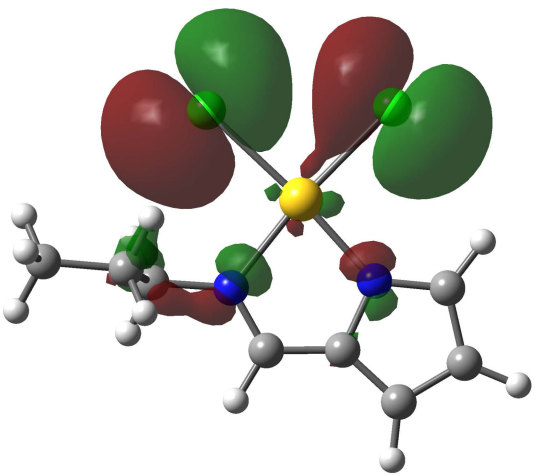
LUMO: Orbital 54



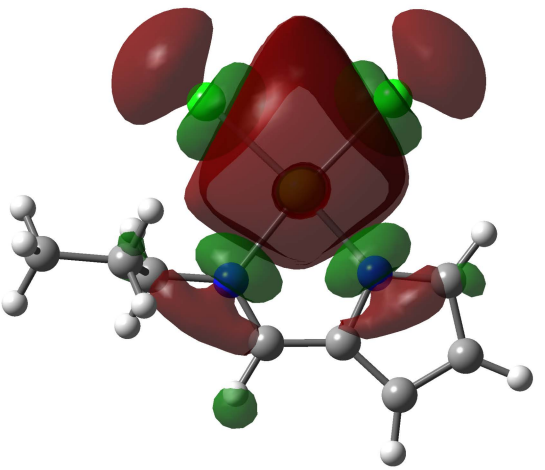
HOMO-1: Orbital 52



LUMO+1: Orbital 55

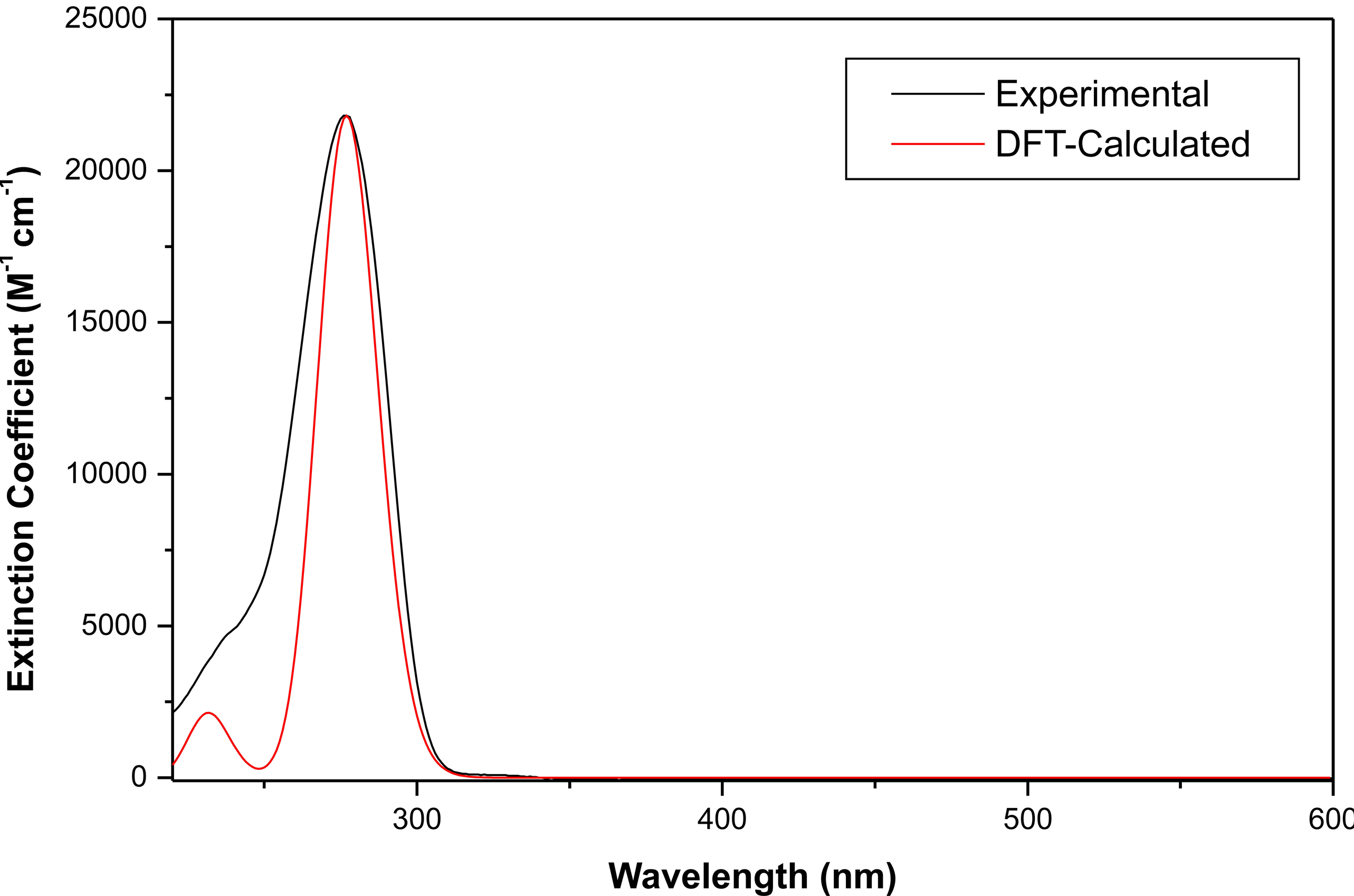


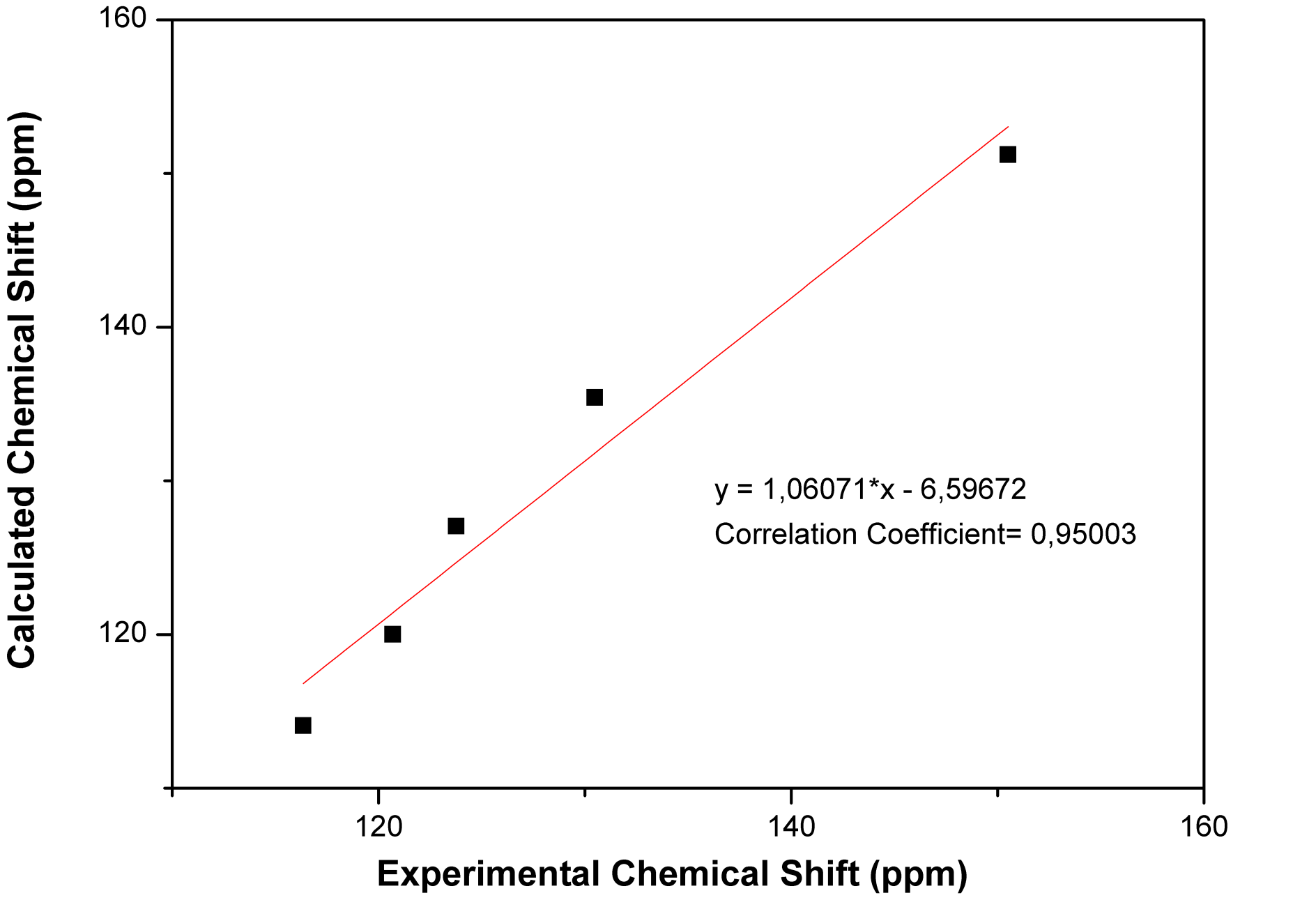
HOMO-2: Orbital 51

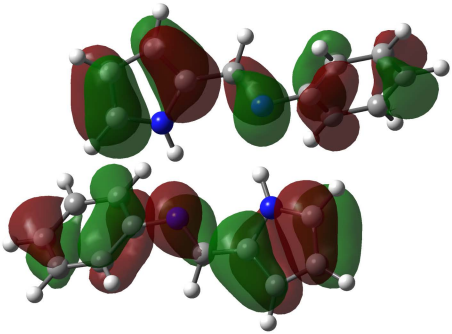


LUMO+1: Orbital 56

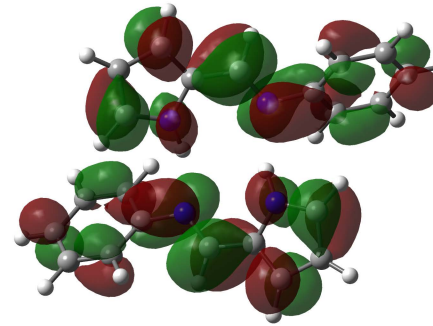
Superposition of Experimental and DFT-Calculated UV-vis Spectra for HL1



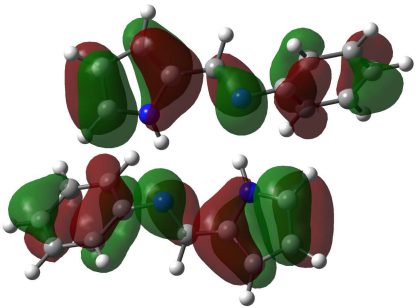

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for HL2
Calculated Chemical Shift (ppm)
160
140
120
120
140
160
Experimental Chemical Shift (ppm)
y = 1,06071*x - 6,59672
Correlation Coefficient= 0,95003



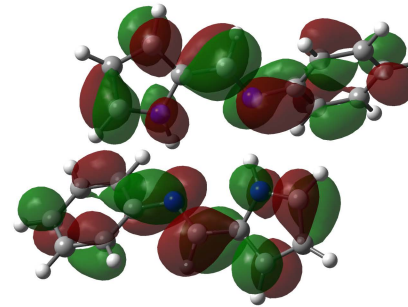
HOMO:Orbital 90



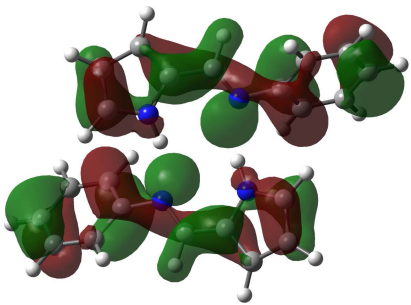
LUMO: Orbital 91



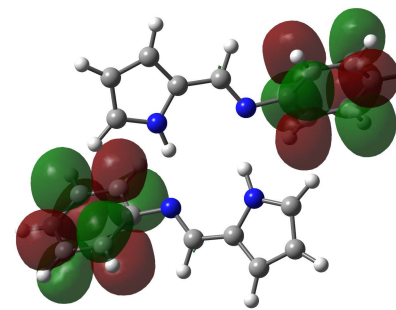
HOMO-1: Orbital 89



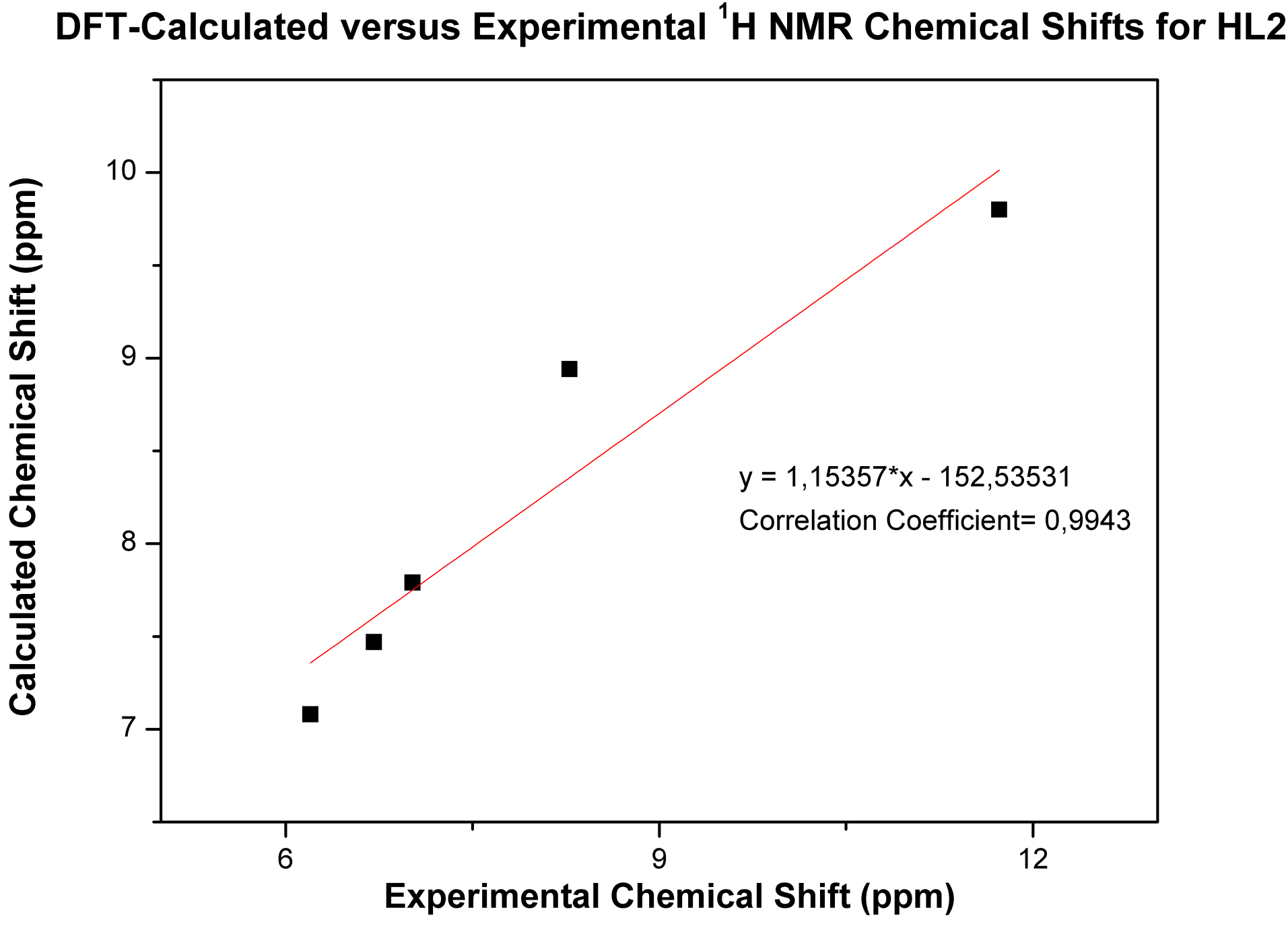
LUMO+1: Orbital 92

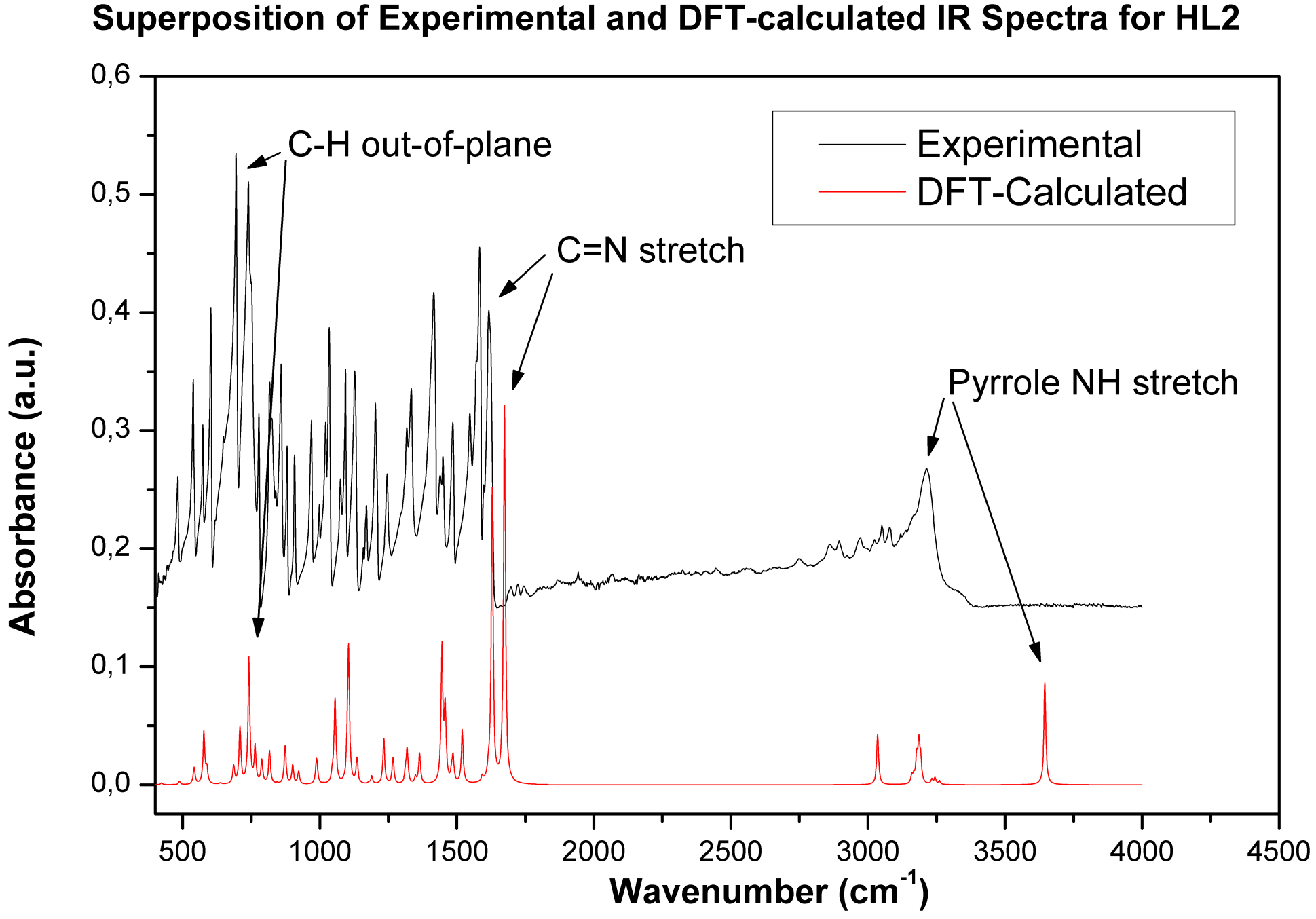


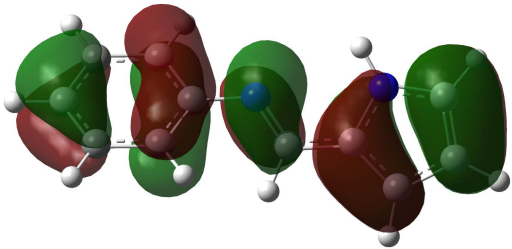
HOMO-2: Orbital 88



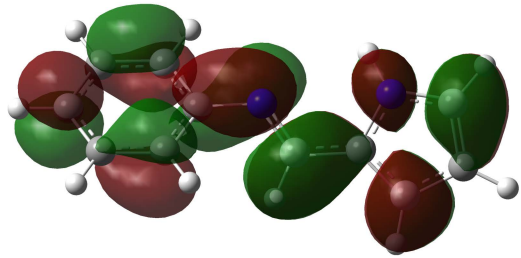
LUMO+2: Orbital 93


DFT-Calculated versus Experimental 1H NMR Chemical Shifts for HL2
Calculated Chemical Shift (ppm)
10
9
8
7
6
9
12
Experimental Chemical Shift (ppm)
y = 1,15357*x - 152,53531
Correlation Coefficient= 0,9943

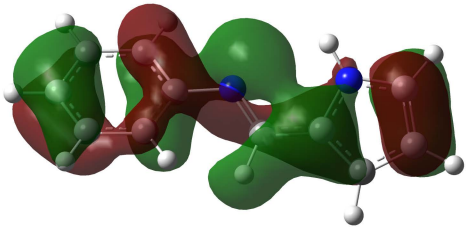

Superposition of Experimental and DFT-calculated IR Spectra for HL2
C-H out-of-plane
C=N stretch
Pyrrole NH stretch
Experimental
DFT-Calculated
Absorbance (a.u.)
Wavenumber (cm-1)
0,0
0,1
0,2
0,3
0,4
0,5
0,6
500
1000
1500
2000
2500
3000
3500
4000
4500



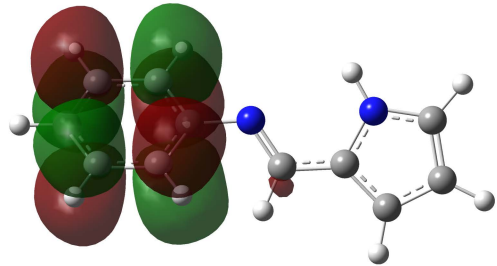
HOMO:Orbital 45



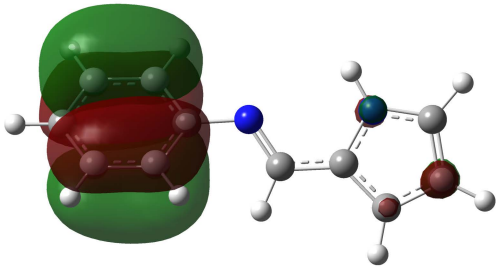
LUMO: Orbital 46



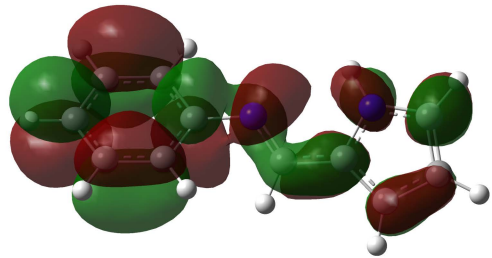
HOMO-1: Orbital 44



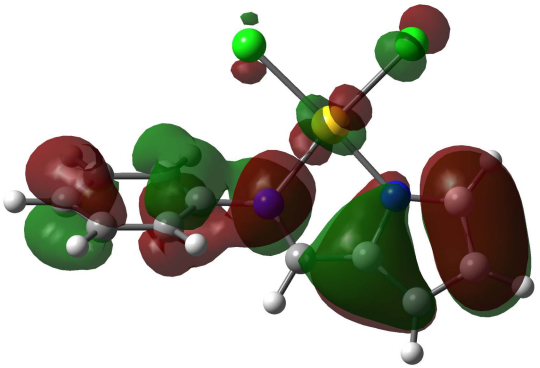
LUMO+1: Orbital 47



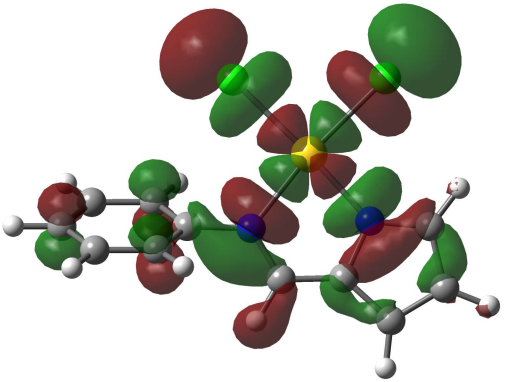
HOMO-2: Orbital 43



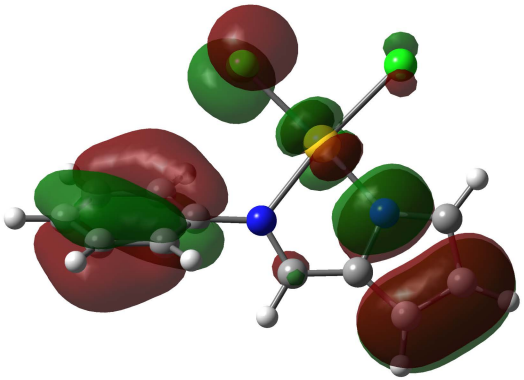
LUMO+2: Orbital 48



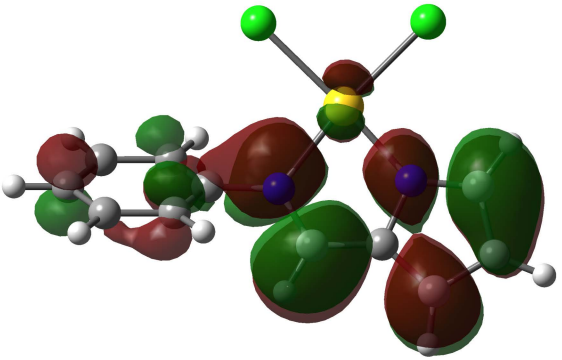
HOMO: Orbital 61



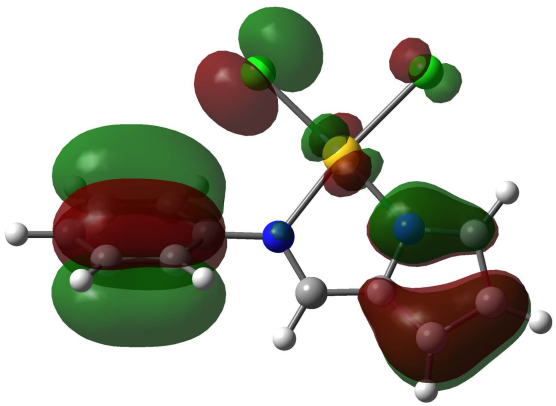
LUMO: Orbital 62



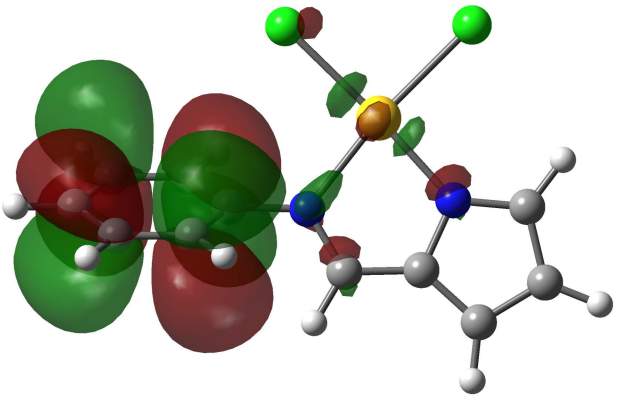
HOMO-1: Orbital 60



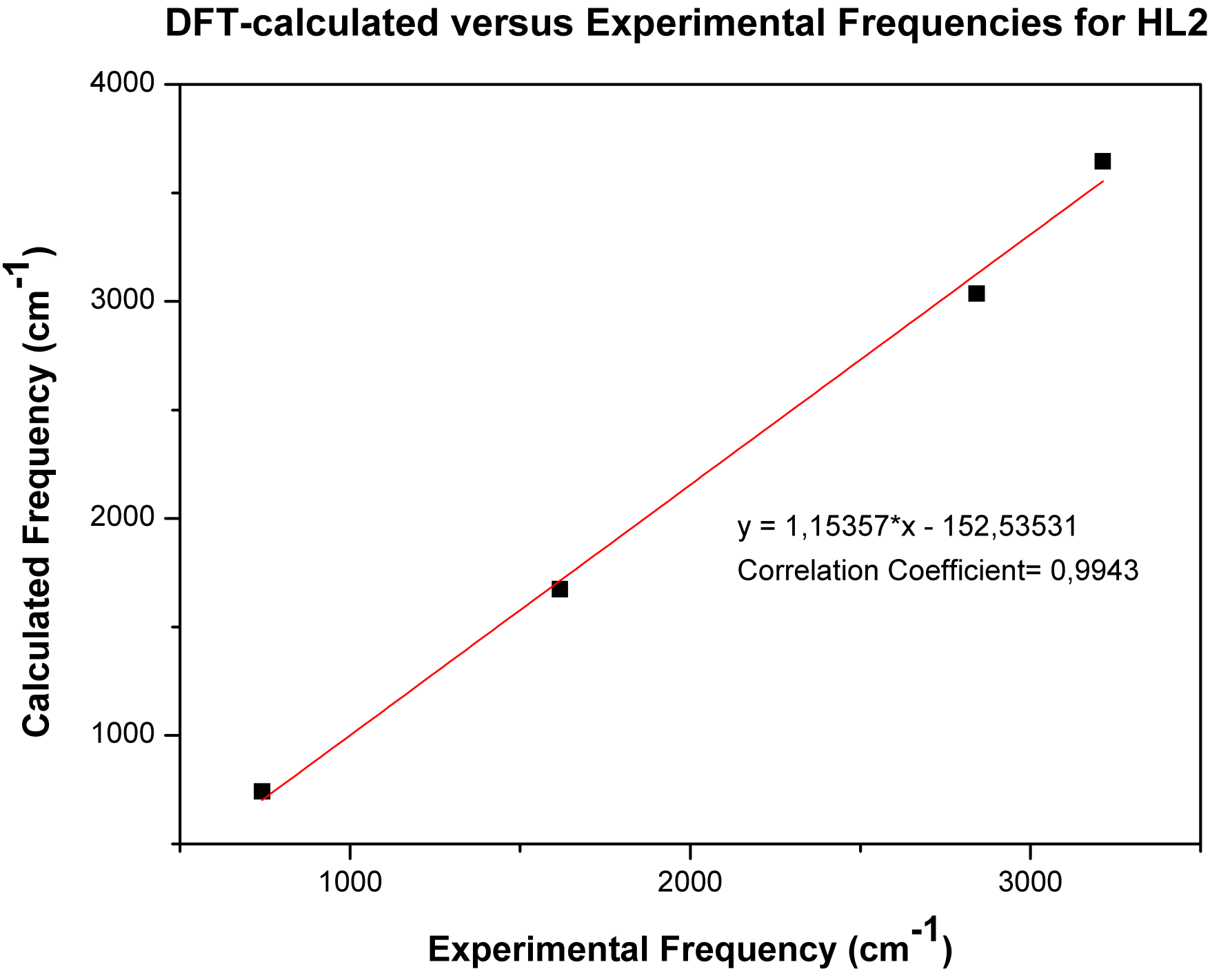
LUMO+1: Orbital 63



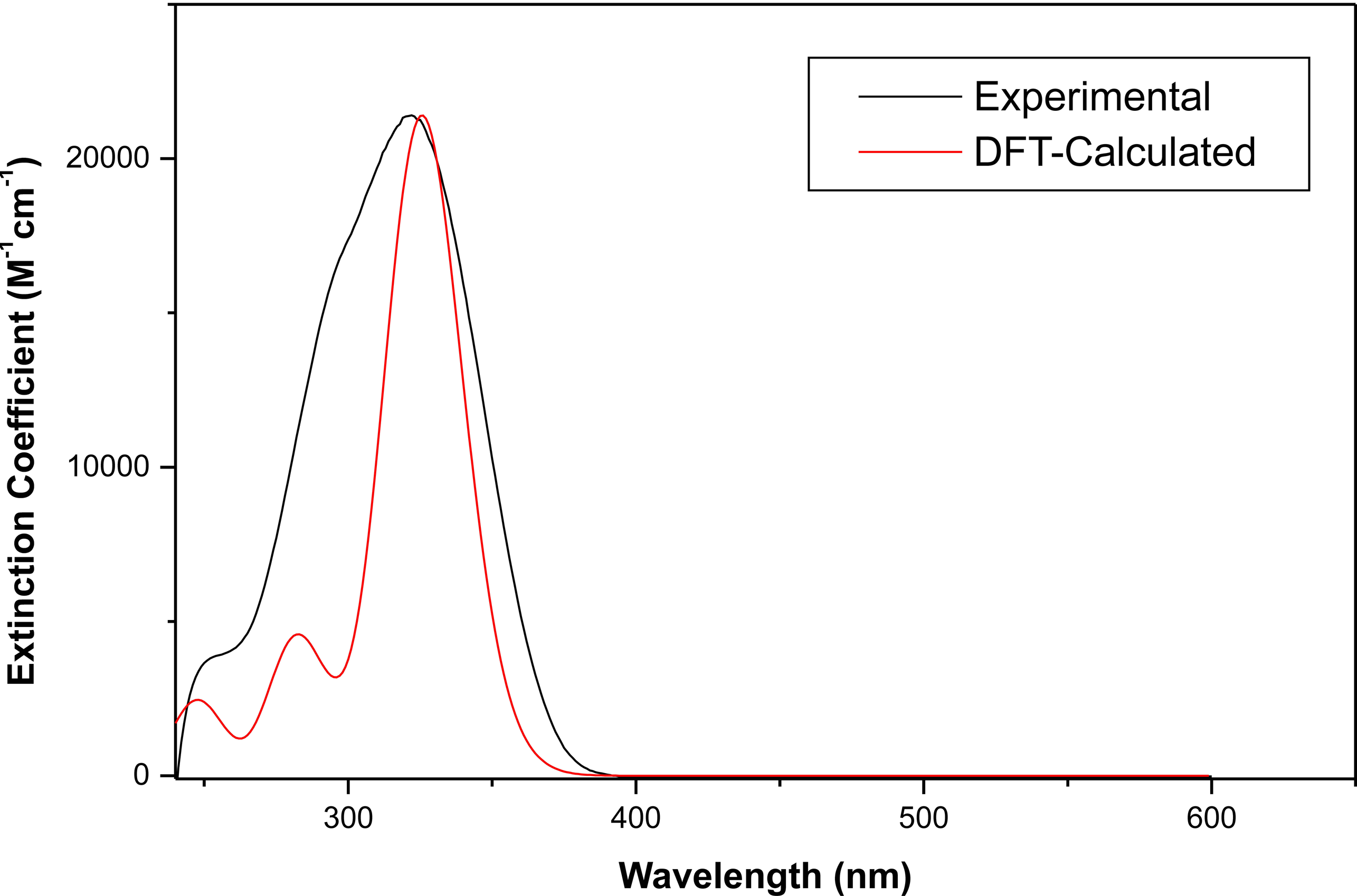
HOMO-2: Orbital 59

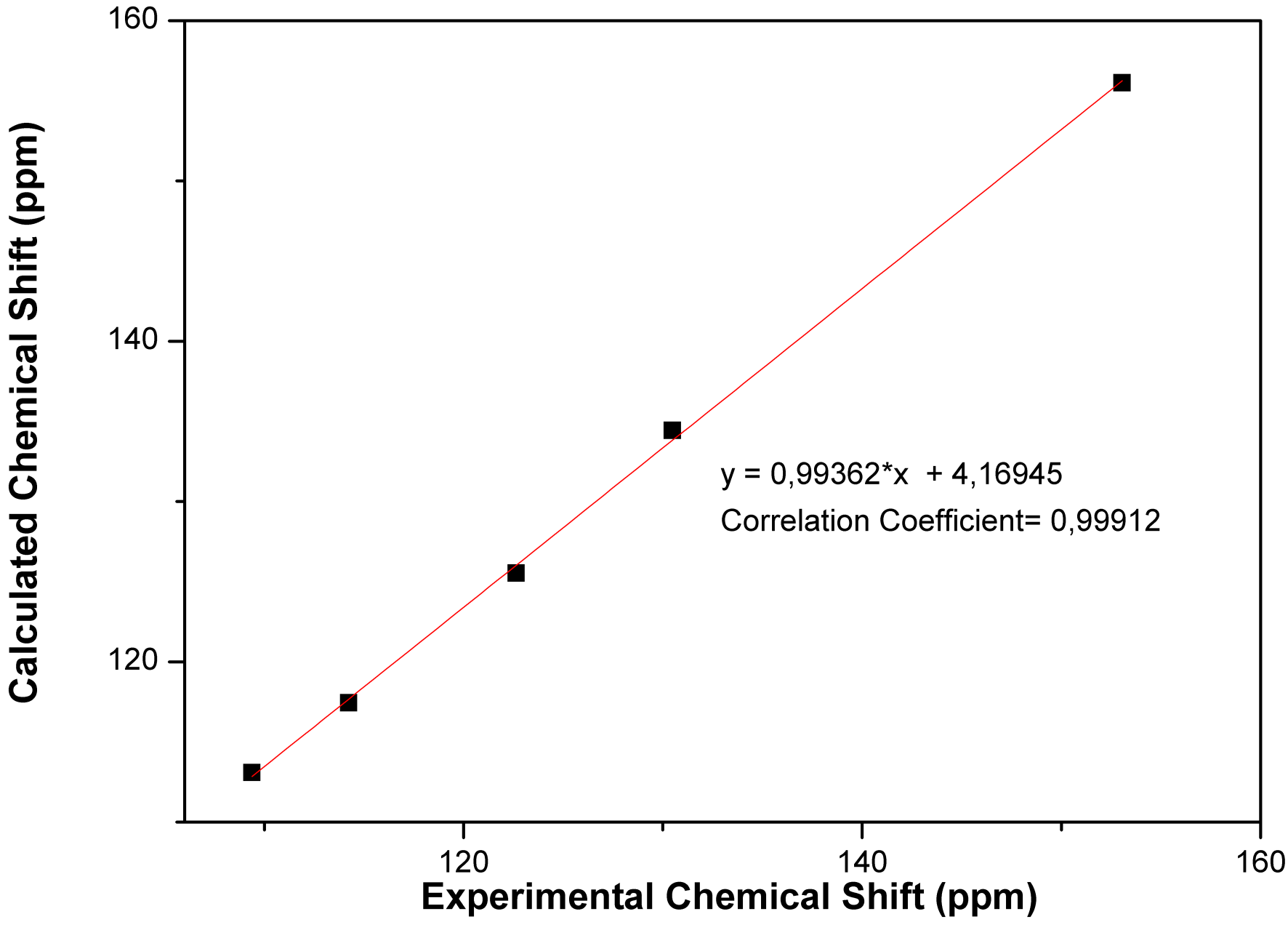


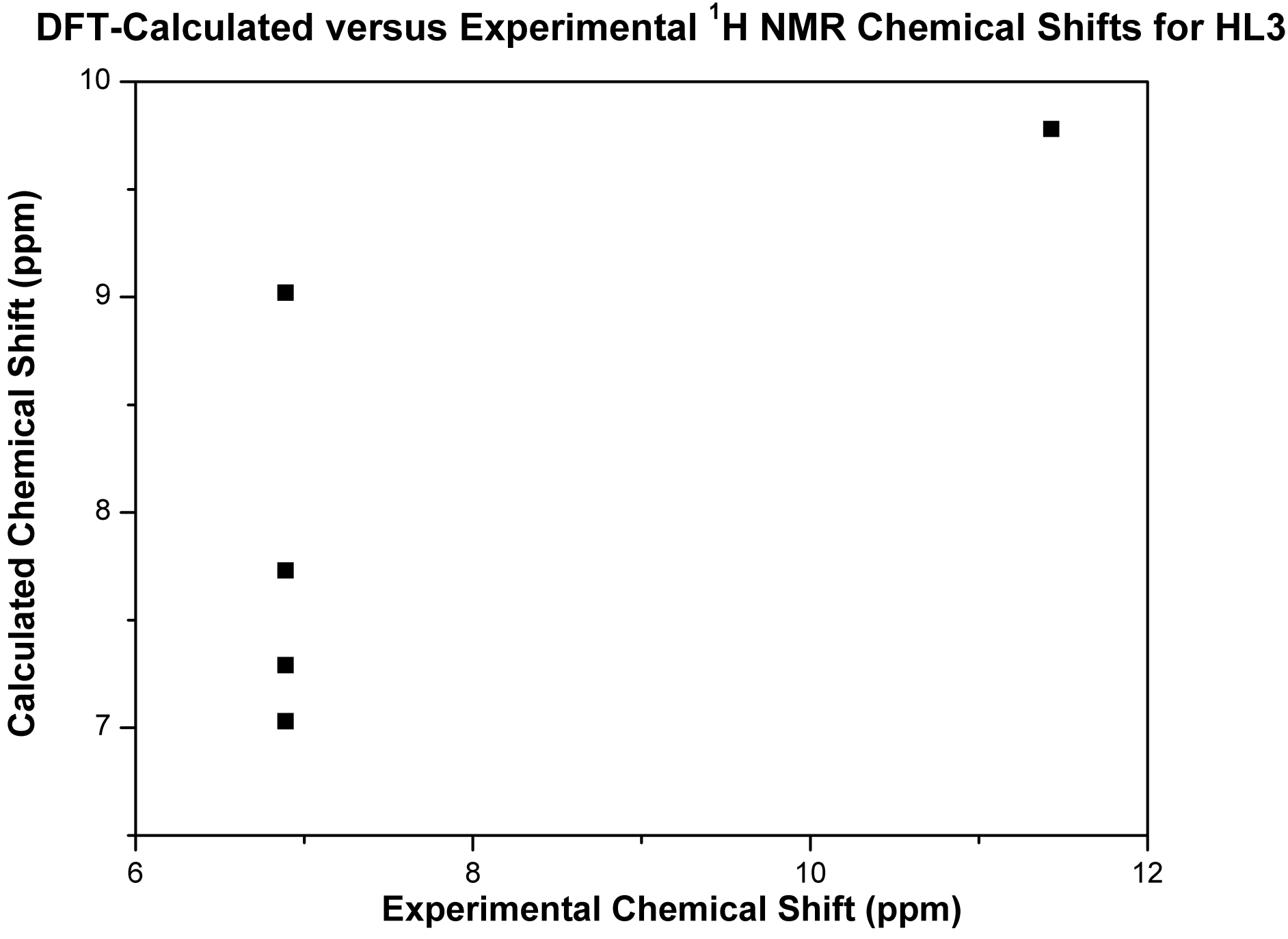
LUMO+2: Orbital 64

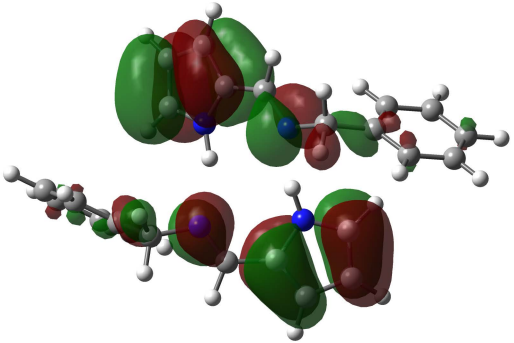

DFT-calculated versus Experimental Frequencies for HL2
Calculated Frequency (cm-1)
Experimental Frequency (cm-1)
4000
3000
2000
1000
1000
2000
3000
y = 1,15357*x - 152,53531
Correlation Coefficient= 0,9943

Superposition of Experimental and DFT-Calculated UV-vis Spectra for HL2

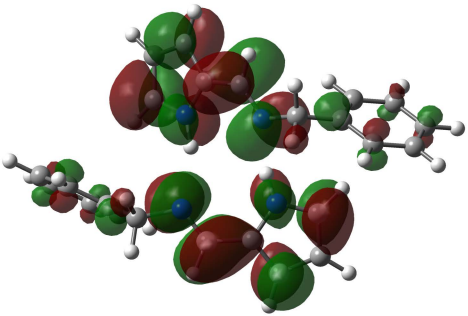



DFT-Calculated versus Experimental 13C NMR Chemical Shifts for HL3
Calculated Chemical Shift (ppm)
160
140
120
120
140
160
Experimental Chemical Shift (ppm)
y = 0,99362*x + 4,16945
Correlation Coefficient= 0,99912

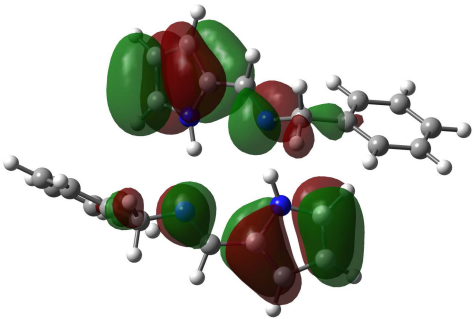

DFT-Calculated versus Experimental ^{1}H NMR Chemical Shifts for HL3
Calculated Chemical Shift (ppm)
10
9
8
7
6
8
10
12
Experimental Chemical Shift (ppm)



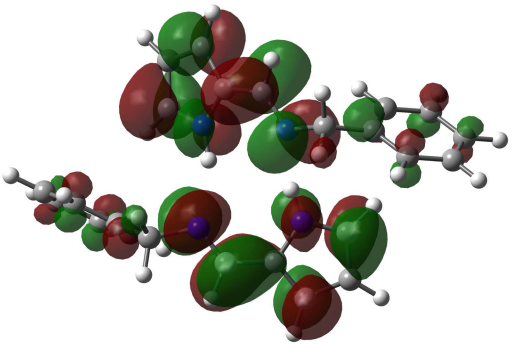
HOMO:Orbital 98



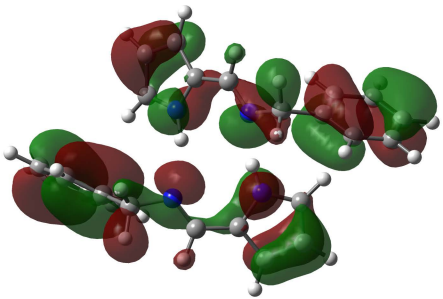
LUMO: Orbital 99



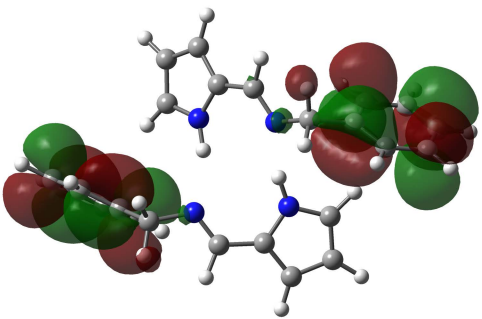
HOMO-1: Orbital 97



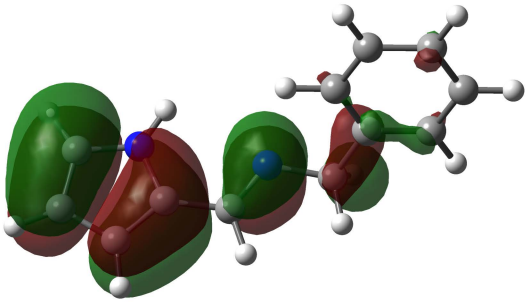
LUMO+1: Orbital 100



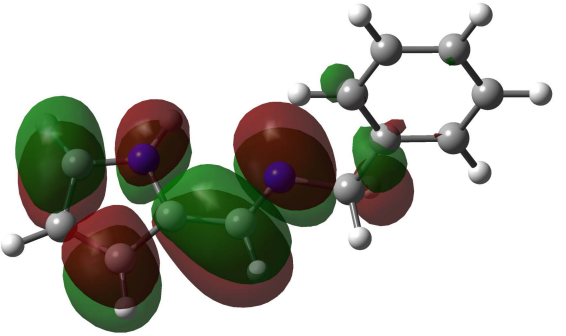
HOMO-2: Orbital 96



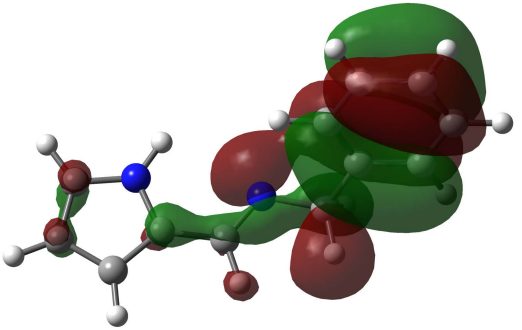
LUMO+2: Orbital 101



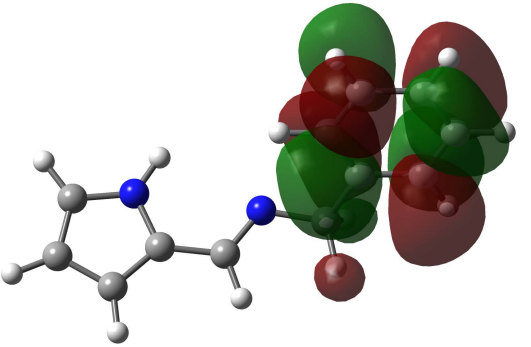
HOMO:Orbital 49



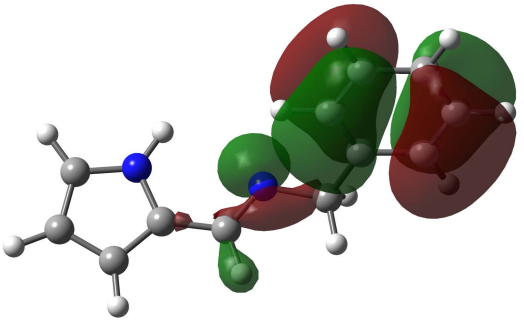
LUMO: Orbital 50



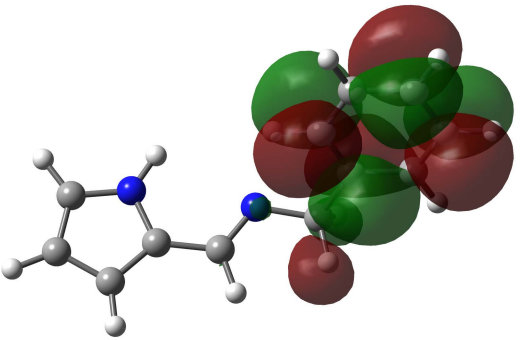
HOMO-1: Orbital 48



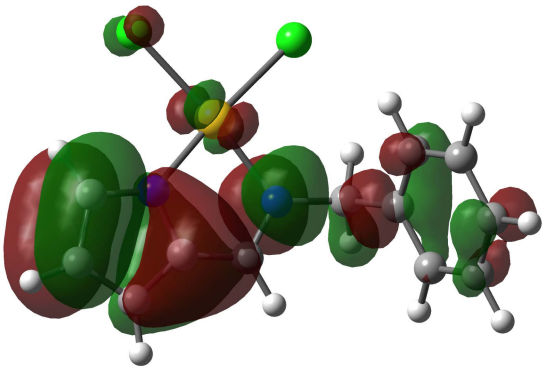
LUMO+1: Orbital 51



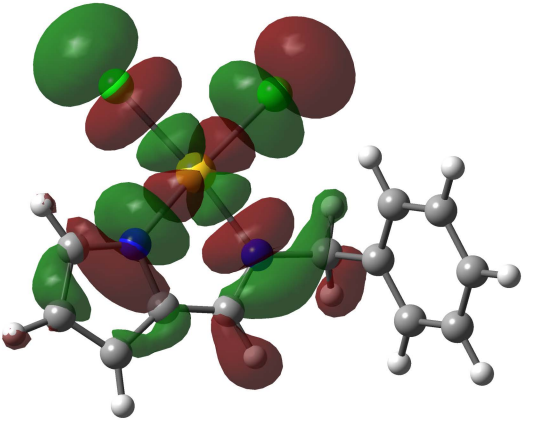
HOMO-2: Orbital 47



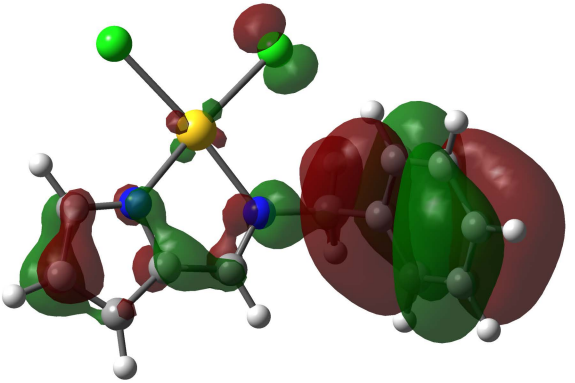
LUMO+2: Orbital 52



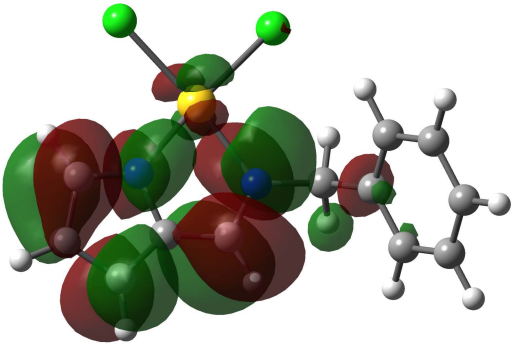
HOMO: Orbital 65



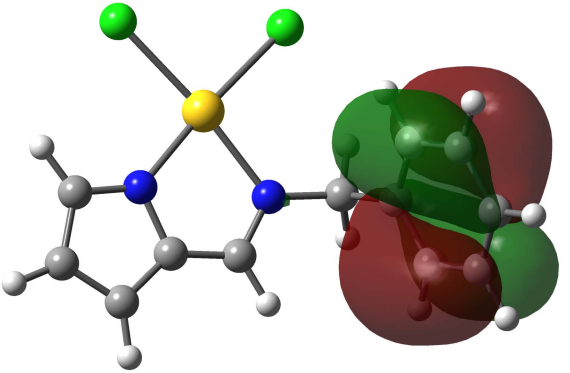
LUMO: Orbital 66



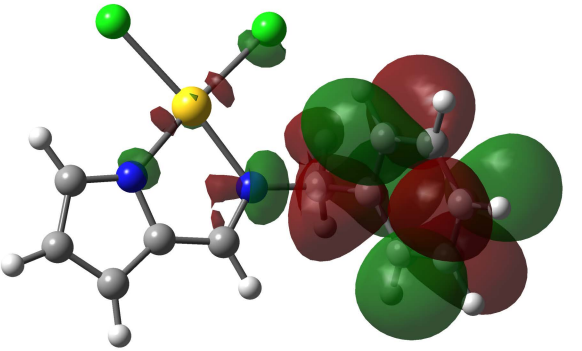
HOMO-1: Orbital 64



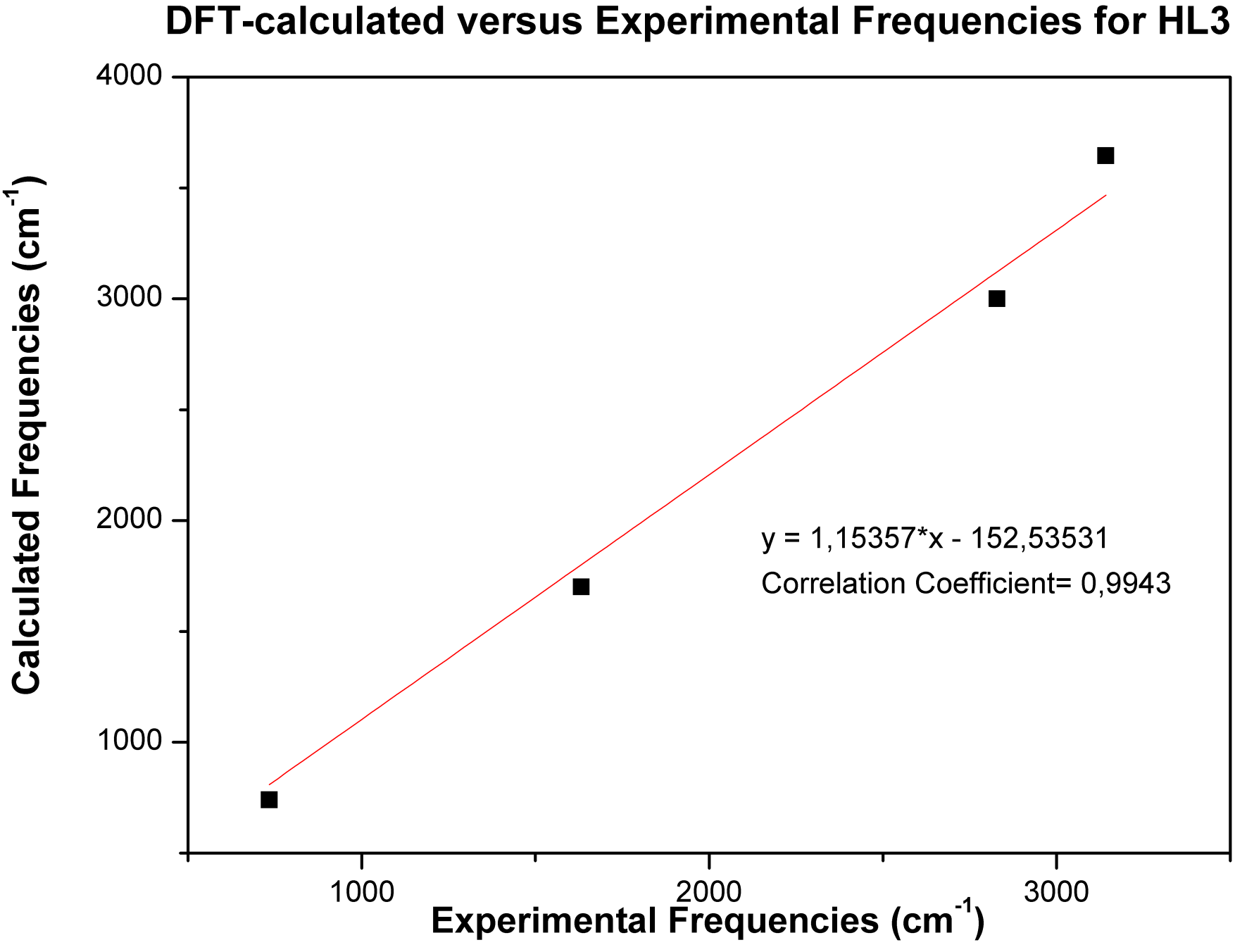
LUMO+1: Orbital 67



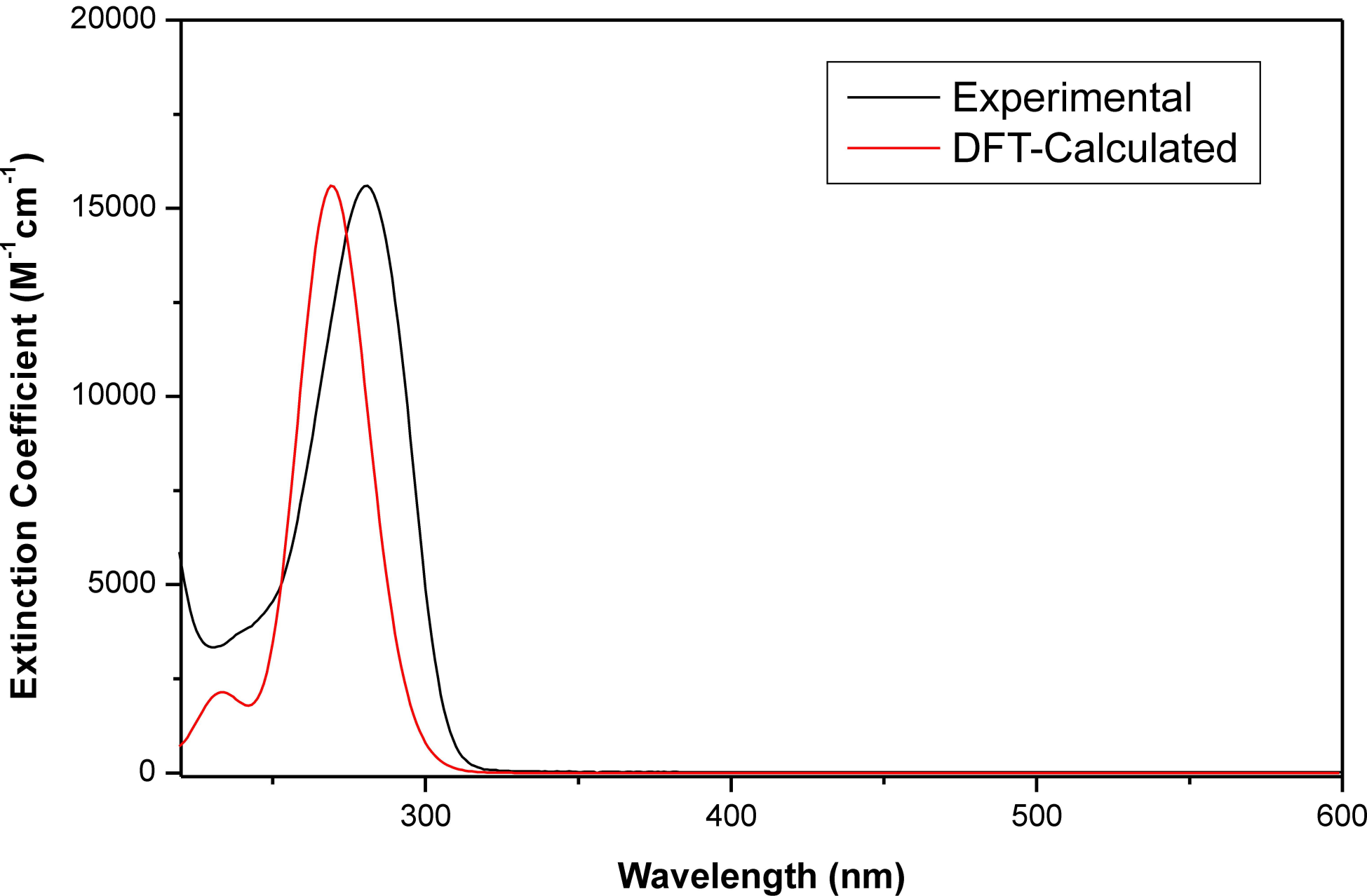
HOMO-2: Orbital 63

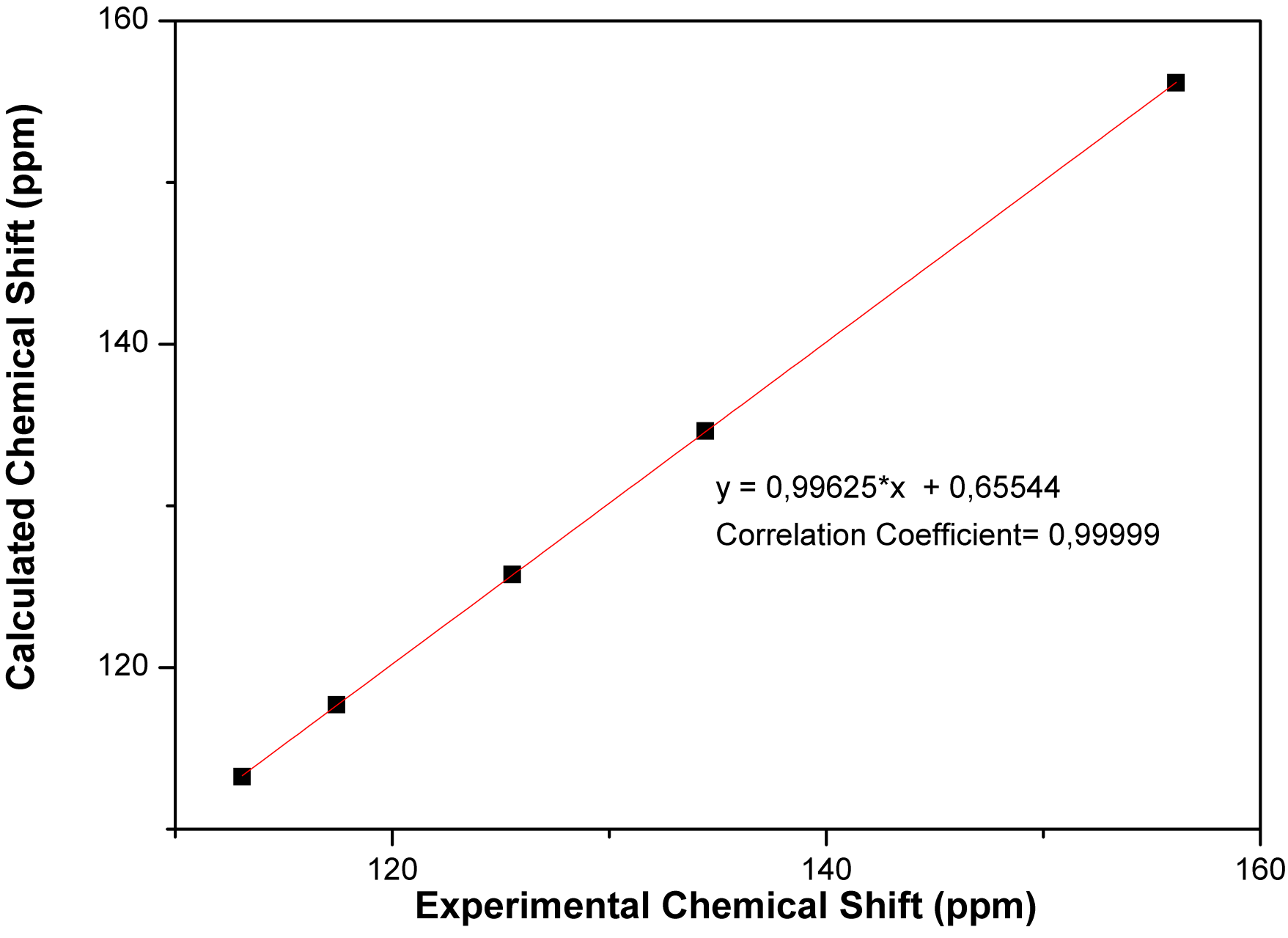


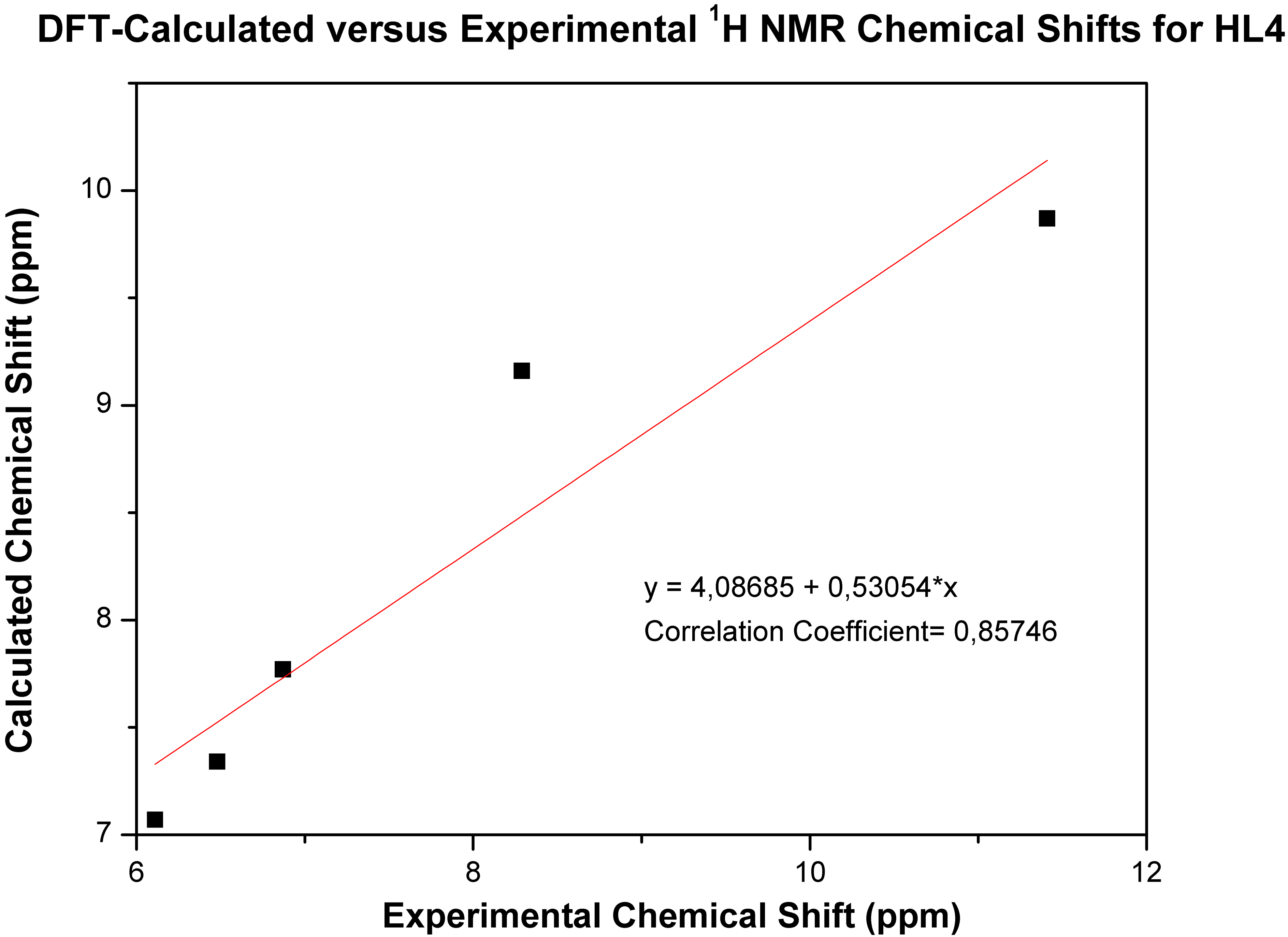
LUMO+2: Orbital 68


DFT-calculated versus Experimental Frequencies for HL3
Calculated Frequencies (cm-1)
Experimental Frequencies (cm-1)
4000
3000
2000
1000
1000
2000
3000
y = 1,15357*x - 152,53531
Correlation Coefficient= 0,9943

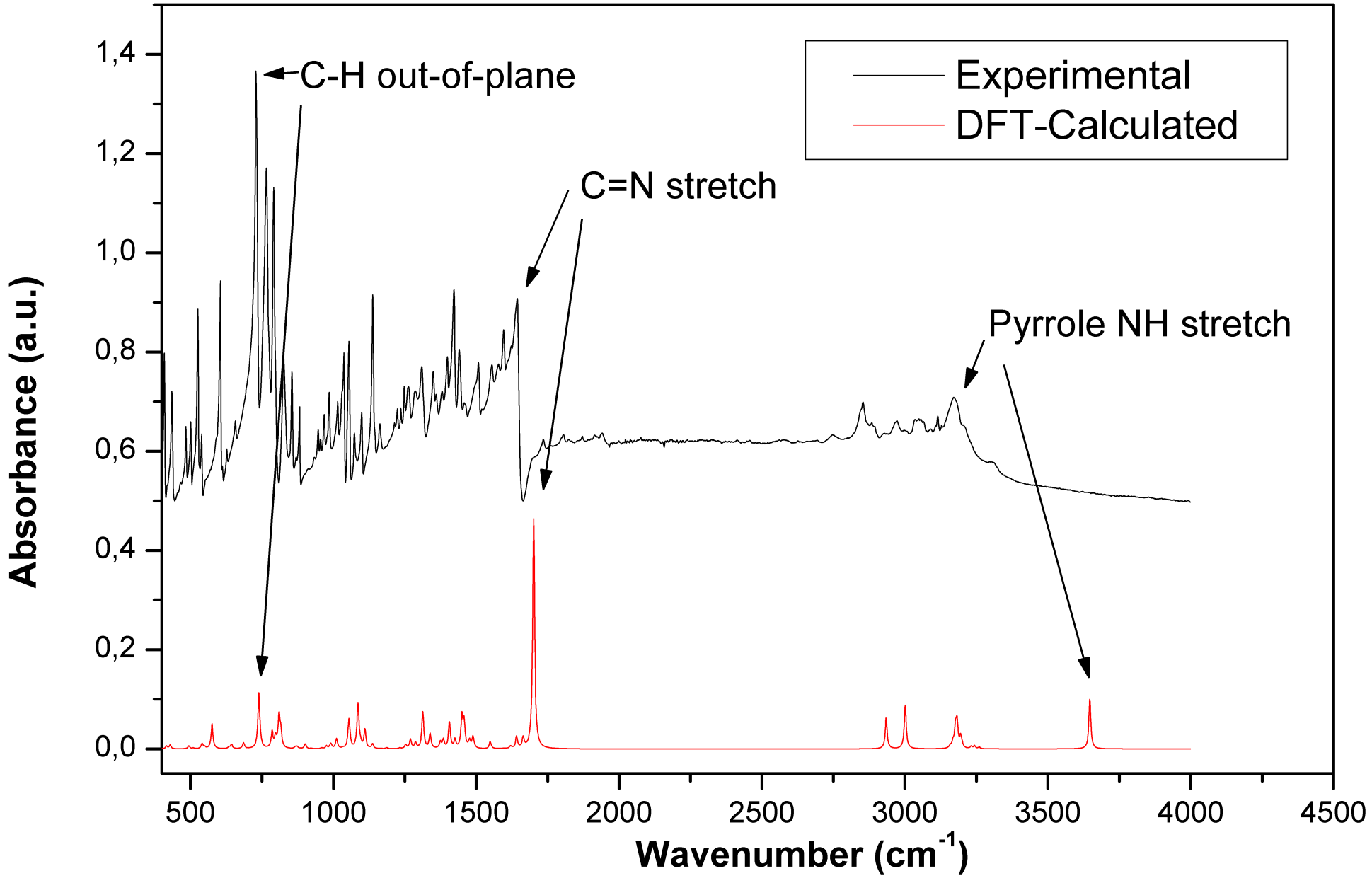
Superposition of Experimental and DFT-Calculated UV-vis Spectra for HL3

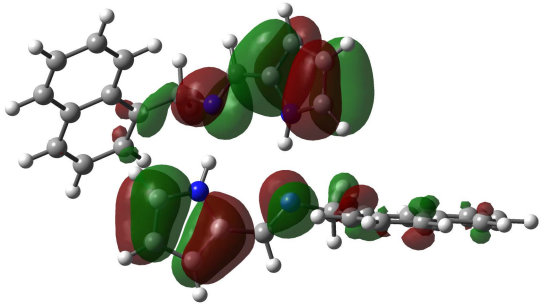



DFT-Calculated versus Experimental 13C NMR Chemical Shifts for HL4
Calculated Chemical Shift (ppm)
160
140
120
120
140
160
Experimental Chemical Shift (ppm)
y = 0,99625*x + 0,65544
Correlation Coefficient= 0,99999

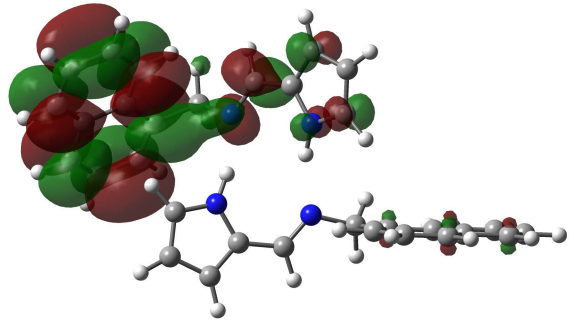


DFT-Calculated versus Experimental 1H NMR Chemical Shifts for HL4
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
10
9
8
7
6
8
10
12
y = 4,08685 + 0,53054*x
Correlation Coefficient= 0,85746

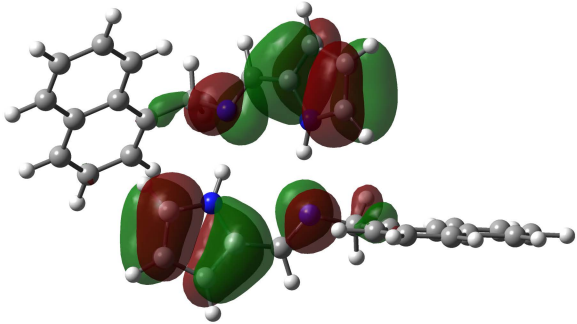

Superposition of Experimental and DFT-calculated IR Spectra for HL4
C-H out-of-plane
C=N stretch
Pyrrole NH stretch
Experimental
DFT-Calculated
Absorbance (a.u.)
Wavenumber (cm-1)
0,0
0,2
0,4
0,6
0,8
1,0
1,2
1,4
500
1000
1500
2000
2500
3000
3500
4000
4500



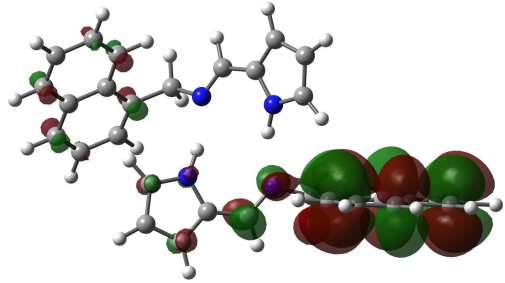
HOMO:Orbital 124



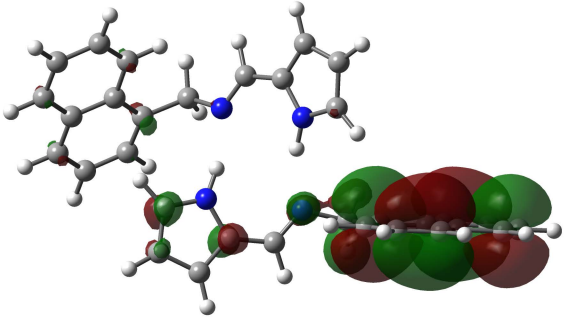
LUMO: Orbital 125



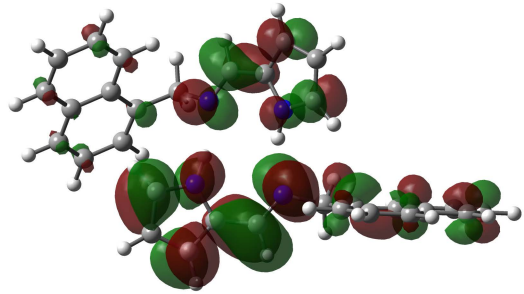
HOMO-1: Orbital 123



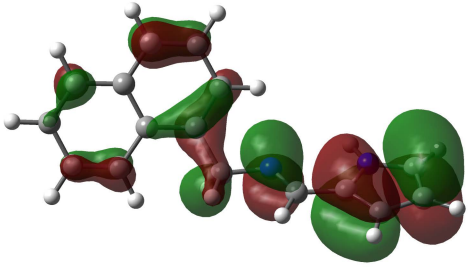
LUMO+1: Orbital 126



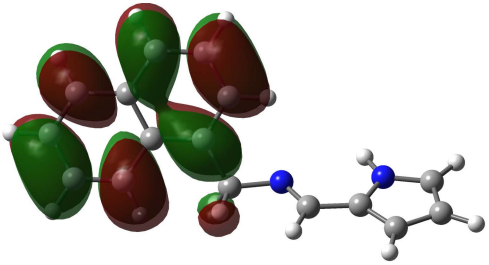
HOMO-2: Orbital 122



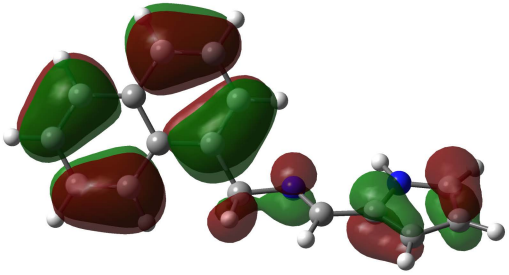
LUMO+2: Orbital 127



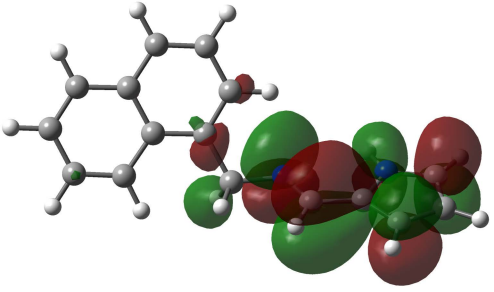
HOMO:Orbital 62



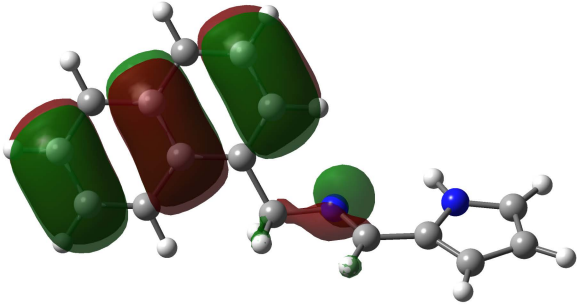
LUMO: Orbital 63



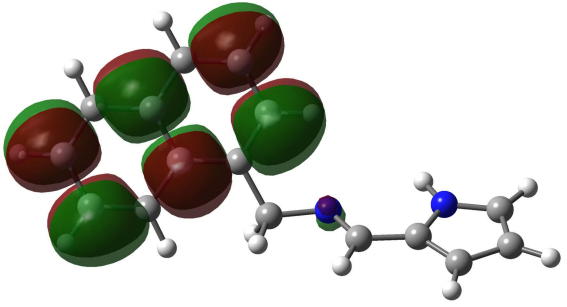
HOMO-1: Orbital 61



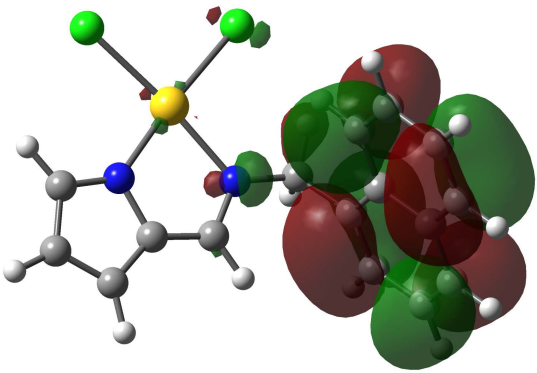
LUMO+1: Orbital 64



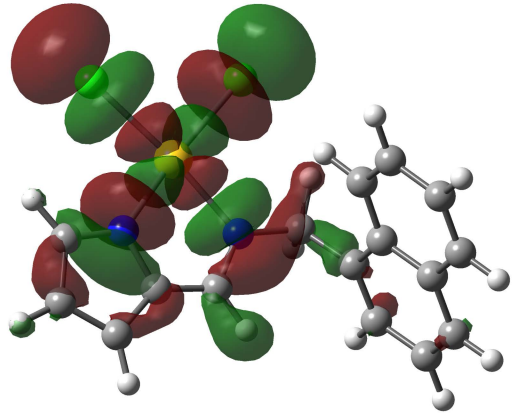
HOMO-2: Orbital 60



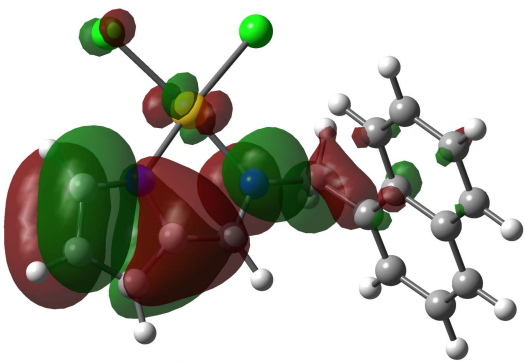
LUMO+2: Orbital 65



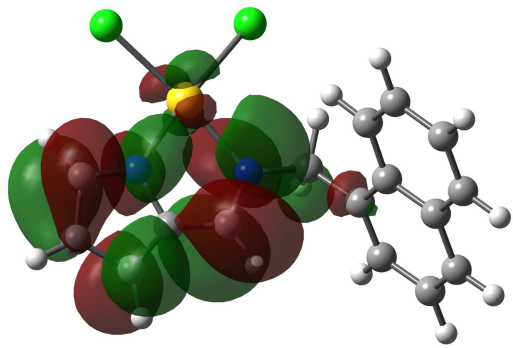
HOMO: Orbital 78



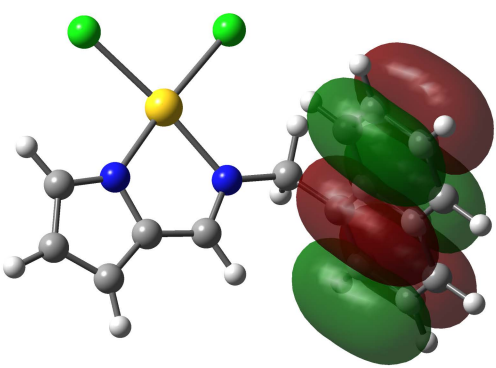
LUMO: Orbital 79



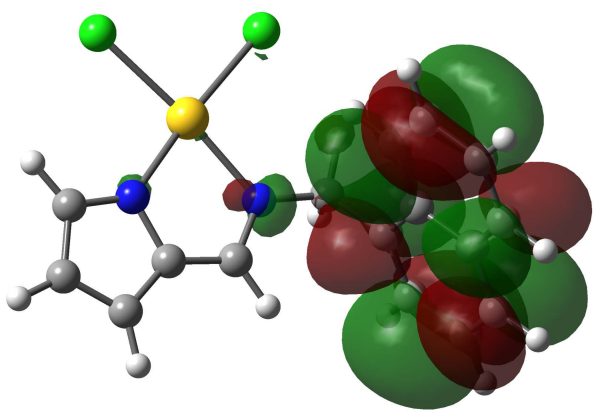
HOMO-1: Orbital 77



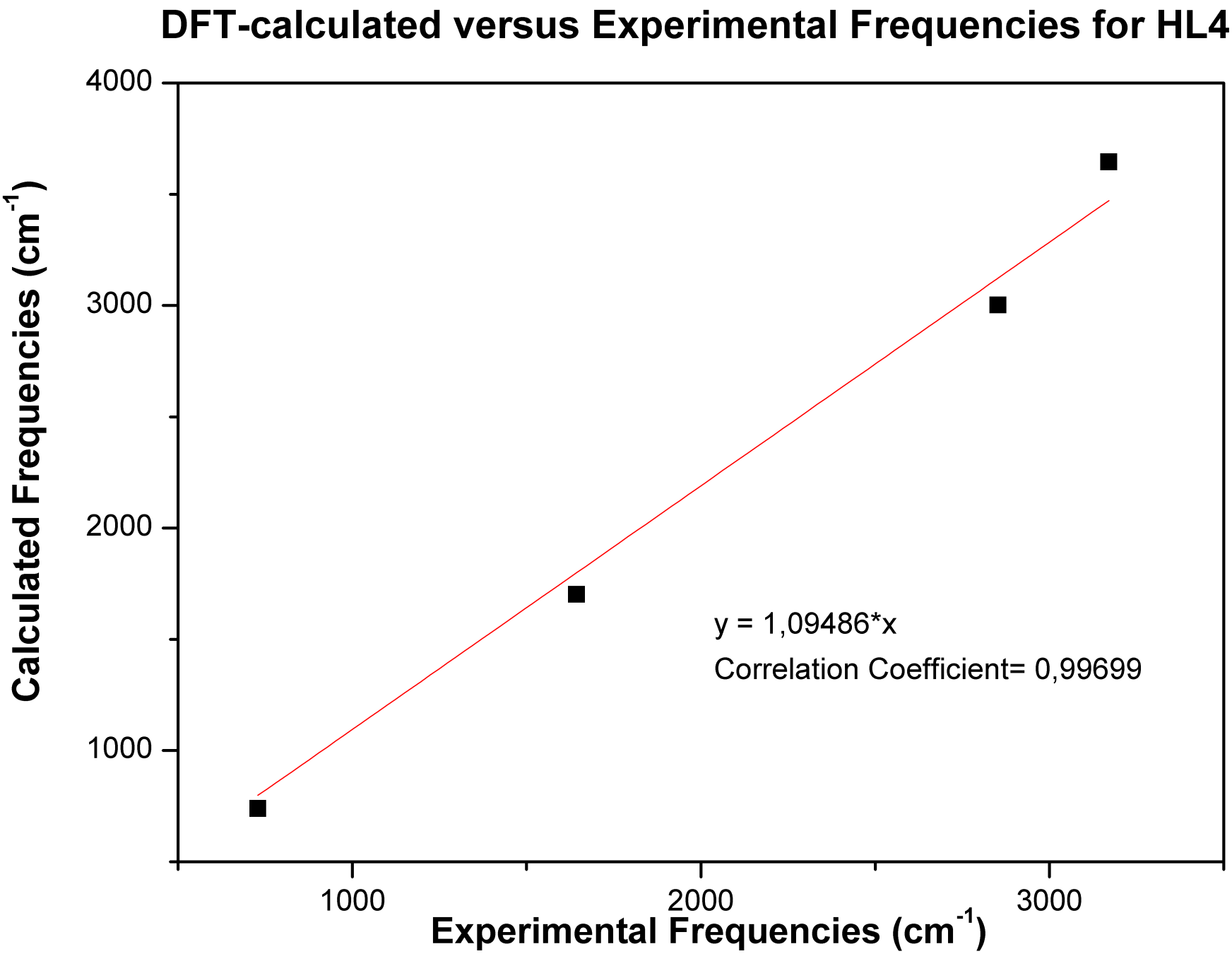
LUMO+1: Orbital 80



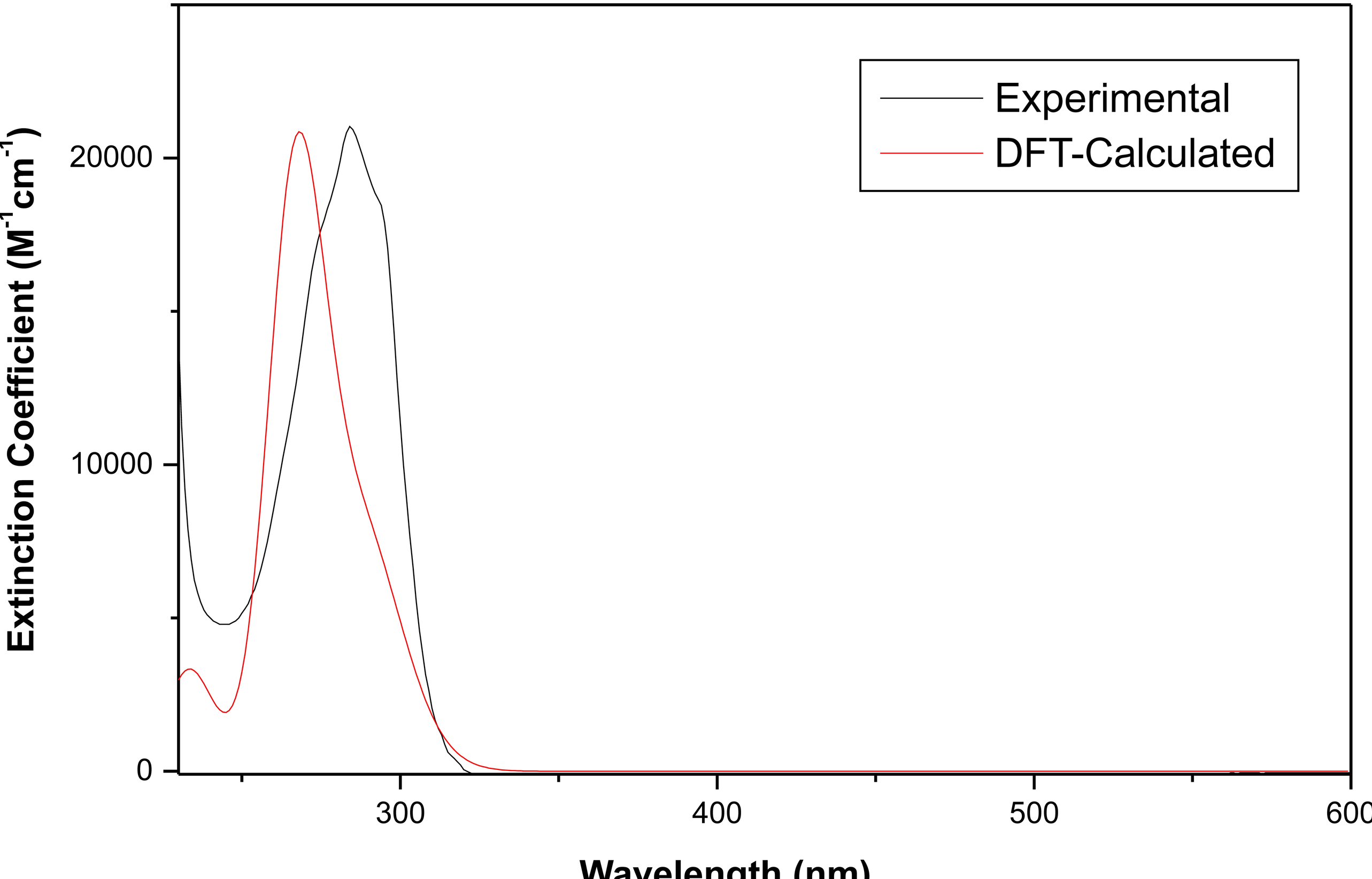
HOMO-2: Orbital 76

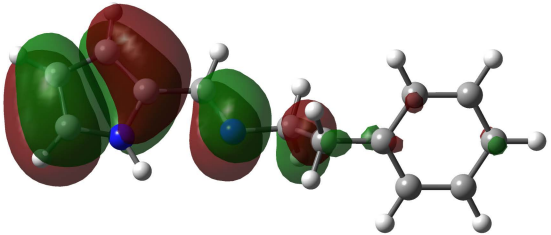


LUMO+2: Orbital 81

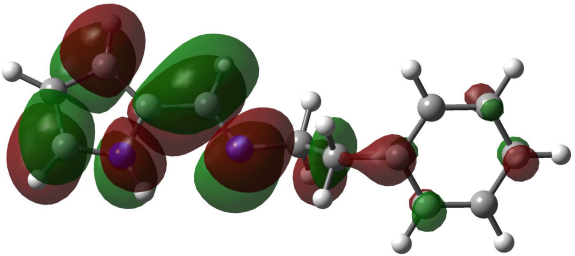

DFT-calculated versus Experimental Frequencies for HL4
Calculated Frequencies (cm-1)
Experimental Frequencies (cm-1)
4000
3000
2000
1000
1000
2000
3000
y = 1,09486*x
Correlation Coefficient= 0,99699

Superposition of Experimental and DFT-Calculated UV-vis Spectra for HL4

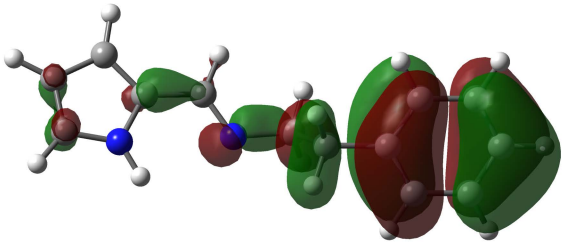




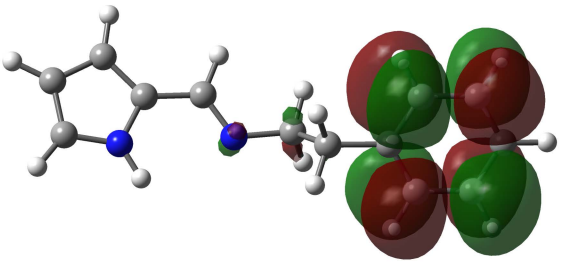
HOMO:Orbital 53



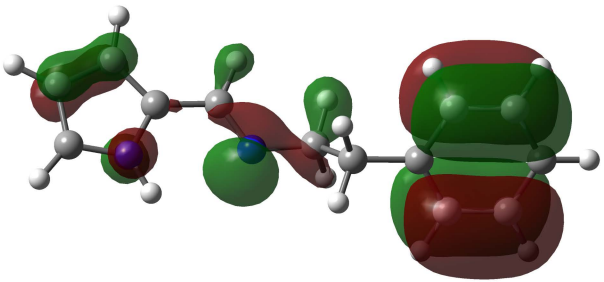
LUMO: Orbital 54



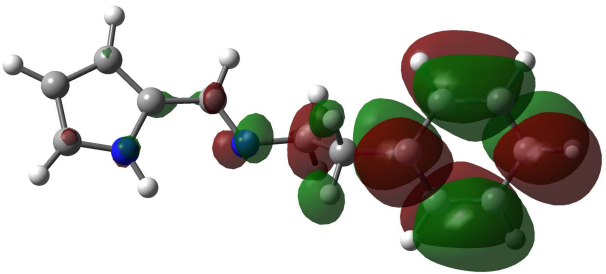
HOMO-1: Orbital 52



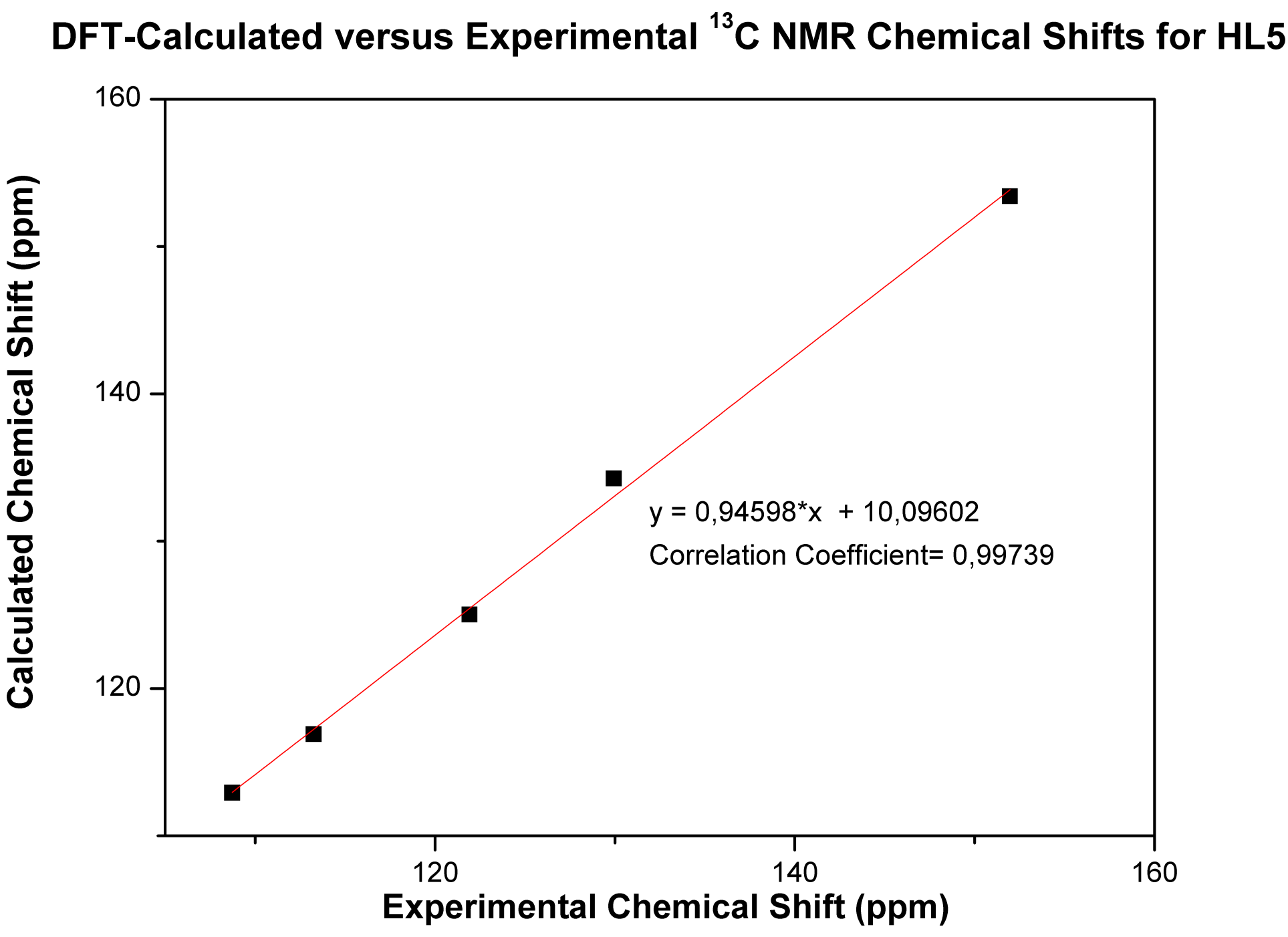
LUMO+1: Orbital 55

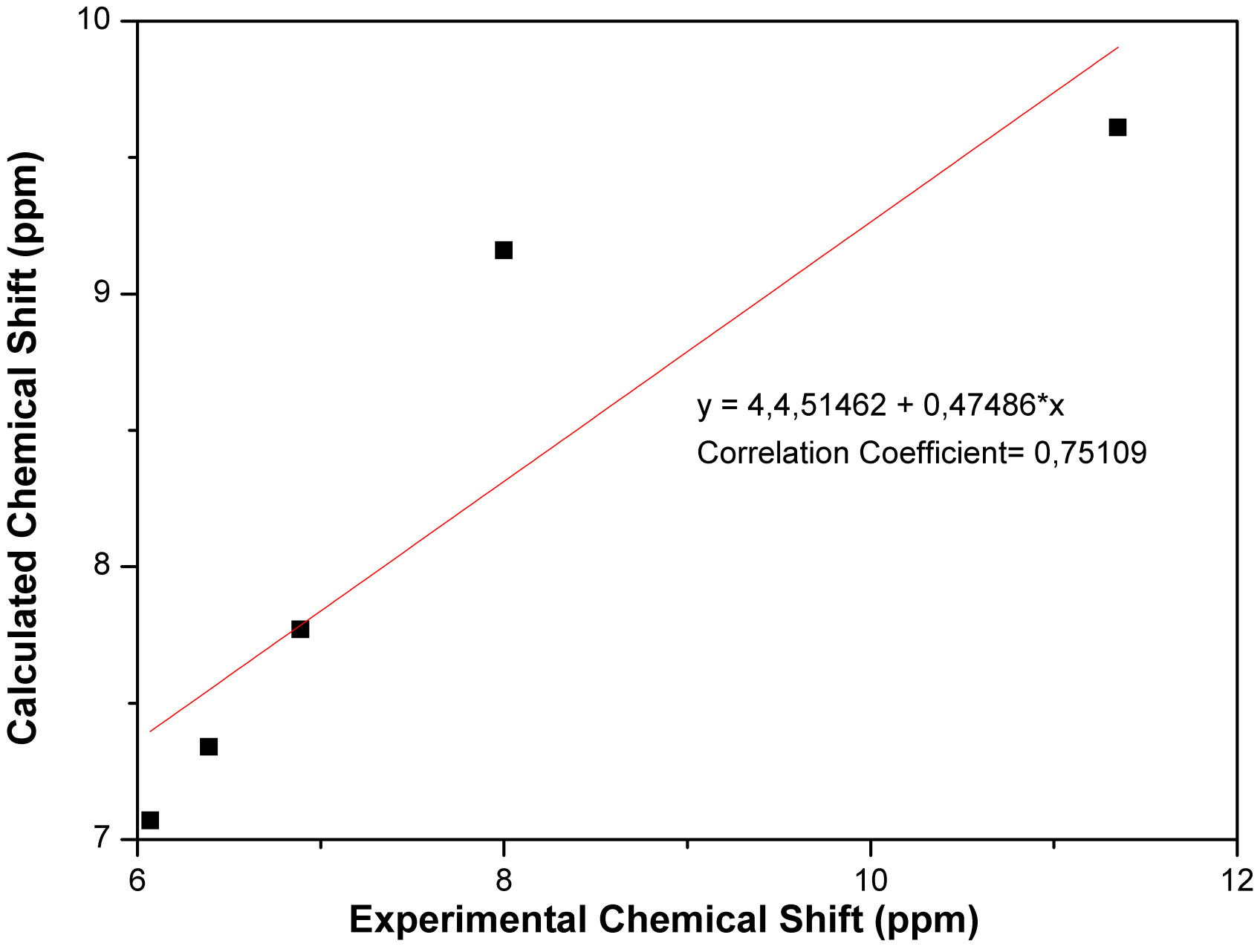


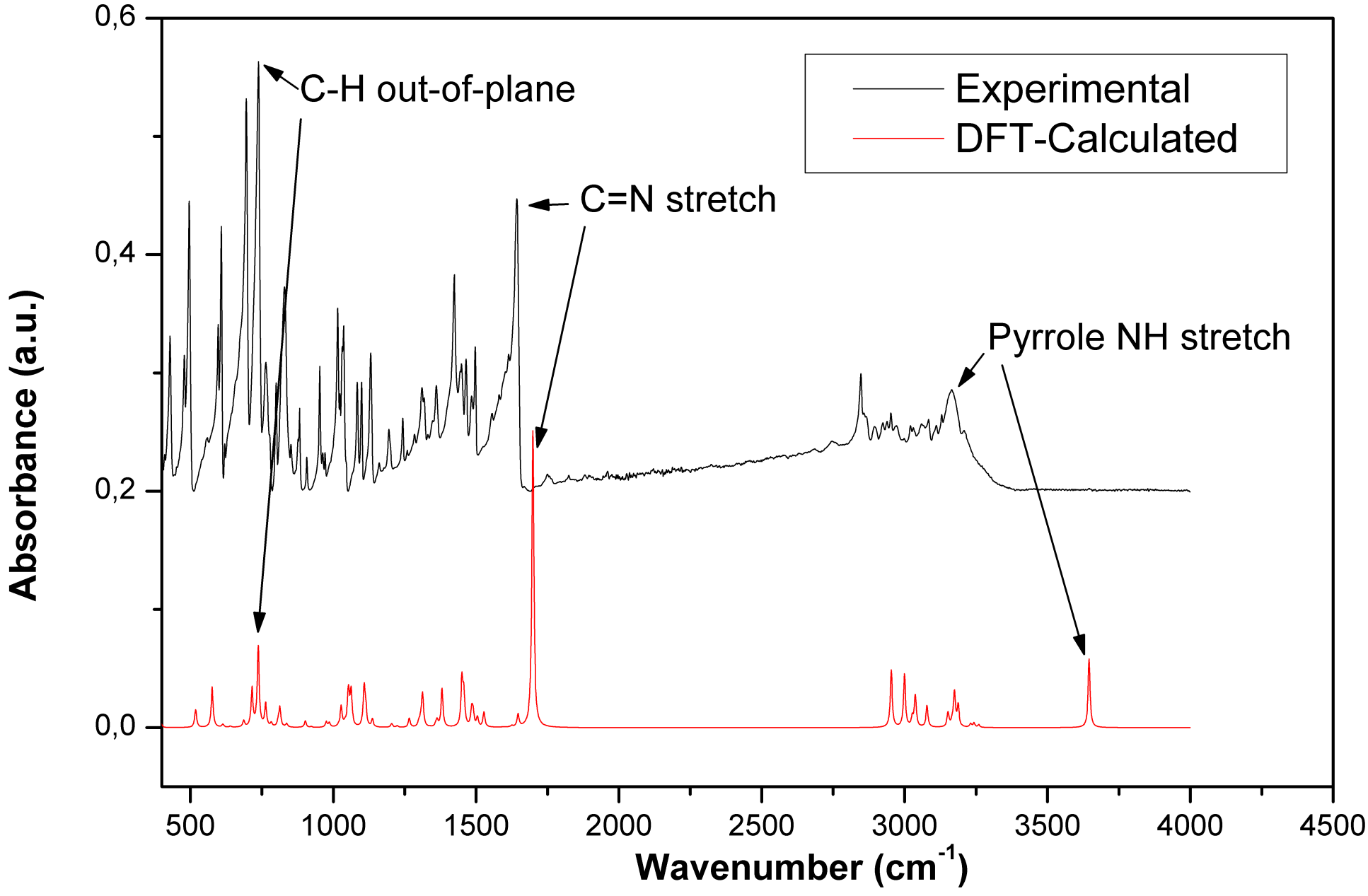
HOMO-2: Orbital 51

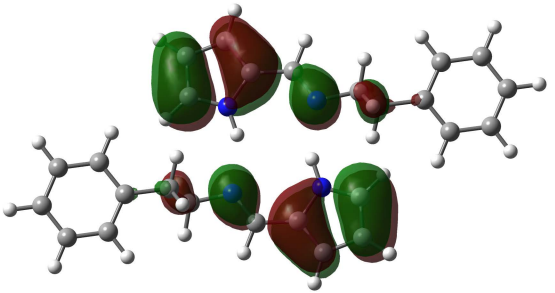


LUMO+2: Orbital 56

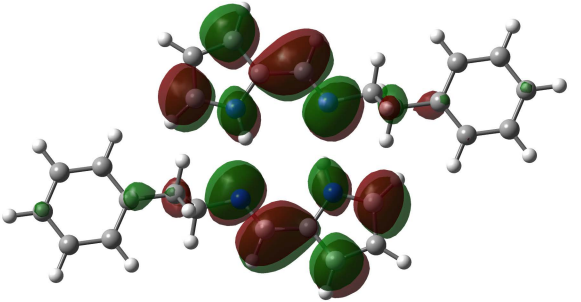

DFT-Calculated versus Experimental 13C NMR Chemical Shifts for HL5
Calculated Chemical Shift (ppm)
160
140
120
120
140
160
Experimental Chemical Shift (ppm)
y = 0,94598*x + 10,09602
Correlation Coefficient= 0,99739


DFT-Calculated versus Experimental 1H NMR Chemical Shifts for HL5
Calculated Chemical Shift (ppm)
Experimental Chemical Shift (ppm)
y = 4,4,51462 + 0,47486*x
Correlation Coefficient= 0,75109
10
9
8
7
6
8
10
12

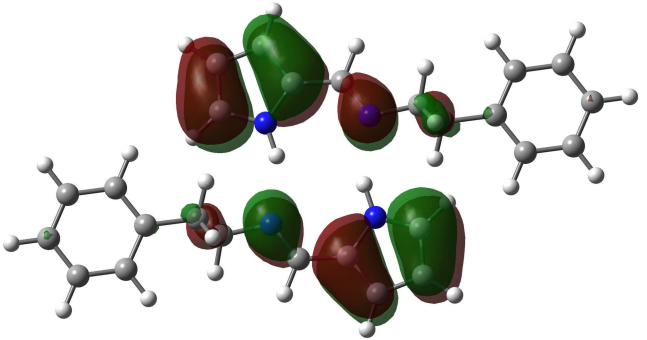

Superposition of Experimental and DFT-calculated IR Spectra for HL5
Absorbance (a.u.)
0,6
0,4
0,2
0,0
500
1000
1500
2000
2500
3000
3500
4000
4500
Wavenumber (cm-1)
C-H out-of-plane
C=N stretch
Pyrrole NH stretch
Experimental
DFT-Calculated



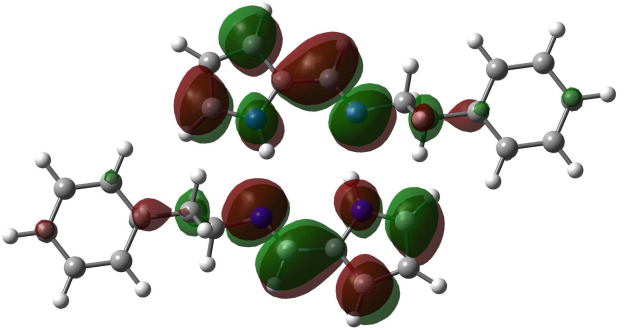
HOMO:Orbital 106



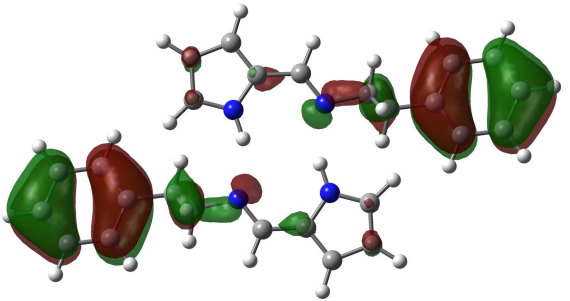
LUMO: Orbital 107



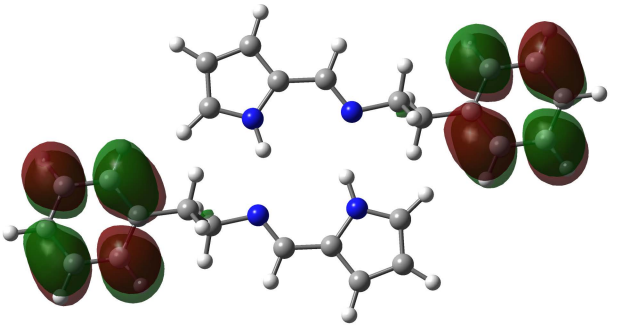
HOMO-1: Orbital 105



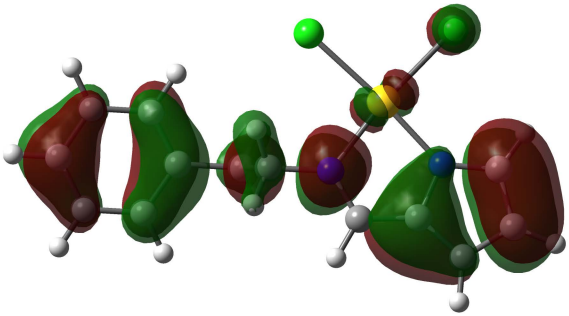
LUMO+1: Orbital 108



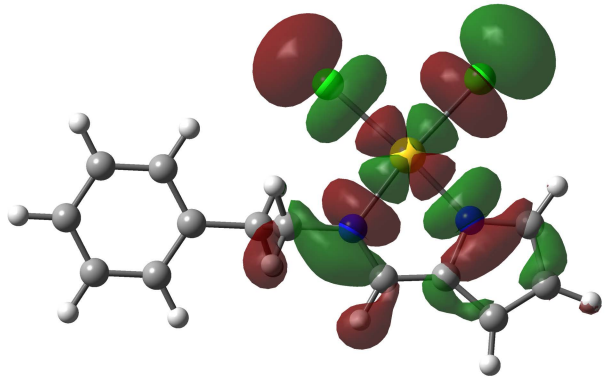
HOMO-2: Orbital 104



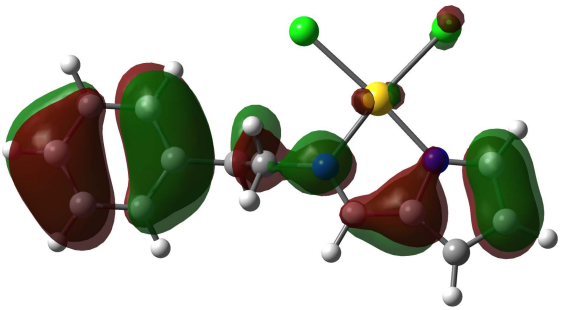
LUMO+2: Orbital 109



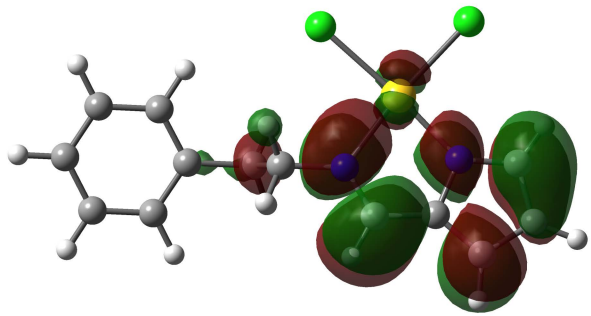
HOMO: Orbital 69



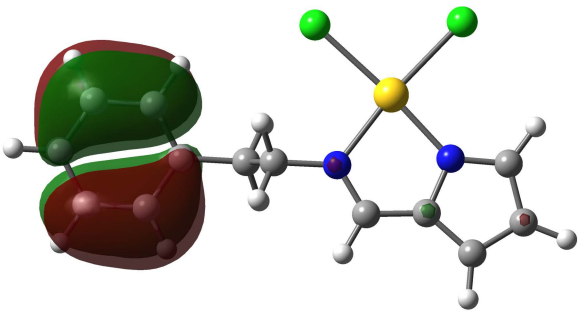
LUMO: Orbital 70



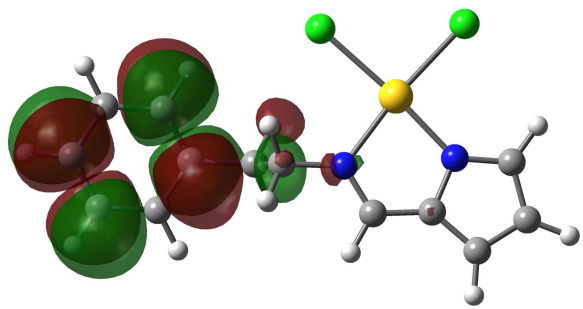
HOMO-1: Orbital 68



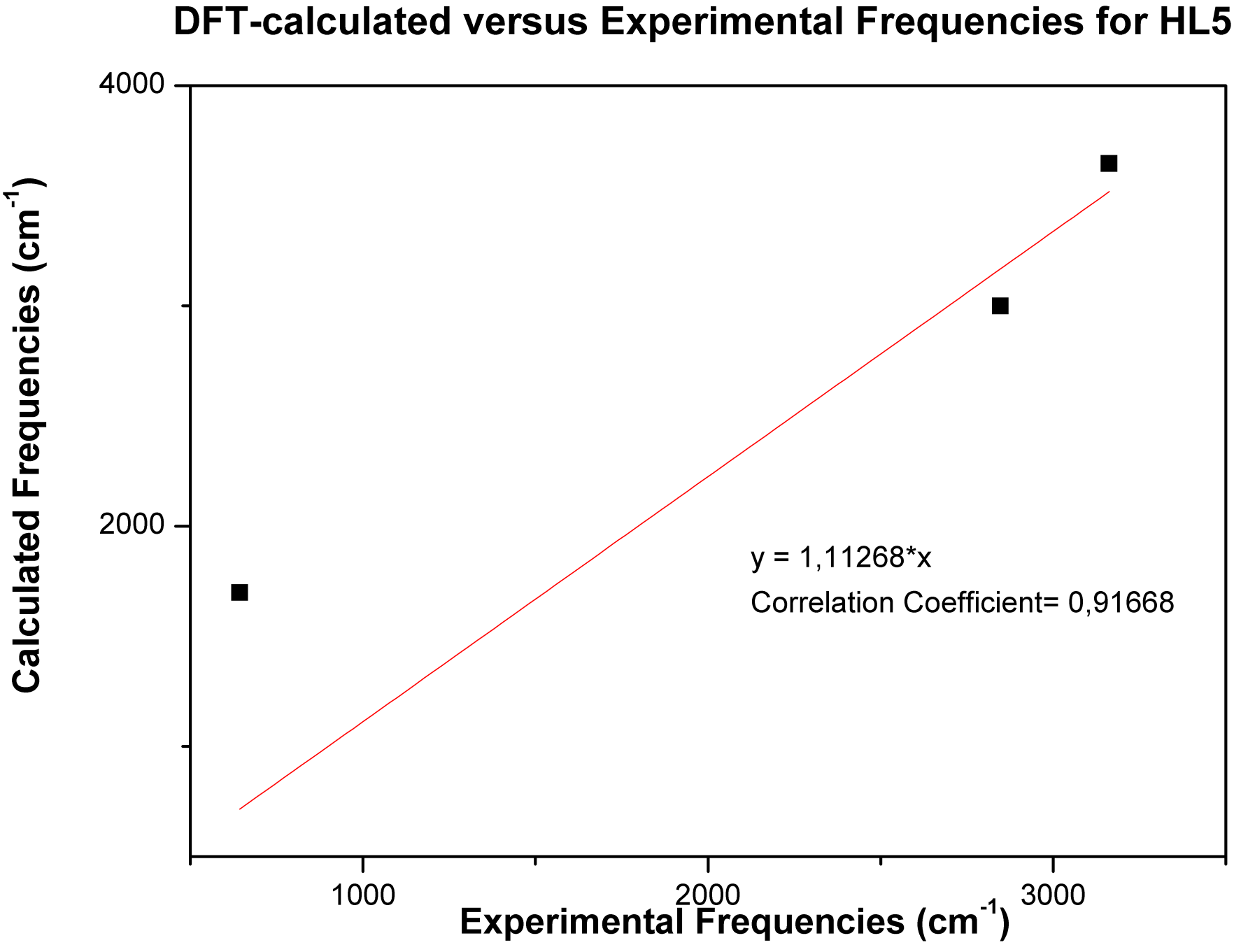
LUMO+1: Orbital 71



HOMO-2: Orbital 67



LUMO+2: Orbital 72


DFT-calculated versus Experimental Frequencies for HL5
Calculated Frequencies (cm-1)
Experimental Frequencies (cm-1)
4000
2000
1000
2000
3000
y = 1,11268*x
Correlation Coefficient= 0,91668

Superposition of Experimental and DFT-Calculated UV-vis Spectra for HL5