Supporting Informations

An Approach to Long and Unsubstituted Molecular wires : Synthesis of Redox-Active, Cationic Phenylethynyl Oligomers Designed for Self-Assembled Monolayers.

Cédric Hortholary and Christophe Coudret

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^1H and ^{13}C NMR spectra

for molecules **7-12**.

13C- {1H}

7

1.24
1.03
0.63
0.62
0.41
0.21
0.00
-0.75

199.43
166.80
157.10
154.49
150.85
150.70
150.53
149.46
146.78
136.95
136.29
136.15
135.63
134.57
134.48
132.22
131.51
130.63
127.44
126.84
126.75
126.59
124.60
123.87
123.61
123.47
123.44
123.21
119.57
117.57
114.49
104.89
96.37
93.69
87.31
62.71

ppm 200 175 150 125 100 75 50 25 0

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*****
* AMX400 / LCC-CNRS *
*****
Current Data Parameters
NAME      hor10411
EXPNO     6
PROCNO    1

F2 - Acquisition Parameters
Date_     20020412
Time      3.21
INSTRUM   amx400
PROBHD    5 mm 1H1 Z-9
PULPROG   zgpg00csave
TD         52628
SOLVENT    MeCN-CD3CN
NS         9957
DS         8
SMH        23809.523 Hz
FIDRES     0.452412 Hz
AQ         1.1052380 sec
RG         32768
OR         21.000 usec
DE         30.00 usec
TE         293.2 K
NUC1       13C
NUC2       1H
NUC3
NUCLEUS    13C
L4
L5

F2 - Processing parameters
SI         65536
SF         100.6127290 MHz
KOH        EM
SSB        0
LB         1.00 Hz
GB         0

1D NMR plot parameters
CX         22.00 cm
F1P        217.091 ppm
F1         21842.10 Hz
F2P        -19.554 ppm
F2         -1967.43 Hz
PPMCH      10.75660 ppm/cm
HZCH       1082.25110 Hz/cm
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1H

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*****
* AMX400 / LCC-CNRS *
*****

Current Data Parameters
NAME      hort0411
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20020411
Time      17.44
INSTRUM   amx400
PROBHD    5 mm TBI Z-g
PULPROG   zgpg
TD         13760
SOLVENT   CD3CN
NS         8
DS         2
SMH        3846.154 Hz
FIDRES     0.279517 Hz
AQ         1.7888499 sec
RG         256
DW         130.000 usec
DE         162.50 usec
TE         -293.0 K
HL1        1 dB
D1         30.00000000 sec
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SF01       400.1317262 MHz
NUCLEUS    1H

F2 - Processing parameters
SI         65536
SF         400.1300000 MHz
WDW        EM
SSB        0
LB         0.20 Hz
GB         0

1D NMR plot parameters
CX         22.00 cm
F1P        9.120 ppm
F1         3649.29 Hz
F2P        -0.492 ppm
F2         -196.86 Hz
PPMCH      0.43692 ppm/cm
HZCM       174.82518 Hz/cm
  
```


¹H

* AMX400 / LCC-CNRS *

Current Data Parameters
NAME hort0411
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20020411
Time 17.44
INSTRUM amx400
PROBHD 5 mm TBI Z-9
PULPROG zgpg30
TD 13760
SOLVENT CD3CN
NS 8
DS 2
SMH 3846.154 Hz
FIDRES 0.279517 Hz
AQ 1.7888499 sec
RG 256
DM 130.000 usec
DE 162.50 usec
TE 293.0 K
HL1 1 dB
D1 30.00000000 sec
P1 6.20 usec
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NUCLEUS ¹H
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
1D NMR plot parameters
CX 22.00 cm
F1P 8.697 ppm
F1 3479.80 Hz
F2P 6.318 ppm
F2 2528.04 Hz
PPMCM 0.10812 ppm/cm
HZCM 43.26183 Hz/cm

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*****
* AMX400 / LCC-QMPS *
*****

Current Data Parameters
NAME             hor10422
EXPNO            6
PROCNO           1

F2 - Acquisition Parameters
Date_            20020423
Time             3.43
INSTRUM          amx400
PROBHD           5 mm 1B1 Z-g
PULPROG          zgpgdcsave
TD               52628
SOLVENT          MeCN
NS               9740
DS               8
SMH              23809.523 Hz
FIDRES           0.452412 Hz
AQ              1.1052380 sec
RG              32768
DM              21.000 usec
DE              30.00 usec
TE              293.2 K
D1              0.030000 sec
CPOPRG           waltz16
P31              92.00 usec
S2              25 dB
HL1             90 dB
D1              1.00000000 sec
P1              11.50 usec
SF01            100.6286653 MHz
NUCLEUS          13C
L4              70

F2 - Processing parameters
SI              65536
SF              100.6127290 MHz
WDW             EM
SSB             0
LB              1.00 Hz
GB              0

1D NMR plot parameters
CX              22.00 cm
F1P            217.091 ppm
F1             21842.10 Hz
F2P            -19.554 ppm
F2             -1967.43 Hz
PQPMCH         10.75660 ppm/cm
HZCH           1082.25110 Hz/cm

```

¹H

H₂O

8

 * AMX400 / LCC-CNRS *

 Current Data Parameters
 NAME hor10422
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020422
 Time 17.41
 INSTRUM amx400
 PROBD 5 mm TBI Z-g
 PULPROG zgpg30
 TD 13760
 SOLVENT CD3CN
 NS 8
 DS 2
 SMH 3846.154 Hz
 FIDRES 0.279517 Hz
 AQ 1.7888499 sec
 RG 256
 DW 130.000 usec
 DE 162.50 usec
 TE -293.0 K 303 K
 HL 1 1 dB
 D1 30.00000000 sec
 P1 6.20 usec
 SF01 400.1317262 MHz
 NUCLEUS ¹H

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 MDW no
 SSB 0
 LB 0.00 Hz
 GB 0

1D NMR plot parameters
 CX 22.00 cm
 F1P 9.120 ppm
 F1 3649.29 Hz
 F2P -0.492 ppm
 F2 -196.86 Hz
 PPMCM 0.43592 ppm/cm
 HZCM 174.82518 Hz/cm

¹H

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*****
* AMX400 / LCC-CNRS *
*****

Current Data Parameters
NAME      hort0422
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20020422
Time      17.41
INSTRUM   amx400
PROBHD    5 mm TBI Z-9
PULPROG   zg50
TD         13760
SOLVENT   CD3CN
NS         8
DS         2
SMH        3846.154 Hz
FIDRES     0.279517 Hz
AQ         1.7888499 sec
RG         256
DM         130.000 usec
DE         162.50 usec
TE         293.0 K
HL1        1 dB
D1         30.00000000 sec
P1         6.20 usec
SFO1       400.1317262 MHz
NUCLEUS    1H

F2 - Processing parameters
SI         65536
SF         400.1300000 MHz
WDW         no
SSB         0
LB         0.00 Hz
GB         0

1D NMR plot parameters
CX         22.00 cm
F1P        8.639 ppm
F1         3456.58 Hz
F2P        6.438 ppm
F2         2576.01 Hz
PPM/QM     0.10003 ppm/cm
HZ/CM      40.02587 Hz/cm
  
```

¹H

CD₃CN

9

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*****
* AMX400 / LCC-CNRS *
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Current Data Parameters
NAME      hort0410
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20020410
Time      17.44
INSTRUM   amx400
PROBHD    5 mm TBI Z-g
PULPROG   zgpg
TD         13760
SOLVENT   CD3CN
NS         8
DS         2
SMH        3846.154 Hz
FIDRES     0.279517 Hz
AQ         1.7888439 sec
RG         256
DM         130.000 usec
DE         162.50 usec
TE         293.2 K 313K
HL1        1 dB
D1         30.00000000 sec
P1         6.20 usec
SF01       400.1317262 MHz
NUCLEUS    1H

F2 - Processing parameters
SI         65536
SF         400.1300000 MHz
WDW        EM
SSB        0
LB         0.20 Hz
GB         0

1D NMR plot parameters
CX         22.00 cm
F1P        9.120 ppm
F1         3649.29 Hz
F2P        -0.492 ppm
F2         -196.86 Hz
PPMCH      0.43692 ppm/cm
HZCM       174.82518 Hz/cm
  
```

1H

CD₃CN

9

 * AMX400 / LCC-CNRS *

 Current Data Parameters
 NAME hort0410
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020410
 Time 17.44
 INSTRUM amx400
 PROBHD 5 mm TBI Z-9
 PULPROG zgpg30
 TD 13760
 SOLVENT CD3CN
 NS 8
 DS 2
 SMH 3846.154 Hz
 FIDRES 0.279517 Hz
 AQ 1.7888499 sec
 RG 256
 DW 130.000 usec
 DE 162.50 usec
 TE 293.0 K
 HL1 1 dB
 D1 30.0000000 sec
 P1 6.20 usec
 SF01 400.1317262 MHz
 NUCLEUS 1H

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0

1D NMR plot parameters
 CX 22.00 cm
 F1P 8.805 ppm
 F1 3523.26 Hz
 F2P 6.318 ppm
 F2 2528.04 Hz
 PPMCM 0.11306 ppm/cm
 HZCM 45.23725 Hz/cm

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

DMF

11

2D-NMR spectra (COSY 45)
of molecules 7, 8 and 9

NAME	PORT0422
EXPND	3
PRDCNO	1

F2 - Acquisition Parameters

Date_	Time	INSTRUM	PROBHD	PULPROG	TD	SOLVENT	NS
20020422	17.41	amy400	5 mm TBI 2-g	COSYgs	2048	CDCl ₃	4

SMH	2232.143 Hz
FIDRES	1.069913 Hz
AQ	0.4586020 sec
RG	4096
DW	224.000 usec
DE	320.00 usec
TE	200.0 K
P16	1700.00 usec
	355

	230
LC1	1 dB
D1	1.00000000 sec
P1	5.00 usec
D0	0.00000030 sec
D27	0.00000046 sec
D16	0.00020000 sec
P0	3.00 usec
D13	0.00000040 sec
SFO1	400.1324200 MHz
NUCLEUS	¹ H
TMO	0.00004600 sec

F1 - Acquisition parameters

NDO	1
TD	256
SFO1	400.1324 MHz
FIDRES	8.719309 Hz
SM	5.579 ppm

F2 - Processing parameters
769

SI	768
SF	400.130000 MHz
MDW	GM
SSB	0
LB	-5.00 Hz
GB	0.9

F1 - Processing parameters

SI	112
MC2	GF
SF	400.130000 MHz
MDM	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

F2PLO	8.551 ppm
F2PHI	6.459 ppm
F1PLO	8.619 ppm
F1PHI	6.179 ppm
F2HZCM	55.80358 Hz/cm
F1HZCM	65.10417 Hz/cm

NAME h010410
EXPNO 3
PROCNO 1

COSY45-9S

F2 - Acquisition Parameters

Date_ 20020410
Time 17.06
INSTRUM amx400
PROBHD 5 mm TBI Z-9
PULPROG zgpg30
TD 2048
SOLVENT CDCl3
NS 4
DS 4
SWH 2232.143 Hz
FIDRES 1.099913 Hz
AQ 0.4588020 sec
RG 8192
DM 224.000 usec
DE 320.00 usec
TE 293.2 K
P16 1700.00 usec
P1 6.00 usec
P2 0.0000000 sec
P3 0.0000030 sec
P4 0.0000046 sec
P5 0.0002000 sec
P6 3.00 usec
P7 0.0000040 sec
P8 400.1324200 MHz
NUCLEUS 1H
INQ 0.00044800 sec

F1 - Acquisition Parameters
NDO 1
TD 256
SF01 400.1324 MHz
FIDRES 8.719309 Hz
SW 5.579 ppm
SI 768
SF 400.1300000 MHz
WDW GM
SSB 0
LB -6.00 Hz
GB 0.9

F2 - Processing parameters
SI 768
SF 400.1300000 MHz
WDW GM
SSB 0
LB -6.00 Hz
GB 0.9

F1 - Processing parameters
SI 208
WC2 0F
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
F2PUL 8.576 ppm
F2PAI 6.484 ppm
F1PUL 8.598 ppm
F1PAI 6.331 ppm
F2HZCM 55.80358 Hz/cm
F1HZCM 50.45388 Hz/cm

6

Attributions of the protons in the aromatic region for complexes **7**, **8** and **9**.

Proton	δ (ppm)	signal	Coupling constant
9	6.56	d	$J = 8$ Hz
10	6.98	dd	$J_1 = 8$ Hz, $J_2 = 1.6$ Hz
18	7.00	pseudo td	$J_1 = 5.6$ Hz, $J_2 = 1.6$ Hz
2, 7, 15	7.22-7.28	m	
23, 25-28	7.43-7.47	m	
17	7.63	d	$J = 5.6$ Hz
6, 8, 19	7.73-7.77	m	
1	7.79	d	$J = 6$ Hz
3, 14, 24	7.81-7.89	m	
22	8.01	td	$J_1 = 6$ Hz, $J_2 = 1.6$ Hz
12	8.02	d	$J = 1.6$ Hz
16	8.06	dd	$J_1 = 4.8$ Hz, $J_2 = 1.2$ Hz
20	8.10	d	$J = 8.4$ Hz
4, 5	8.33-8.37	m	
13	8.40	d	$J = 8$ Hz
21	8.48	d	$J = 8$ Hz

Proton	δ (ppm)	signal	Coupling constant
9	6.56	d	J= 8 Hz
10	6.98	dd	J ₁ = 8 Hz, J ₂ = 1.6 Hz
18	7.00	pseudo td	J ₁ = 5.6 Hz, J ₂ = 1.6 Hz
2, 7, 15	7.22-7.28	m	
23, 25-32	7.43-7.57	m	
17	7.63	d	J= 5.6 Hz
6, 8, 19	7.73-7.78	m	
1	7.79	d	J= 5.6 Hz
3, 14, 24	7.81-7.89	m	
22	8.01	td	J ₁ = 8 Hz, J ₂ = 1.6 Hz
12	8.03	d	J= 1.6 Hz
16	8.06	dd	J ₁ = 5.6 Hz, J ₂ = 1.6 Hz
20	8.10	d	J= 8 Hz
4, 5	8.33-8.37	m	
13	8.40	d	J= 8 Hz
21	8.48	d	J= 8 Hz

Proton	δ (ppm)	signal	Coupling constant
9	6.56	d	$J = 8$ Hz
10	6.98	dd	$J_1 = 8$ Hz, $J_2 = 1.6$ Hz
18	7.00	pseudo td	$J_1 = 5.6$ Hz, $J_2 = 1.6$ Hz
2, 7, 15	7.22-7.28	m	
23, 25-36	7.43-7.59	m	
17	7.63	d	$J = 6$ Hz
6, 8, 19	7.74-7.78	m	
1	7.80	d	$J = 6$ Hz
3, 14, 24	7.81-7.89	m	
22	8.02	td	$J_1 = 8$ Hz, $J_2 = 1.6$ Hz
12	8.03	d	$J = 1.6$ Hz
16	8.07	dd	$J_1 = 6$ Hz, $J_2 = 1.2$ Hz
20	8.10	d	$J = 8$ Hz
4, 5	8.33-8.37	m	
13	8.40	d	$J = 8$ Hz
21	8.48	d	$J = 8$ Hz

UV-visible spectra for molecules **7-12**

Molecule **7** (concentration : $1.7 \cdot 10^{-5}$ mol/L in ethanol)

Molecule **8** (concentration : $1.7 \cdot 10^{-5}$ mol/L in ethanol)

Molecule **9** (concentration : $1.7 \cdot 10^{-5}$ mol/L in ethanol)

Molecule **10** (concentration : $5 \cdot 10^{-5}$ mol/L in ethanol)

Molecule **11** (concentration : $5 \cdot 10^{-5}$ mol/L in ethanol)

Molecule **12** (concentration : $3 \cdot 10^{-5}$ mol/L in ethanol)

MLCT transitions of the calculated UV-visible spectra and Z-matrixes for the complexes **10**, **11** and **12**, with a representations of the molecular orbitals involved in these transitions.

(configurations interactions have been computed with 12 occupied and 12 unoccupied molecular orbitals).

Computed total energy of the optimised structure : 116.6 kcal/mol

Z-matrix of molecule **10**

Ru	0.0000000	0	0.0000000	0	0.0000000	0	0	0	0	0.0000000
N	2.0467584	1	0.0000000	0	0.0000000	0	1	0	0	0.0000000
C	1.3630658	1	112.8247581	1	0.0000000	0	2	1	0	0.0000000
C	1.4881165	1	116.2056619	1	0.4690797	1	3	2	1	0.0000000
N	2.0525264	1	82.1319515	1	-0.1946479	1	1	2	3	0.0000000
C	1.3622914	1	125.1931872	1	-179.7094709	1	5	1	4	0.0000000
C	1.3956045	1	119.7050617	1	179.7648465	1	6	5	1	0.0000000
C	1.3961573	1	119.3951941	1	-0.0577129	1	7	6	5	0.0000000
C	1.4049769	1	119.4586149	1	179.7962894	1	4	5	3	0.0000000
H	1.0797866	1	122.0323103	1	179.9972632	1	9	4	8	0.0000000
H	1.0823680	1	119.9270326	1	179.9715228	1	8	7	9	0.0000000
H	1.0822945	1	120.3015461	1	179.9617962	1	7	6	8	0.0000000
H	1.0787067	1	121.0450737	1	179.6944071	1	6	5	7	0.0000000
C	1.4050073	1	119.4017920	1	179.7956245	1	3	2	4	0.0000000
C	1.3974123	1	119.1218038	1	0.0671444	1	14	3	2	0.0000000
C	1.3965108	1	120.1059062	1	0.0032052	1	15	14	3	0.0000000
C	1.3613326	1	124.8361711	1	-179.5694567	1	2	1	3	0.0000000
H	1.0788449	1	120.8874498	1	179.7181659	1	17	2	16	0.0000000

H	1.0822791	1	120.3179531	1	-179.9773521	1	16	15	17	0.0000000
H	1.0823627	1	119.9737046	1	-179.9925537	1	15	14	16	0.0000000
H	1.0797874	1	122.0376403	1	179.9881836	1	14	3	15	0.0000000
N	2.0444499	1	88.5005478	1	94.8282625	1	1	2	5	0.0000000
C	1.3635233	1	112.5894680	1	94.6957038	1	22	1	2	0.0000000
C	1.4894163	1	116.2209554	1	0.4186564	1	23	22	1	0.0000000
N	2.0452923	1	94.6512747	1	177.0867553	1	1	2	5	0.0000000
C	1.3612126	1	125.0480159	1	-179.8327555	1	25	1	24	0.0000000
C	1.3956638	1	119.6200962	1	179.8364376	1	26	25	1	0.0000000
C	1.3967632	1	119.3788701	1	-0.0239464	1	27	26	25	0.0000000
C	1.4047394	1	119.3848615	1	179.8372119	1	24	25	23	0.0000000
H	1.0798470	1	122.0086710	1	-179.9942652	1	29	24	28	0.0000000
H	1.0823620	1	119.9126480	1	179.9657659	1	28	27	29	0.0000000
H	1.0822733	1	120.3043301	1	179.9590761	1	27	26	28	0.0000000
H	1.0789227	1	120.8782578	1	179.7518149	1	26	25	27	0.0000000
C	1.4047527	1	119.3836557	1	179.7114906	1	23	22	24	0.0000000
C	1.3975817	1	119.1083097	1	0.0177711	1	34	23	22	0.0000000
C	1.3967616	1	120.1207528	1	-0.0284536	1	35	34	23	0.0000000
C	1.3610619	1	125.0230742	1	-179.8513270	1	22	1	23	0.0000000
H	1.0789004	1	120.8838903	1	179.7408585	1	37	22	36	0.0000000
H	1.0822783	1	120.3159089	1	-179.9584897	1	36	35	37	0.0000000
H	1.0823588	1	119.9653530	1	-179.9520887	1	35	34	36	0.0000000
H	1.0798476	1	122.0093132	1	-179.9698964	1	34	23	35	0.0000000
N	2.0558992	1	94.3624495	1	-87.9423270	1	1	2	5	0.0000000
C	1.3625843	1	113.2402056	1	177.2789929	1	42	1	2	0.0000000
C	1.4827034	1	116.0330796	1	0.5442571	1	43	42	1	0.0000000
C	2.0204181	1	95.4005607	1	176.4710042	1	1	5	2	0.0000000
C	1.3975845	1	125.5274048	1	179.9736308	1	45	1	44	0.0000000
C	1.3980321	1	119.4399522	1	-179.9800851	1	46	45	1	0.0000000
C	1.4031400	1	120.1931622	1	-0.0038274	1	47	46	45	0.0000000
C	1.4053688	1	125.2398600	1	-179.8499530	1	44	43	45	0.0000000
H	1.0810839	1	121.0883750	1	-179.9881493	1	49	44	48	0.0000000
C	1.4390060	1	119.9040825	1	179.9745410	1	48	47	49	0.0000000
C	1.2054806	1	150.3992197	1	-179.9844670	1	51	47	48	0.0000000

C	1.4389177	1	160.0477552	1	-179.9607283	1	52	47	51	0.0000000
C	1.4011511	1	120.0760163	1	4.7187494	1	53	52	47	0.0000000
C	1.3987342	1	120.0740169	1	179.9904525	1	54	53	52	0.0000000
C	1.4011411	1	120.0762589	1	0.0012271	1	55	54	53	0.0000000
C	1.4011995	1	119.8493614	1	0.0033607	1	56	55	54	0.0000000
C	1.4011557	1	120.0722331	1	179.9950399	1	53	52	54	0.0000000
H	1.0834698	1	120.4512175	1	179.9959376	1	58	53	57	0.0000000
H	1.0834618	1	120.4524583	1	-179.9960660	1	57	56	58	0.0000000
C	1.4389833	1	120.0771473	1	-179.9976595	1	56	55	57	0.0000000
C	1.2055523	1	150.4578561	1	-179.9839709	1	61	55	56	0.0000000
C	1.4389769	1	160.0497723	1	-179.9885936	1	62	55	61	0.0000000
C	1.4005364	1	120.0915143	1	5.0061121	1	63	62	55	0.0000000
C	1.3983677	1	120.0655757	1	179.9222939	1	64	63	62	0.0000000
C	1.4040077	1	120.2204026	1	0.8835884	1	65	64	63	0.0000000
S	1.8160819	1	121.3231398	1	-177.9390214	1	66	65	64	0.0000000
C	1.8194255	1	98.6899208	1	-50.5195252	1	67	66	65	0.0000000
O	1.2216532	1	121.1685535	1	-17.4886187	1	68	67	66	0.0000000
C	1.4947538	1	118.9868745	1	-177.6932616	1	68	67	69	0.0000000
H	1.1098126	1	109.5140763	1	58.8739548	1	70	68	67	0.0000000
H	1.1110350	1	110.7876352	1	120.1842869	1	70	68	71	0.0000000
H	1.1097881	1	109.4537641	1	-119.6990509	1	70	68	71	0.0000000
C	1.4003341	1	119.0481032	1	-175.7430565	1	66	67	65	0.0000000
C	1.4006469	1	120.0891496	1	179.4769736	1	63	62	64	0.0000000
H	1.0834571	1	120.4580823	1	179.7706370	1	75	63	74	0.0000000
H	1.0826146	1	120.1492665	1	179.5137736	1	74	66	75	0.0000000
H	1.0823555	1	119.3358834	1	-179.1979319	1	65	64	66	0.0000000
H	1.0834599	1	120.4557341	1	-179.5135601	1	64	63	65	0.0000000
H	1.0834635	1	119.4730518	1	-179.9964019	1	55	54	56	0.0000000
H	1.0834643	1	120.4515879	1	-179.9951275	1	54	53	55	0.0000000
H	1.0834237	1	119.3940354	1	179.9530724	1	47	46	48	0.0000000
H	1.0795837	1	120.9292494	1	179.7748781	1	46	45	47	0.0000000
C	1.4043931	1	119.5990956	1	179.7045402	1	43	42	44	0.0000000
C	1.3971053	1	119.0756241	1	0.0541738	1	84	43	42	0.0000000
C	1.3964593	1	120.0705770	1	-0.0182203	1	85	84	43	0.0000000

C	1.3617180	1	124.6179132	1	-179.6440401	1	42	1	43	0.0000000
H	1.0786576	1	120.9098087	1	179.7415950	1	87	42	86	0.0000000
H	1.0822830	1	120.3081402	1	-179.9719948	1	86	85	87	0.0000000
H	1.0823544	1	119.9878889	1	-179.9674545	1	85	84	86	0.0000000
H	1.0800198	1	121.9632757	1	-179.9774683	1	84	43	85	0.0000000

Transition : 530.8 nm

Spin Up : Occ. MO --> Unocc. MO Coefficients

135 --> 138 0.415707

134 --> 138 -0.441077

Spin Down: Occ. MO --> Unocc. MO Coefficients

135 --> 138 -0.415707

134 --> 138 0.441077

Transition : 476.9 nm

Spin Up : Occ. MO --> Unocc. MO Coefficients

135 --> 139 -0.454517

134 --> 139 0.338442

Spin Down: Occ. MO --> Unocc. MO Coefficients

135 --> 139 0.454517

134 --> 139 -0.338442

Orbital 134

Orbital 135

Orbital 138

Orbital 139

Computed total energy of the optimised structure : 126.9 kcal/mol

Z-matrix of molecule **11**

Ru	0.0000000	0	0.0000000	0	0.0000000	0	0	0	0	0.0000000
N	2.0467528	1	0.0000000	0	0.0000000	0	1	0	0	0.0000000
C	1.3630632	1	112.8249602	1	0.0000000	0	2	1	0	0.0000000
C	1.4881205	1	116.2053807	1	0.4672675	1	3	2	1	0.0000000
N	2.0525227	1	82.1320813	1	-0.1924836	1	1	2	3	0.0000000
C	1.3622928	1	125.1931233	1	-179.7090390	1	5	1	4	0.0000000
C	1.3956039	1	119.7049958	1	179.7630624	1	6	5	1	0.0000000
C	1.3961581	1	119.3950185	1	-0.0578680	1	7	6	5	0.0000000
C	1.4049752	1	119.4585171	1	179.7966751	1	4	5	3	0.0000000
H	1.0797869	1	122.0320830	1	179.9971711	1	9	4	8	0.0000000
H	1.0823678	1	119.9269217	1	179.9711382	1	8	7	9	0.0000000
H	1.0822957	1	120.3017507	1	179.9619788	1	7	6	8	0.0000000
H	1.0787080	1	121.0451906	1	179.6947884	1	6	5	7	0.0000000
C	1.4050083	1	119.4018155	1	179.7947194	1	3	2	4	0.0000000
C	1.3974145	1	119.1216495	1	0.0665321	1	14	3	2	0.0000000
C	1.3965104	1	120.1059896	1	0.0032371	1	15	14	3	0.0000000
C	1.3613345	1	124.8358835	1	-179.5729727	1	2	1	3	0.0000000
H	1.0788441	1	120.8872896	1	179.7170526	1	17	2	16	0.0000000
H	1.0822801	1	120.3182411	1	-179.9769691	1	16	15	17	0.0000000
H	1.0823637	1	119.9736808	1	-179.9923038	1	15	14	16	0.0000000
H	1.0797869	1	122.0376713	1	179.9886774	1	14	3	15	0.0000000
N	2.0444468	1	88.5012404	1	94.8280252	1	1	2	5	0.0000000
C	1.3635244	1	112.5893152	1	94.6974073	1	22	1	2	0.0000000
C	1.4894176	1	116.2209272	1	0.4167652	1	23	22	1	0.0000000
N	2.0452939	1	94.6513215	1	177.0868046	1	1	2	5	0.0000000
C	1.3612146	1	125.0482400	1	-179.8330555	1	25	1	24	0.0000000
C	1.3956617	1	119.6200741	1	179.8367060	1	26	25	1	0.0000000

C	1.3967661	1	119.3789574	1	-0.0242309	1	27	26	25	0.0000000
C	1.4047409	1	119.3848690	1	179.8369268	1	24	25	23	0.0000000
H	1.0798462	1	122.0086747	1	-179.9938504	1	29	24	28	0.0000000
H	1.0823587	1	119.9125991	1	179.9656827	1	28	27	29	0.0000000
H	1.0822743	1	120.3046711	1	179.9592471	1	27	26	28	0.0000000
H	1.0789237	1	120.8782095	1	179.7515656	1	26	25	27	0.0000000
C	1.4047500	1	119.3836303	1	179.7108916	1	23	22	24	0.0000000
C	1.3975801	1	119.1084514	1	0.0174669	1	34	23	22	0.0000000
C	1.3967612	1	120.1207920	1	-0.0285283	1	35	34	23	0.0000000
C	1.3610629	1	125.0233241	1	-179.8543508	1	22	1	23	0.0000000
H	1.0789026	1	120.8839062	1	179.7403016	1	37	22	36	0.0000000
H	1.0822769	1	120.3158115	1	-179.9584592	1	36	35	37	0.0000000
H	1.0823598	1	119.9652938	1	-179.9517722	1	35	34	36	0.0000000
H	1.0798474	1	122.0091800	1	-179.9697995	1	34	23	35	0.0000000
N	2.0558934	1	94.3619249	1	-87.9419743	1	1	2	5	0.0000000
C	1.3625859	1	113.2401747	1	177.2774359	1	42	1	2	0.0000000
C	1.4827066	1	116.0330163	1	0.5455626	1	43	42	1	0.0000000
C	2.0204096	1	95.4005572	1	176.4707185	1	1	5	2	0.0000000
C	1.3975838	1	125.5270291	1	179.9725169	1	45	1	44	0.0000000
C	1.3980283	1	119.4399994	1	-179.9768773	1	46	45	1	0.0000000
C	1.4031440	1	120.1931326	1	-0.0040222	1	47	46	45	0.0000000
C	1.4053718	1	125.2404657	1	-179.8479556	1	44	43	45	0.0000000
H	1.0810862	1	121.0882126	1	-179.9862600	1	49	44	48	0.0000000
C	1.4390094	1	119.9032235	1	179.9614306	1	48	47	49	0.0000000
C	1.2054831	1	150.3876514	1	-179.9472646	1	51	47	48	0.0000000
C	1.4389197	1	160.0133558	1	-179.9329916	1	52	47	51	0.0000000
C	1.4011618	1	120.0743849	1	4.5260148	1	53	52	47	0.0000000
C	1.3987429	1	120.0748322	1	179.9995811	1	54	53	52	0.0000000
C	1.4011645	1	120.0748651	1	-0.0006719	1	55	54	53	0.0000000
C	1.4011812	1	119.8488945	1	0.0008437	1	56	55	54	0.0000000
C	1.4011455	1	120.0742671	1	179.9981800	1	53	52	54	0.0000000
H	1.0834620	1	120.4510972	1	-179.9987578	1	58	53	57	0.0000000
H	1.0834669	1	120.4515142	1	-179.9995594	1	57	56	58	0.0000000
C	1.4389938	1	120.0809460	1	179.9926392	1	56	55	57	0.0000000

C	1.2055594	1	150.4565776	1	-179.9563132	1	61	55	56	0.0000000
C	1.4389954	1	160.0467537	1	-179.9375064	1	62	55	61	0.0000000
C	1.4011610	1	120.0796797	1	2.5810442	1	63	62	55	0.0000000
C	1.3987512	1	120.0754351	1	179.9971359	1	64	63	62	0.0000000
C	1.4011714	1	120.0757704	1	0.0020567	1	65	64	63	0.0000000
C	1.4011645	1	119.8487123	1	0.0007441	1	66	65	64	0.0000000
C	1.4011772	1	120.0717483	1	-179.9988463	1	63	62	64	0.0000000
H	1.0834628	1	120.4516937	1	179.9981822	1	68	63	67	0.0000000
H	1.0834577	1	120.4510152	1	-179.9990342	1	67	66	68	0.0000000
C	1.4389909	1	120.0775786	1	-179.9979919	1	66	65	67	0.0000000
C	1.2055552	1	150.4530246	1	-179.9612679	1	71	65	66	0.0000000
C	1.4389829	1	160.0399720	1	-179.9551148	1	72	65	71	0.0000000
C	1.4005812	1	120.0901339	1	4.7874220	1	73	72	65	0.0000000
C	1.3983767	1	120.0644615	1	179.9203372	1	74	73	72	0.0000000
C	1.4040108	1	120.2201707	1	0.8822814	1	75	74	73	0.0000000
S	1.8160865	1	121.3237003	1	-177.9365261	1	76	75	74	0.0000000
C	1.8208872	1	98.6967659	1	-50.4985577	1	77	76	75	0.0000000
O	1.2213811	1	121.0551959	1	-17.5485842	1	78	77	76	0.0000000
C	1.4949173	1	119.5751200	1	-177.6772190	1	78	77	79	0.0000000
H	1.1100907	1	109.6081767	1	-121.3324882	1	80	78	77	0.0000000
H	1.1100474	1	110.5431406	1	119.9803638	1	80	78	81	0.0000000
H	1.1101319	1	109.6715285	1	-119.9654781	1	80	78	81	0.0000000
C	1.4003306	1	119.0473623	1	-175.7424095	1	76	77	75	0.0000000
C	1.4006065	1	120.0907831	1	179.4749140	1	73	72	74	0.0000000
H	1.0834547	1	120.4570758	1	179.7706631	1	85	73	84	0.0000000
H	1.0826155	1	120.1493709	1	179.5141356	1	84	76	85	0.0000000
H	1.0823537	1	119.3363063	1	-179.1974959	1	75	74	76	0.0000000
H	1.0834597	1	120.4569067	1	-179.5137071	1	74	73	75	0.0000000
H	1.0834669	1	119.4729973	1	-179.9994331	1	65	64	66	0.0000000
H	1.0834614	1	120.4506109	1	-179.9979107	1	64	63	65	0.0000000
H	1.0834557	1	119.4737435	1	-179.9998415	1	55	54	56	0.0000000
H	1.0834699	1	120.4510832	1	179.9992015	1	54	53	55	0.0000000
H	1.0834240	1	119.3939619	1	179.9506849	1	47	46	48	0.0000000
H	1.0795844	1	120.9293319	1	179.7729082	1	46	45	47	0.0000000

C	1.4043933	1	119.5987855	1	179.7050372	1	43	42	44	0.0000000
C	1.3971079	1	119.0757161	1	0.0535065	1	96	43	42	0.0000000
C	1.3964591	1	120.0706342	1	-0.0180720	1	97	96	43	0.0000000
C	1.3617198	1	124.6177274	1	-179.6425230	1	42	1	43	0.0000000
H	1.0786556	1	120.9099221	1	179.7410746	1	99	42	98	0.0000000
H	1.0822837	1	120.3084749	1	-179.9721043	1	98	97	99	0.0000000
H	1.0823541	1	119.9881338	1	-179.9672901	1	97	96	98	0.0000000
H	1.0800207	1	121.9629850	1	-179.9773959	1	96	43	97	0.0000000

Transition : 529.5 nm

```

Spin Up :  Occ. MO  -->  Unocc. MO  Coefficients
-----
          152  -->   156             0.409549
          151  -->   156          -0.458319

```

```

Spin Down:  Occ. MO  -->  Unocc. MO  Coefficients
-----
          152  -->   156          -0.409549
          151  -->   156             0.458319

```

Transition : 475.1 nm

```

Spin Up :  Occ. MO  -->  Unocc. MO  Coefficients
-----
          152  -->   157             0.461652
          151  -->   157          -0.328497

```

```

Spin Down:  Occ. MO  -->  Unocc. MO  Coefficients
-----

```


152	-->	157	-0.461652
151	-->	157	0.328497

Orbital 151

Orbital 152

Orbital 156

Orbital 157

Computed total energy of the optimised structure : 139.2 kcal/mol

Z-matrix of molecule **12**

Ru	0.0000000	0	0.0000000	0	0.0000000	0	0	0	0	0.0000000
N	2.0467509	1	0.0000000	0	0.0000000	0	1	0	0	0.0000000
C	1.3630643	1	112.8249487	1	0.0000000	0	2	1	0	0.0000000
C	1.4881193	1	116.2053987	1	0.4670355	1	3	2	1	0.0000000
N	2.0525247	1	82.1320911	1	-0.1925934	1	1	2	3	0.0000000
C	1.3622923	1	125.1930926	1	-179.7101013	1	5	1	4	0.0000000
C	1.3956045	1	119.7049417	1	179.7641018	1	6	5	1	0.0000000
C	1.3961584	1	119.3949288	1	-0.0578365	1	7	6	5	0.0000000
C	1.4049752	1	119.4584621	1	179.7964482	1	4	5	3	0.0000000
H	1.0797867	1	122.0320873	1	179.9973140	1	9	4	8	0.0000000
H	1.0823676	1	119.9268763	1	179.9709019	1	8	7	9	0.0000000
H	1.0822944	1	120.3018840	1	179.9619308	1	7	6	8	0.0000000
H	1.0787076	1	121.0451993	1	179.6946476	1	6	5	7	0.0000000
C	1.4050084	1	119.4017640	1	179.7941329	1	3	2	4	0.0000000
C	1.3974150	1	119.1216781	1	0.0661564	1	14	3	2	0.0000000
C	1.3965097	1	120.1059465	1	0.0033426	1	15	14	3	0.0000000
C	1.3613339	1	124.8358889	1	-179.5743002	1	2	1	3	0.0000000
H	1.0788447	1	120.8874076	1	179.7165825	1	17	2	16	0.0000000
H	1.0822811	1	120.3181990	1	-179.9767466	1	16	15	17	0.0000000
H	1.0823637	1	119.9737053	1	-179.9923456	1	15	14	16	0.0000000
H	1.0797870	1	122.0376823	1	179.9889447	1	14	3	15	0.0000000
N	2.0444491	1	88.5012597	1	94.8279260	1	1	2	5	0.0000000
C	1.3635230	1	112.5893584	1	94.6968096	1	22	1	2	0.0000000
C	1.4894181	1	116.2208908	1	0.4173786	1	23	22	1	0.0000000
N	2.0452947	1	94.6513424	1	177.0866453	1	1	2	5	0.0000000

C	1.3612143	1	125.0482151	1	-179.8332063	1	25	1	24	0.0000000
C	1.3956633	1	119.6200307	1	179.8372359	1	26	25	1	0.0000000
C	1.3967649	1	119.3789551	1	-0.0243590	1	27	26	25	0.0000000
C	1.4047418	1	119.3848039	1	179.8366439	1	24	25	23	0.0000000
H	1.0798463	1	122.0085923	1	-179.9937788	1	29	24	28	0.0000000
H	1.0823601	1	119.9126854	1	179.9655068	1	28	27	29	0.0000000
H	1.0822744	1	120.3047389	1	179.9594665	1	27	26	28	0.0000000
H	1.0789243	1	120.8783913	1	179.7515121	1	26	25	27	0.0000000
C	1.4047492	1	119.3837671	1	179.7118003	1	23	22	24	0.0000000
C	1.3975804	1	119.1083510	1	0.0172959	1	34	23	22	0.0000000
C	1.3967602	1	120.1207906	1	-0.0283745	1	35	34	23	0.0000000
C	1.3610640	1	125.0233724	1	-179.8529645	1	22	1	23	0.0000000
H	1.0789030	1	120.8838315	1	179.7408070	1	37	22	36	0.0000000
H	1.0822763	1	120.3158021	1	-179.9585451	1	36	35	37	0.0000000
H	1.0823595	1	119.9652522	1	-179.9521290	1	35	34	36	0.0000000
H	1.0798465	1	122.0091809	1	-179.9699798	1	34	23	35	0.0000000
N	2.0558968	1	94.3617185	1	-87.9421967	1	1	2	5	0.0000000
C	1.3625840	1	113.2401999	1	177.2776123	1	42	1	2	0.0000000
C	1.4827055	1	116.0329877	1	0.5448548	1	43	42	1	0.0000000
C	2.0204120	1	95.4000886	1	176.4704579	1	1	5	2	0.0000000
C	1.3975876	1	125.5274000	1	179.9712923	1	45	1	44	0.0000000
C	1.3980301	1	119.4401298	1	-179.9759003	1	46	45	1	0.0000000
C	1.4031418	1	120.1929081	1	-0.0061945	1	47	46	45	0.0000000
C	1.4053683	1	125.2402533	1	-179.8480863	1	44	43	45	0.0000000
H	1.0810904	1	121.0880014	1	-179.9876185	1	49	44	48	0.0000000
C	1.4390102	1	119.9041774	1	179.9613706	1	48	47	49	0.0000000
C	1.2054806	1	150.4019410	1	179.9749445	1	51	47	48	0.0000000
C	1.4389184	1	160.0514134	1	179.9160842	1	52	47	51	0.0000000
C	1.4011503	1	120.0769858	1	1.8540666	1	53	52	47	0.0000000
C	1.3987408	1	120.0742263	1	179.9988534	1	54	53	52	0.0000000
C	1.4011828	1	120.0752337	1	0.0011026	1	55	54	53	0.0000000
C	1.4011613	1	119.8490095	1	-0.0007166	1	56	55	54	0.0000000
C	1.4011552	1	120.0715112	1	179.9999243	1	53	52	54	0.0000000
H	1.0834666	1	120.4511542	1	179.9991778	1	58	53	57	0.0000000

H	1.0834625	1	120.4511824	1	179.9997190	1	57	56	58	0.0000000
C	1.4389930	1	120.0748562	1	179.9995114	1	56	55	57	0.0000000
C	1.2055586	1	150.4592278	1	179.9437256	1	61	55	56	0.0000000
C	1.4389923	1	160.0560467	1	179.9141098	1	62	55	61	0.0000000
C	1.4011671	1	120.0755322	1	1.7964999	1	63	62	55	0.0000000
C	1.3987434	1	120.0759976	1	-179.9999385	1	64	63	62	0.0000000
C	1.4011652	1	120.0756896	1	0.0002715	1	65	64	63	0.0000000
C	1.4011738	1	119.8485457	1	-0.0005078	1	66	65	64	0.0000000
C	1.4011719	1	120.0759356	1	179.9998187	1	63	62	64	0.0000000
H	1.0834608	1	120.4511405	1	-179.9996074	1	68	63	67	0.0000000
H	1.0834615	1	120.4510823	1	179.9992904	1	67	66	68	0.0000000
C	1.4389938	1	120.0758568	1	179.9986070	1	66	65	67	0.0000000
C	1.2055580	1	150.4632933	1	179.9398568	1	71	65	66	0.0000000
C	1.4389950	1	160.0603346	1	179.9128663	1	72	65	71	0.0000000
C	1.4011751	1	120.0752479	1	0.8644842	1	73	72	65	0.0000000
C	1.3987446	1	120.0752217	1	179.9992433	1	74	73	72	0.0000000
C	1.4011758	1	120.0754925	1	-0.0001851	1	75	74	73	0.0000000
C	1.4011563	1	119.8490274	1	0.0004451	1	76	75	74	0.0000000
C	1.4011607	1	120.0759582	1	179.9991273	1	73	72	74	0.0000000
H	1.0834670	1	120.4511693	1	179.9997902	1	78	73	77	0.0000000
H	1.0834631	1	120.4513170	1	-179.9988523	1	77	76	78	0.0000000
C	1.4389835	1	120.0743975	1	-179.9963332	1	76	75	77	0.0000000
C	1.2055437	1	150.4610964	1	179.9370012	1	81	75	76	0.0000000
C	1.4389237	1	160.0570360	1	179.9162543	1	82	75	81	0.0000000
C	1.4012688	1	120.0766787	1	1.0190667	1	83	82	75	0.0000000
C	1.3984251	1	120.0455945	1	179.9426431	1	84	83	82	0.0000000
C	1.4001738	1	120.0922085	1	-0.4449077	1	85	84	83	0.0000000
S	1.8087417	1	120.0424825	1	179.5203232	1	86	85	84	0.0000000
C	1.8235709	1	98.5003597	1	91.6532789	1	87	86	85	0.0000000
O	1.2205550	1	118.0074515	1	179.5343255	1	88	87	86	0.0000000
C	1.5019450	1	123.1129797	1	179.8764586	1	88	87	89	0.0000000
H	1.1093996	1	109.9161470	1	-60.1155271	1	90	88	87	0.0000000
H	1.1093147	1	109.9389274	1	120.9933944	1	90	88	91	0.0000000
H	1.1110220	1	110.5593977	1	-119.5109148	1	90	88	91	0.0000000

C	1.4002562	1	120.0693676	1	178.4506149	1	86	87	85	0.0000000
C	1.4012718	1	120.0763537	1	-179.8799240	1	83	82	84	0.0000000
H	1.0834139	1	120.4734677	1	-179.9667117	1	95	83	94	0.0000000
H	1.0825108	1	120.1878688	1	-179.5569884	1	94	86	95	0.0000000
H	1.0825102	1	119.7174660	1	-179.5571525	1	85	84	86	0.0000000
H	1.0834202	1	120.4724420	1	179.9678172	1	84	83	85	0.0000000
H	1.0834619	1	119.4734266	1	-179.9989450	1	75	74	76	0.0000000
H	1.0834573	1	120.4512714	1	-179.9997203	1	74	73	75	0.0000000
H	1.0834640	1	119.4732424	1	179.9992212	1	65	64	66	0.0000000
H	1.0834633	1	120.4509722	1	179.9997530	1	64	63	65	0.0000000
H	1.0834604	1	119.4729390	1	179.9995532	1	55	54	56	0.0000000
H	1.0834659	1	120.4511849	1	-179.9990122	1	54	53	55	0.0000000
H	1.0834237	1	119.3942265	1	179.9529115	1	47	46	48	0.0000000
H	1.0795850	1	120.9291382	1	179.7722058	1	46	45	47	0.0000000
C	1.4043933	1	119.5988532	1	179.7051008	1	43	42	44	0.0000000
C	1.3971065	1	119.0757446	1	0.0537104	1	108	43	42	0.0000000
C	1.3964596	1	120.0706101	1	-0.0182705	1	109	108	43	0.0000000
C	1.3617197	1	124.6177914	1	-179.6430133	1	42	1	43	0.0000000
H	1.0786587	1	120.9099350	1	179.7412872	1	111	42	110	0.0000000
H	1.0822837	1	120.3084708	1	-179.9728623	1	110	109	111	0.0000000
H	1.0823534	1	119.9881634	1	-179.9674854	1	109	108	110	0.0000000
H	1.0800190	1	121.9630349	1	-179.9773519	1	108	43	109	0.0000000

Transition : 527.7 nm

Spin Up : Occ. MO --> Unocc. MO Coefficients

```

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                170 --> 174                0.402782
                169 --> 174               -0.382969

```

Spin Down: Occ. MO --> Unocc. MO Coefficients

```

-----
                170 --> 174               -0.402782
                169 --> 174                0.382969

```

Transition : 473.7 nm

Spin Up : Occ. MO --> Unocc. MO Coefficients

170 --> 175 0.460003

Spin Down: Occ. MO --> Unocc. MO Coefficients

170 --> 175 -0.460003

Orbital 169

Orbital 170

Orbital 174

Orbital 175