Optically active Ag(I):o-OPE helicates using a single homochiral sulfoxide as chiral inducer

Sandra Resa,[a]Pablo Reiné,[a] Luis Álvarez de Cienfuegos,[a] Santiago Guisán-Ceinos,[b] María Ribagorda,[b]Giovanna Longhi,[c]GiuseppeMazzeo,[c] Sergio Abbate,[c] Antonio J. Mota,[d]Delia Miguel,[e*]and Juan M. Cuerva[a*]

[a] *Department of Organic Chemistry. University of Granada. C.U. Fuentenueva. Granada, Spain. Unidad de excelencia de Química (UEQ)*

[b]*Department of Organic Chemistry. C.U. Cantoblanco, Universidad Autónoma de Madrid, Spain*[c] *Dipartimento di Medicina Molecolare e Traslazionale, Universitá di Brescia, Viale Europa 11, Brescia, Italy*

[d] *Department of Inorganic Chemistry. University of Granada. C.U. Fuentenueva. Granada, Spain, UEQ*

[e] *Department of Physical Chemistry. University of Granada. C.U. Cartuja. Granada, Spain, UEQ*

jmcuerva@ugr.es, dmalvarez@ugr.es

-Supporting Information -

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^{1}H and ^{13}C NMR spectra of new compounds

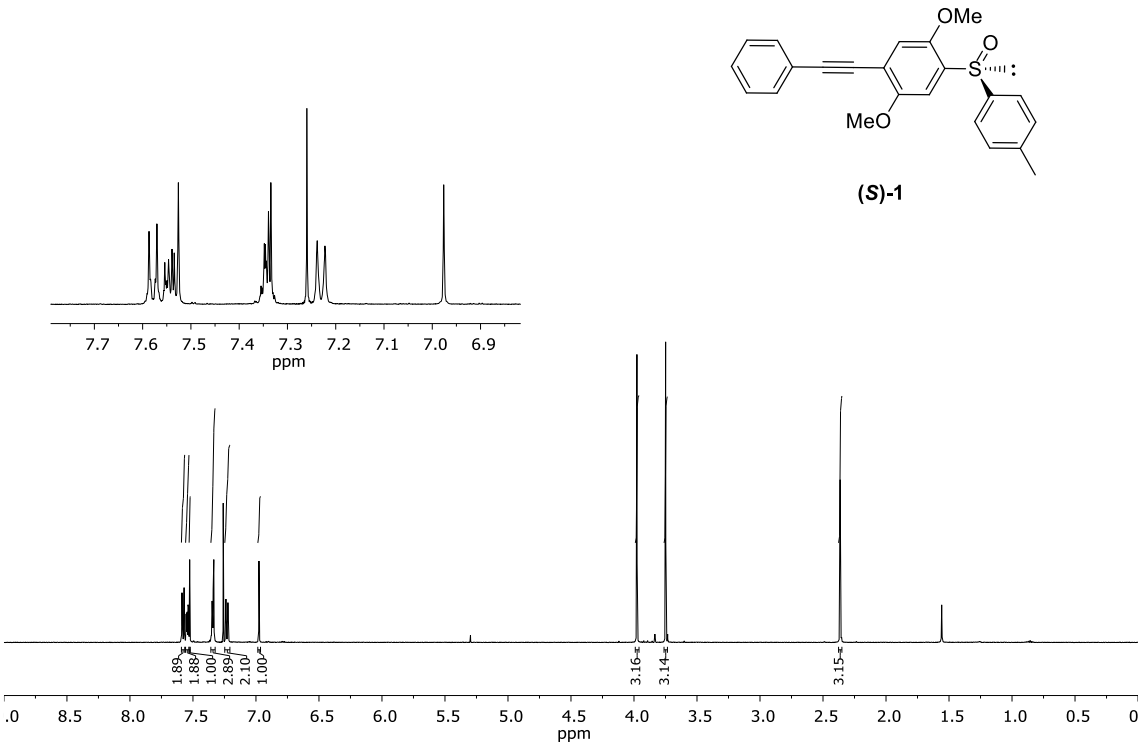


Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound (*S*)-**1**.

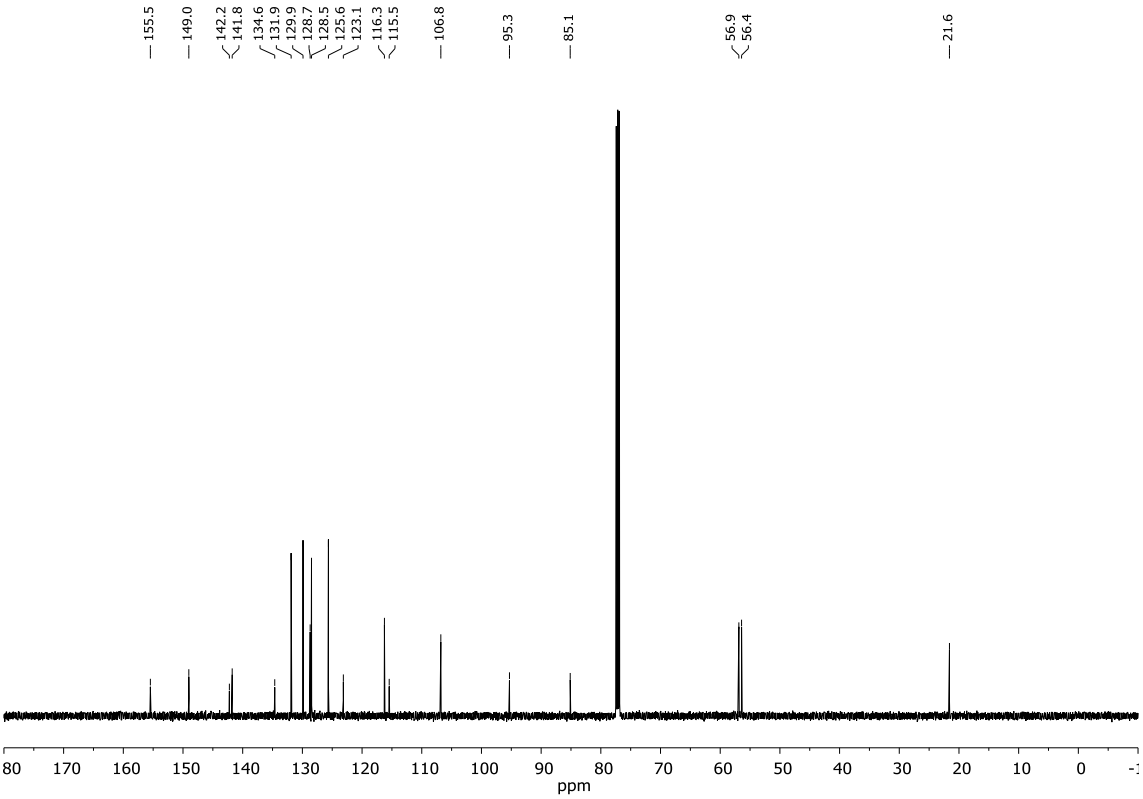


Figure S2. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (*S*)-**1**.

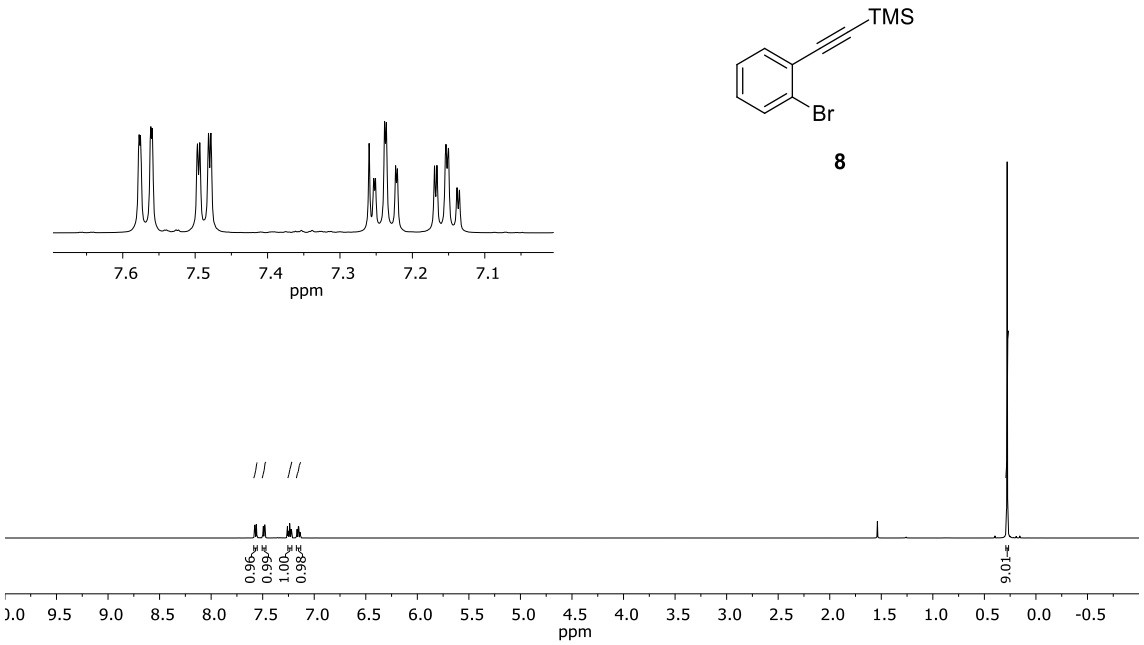


Figure S3. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **8.**

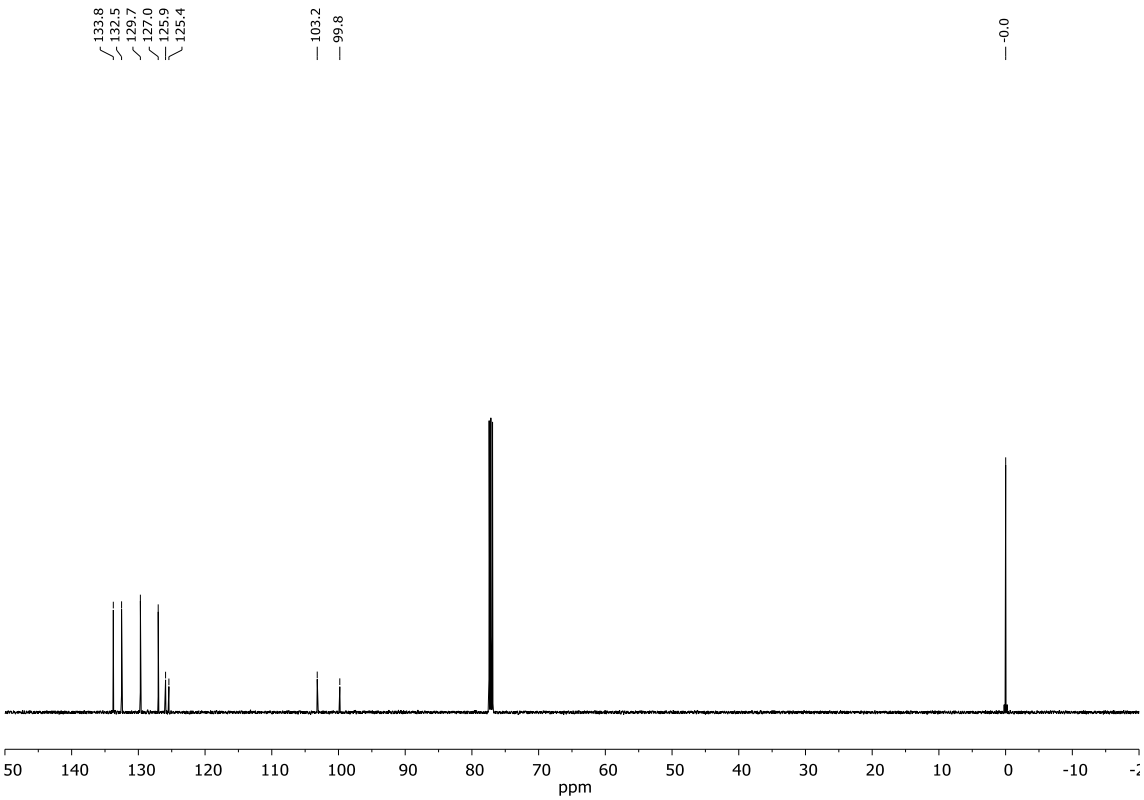


Figure S4. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **8**.

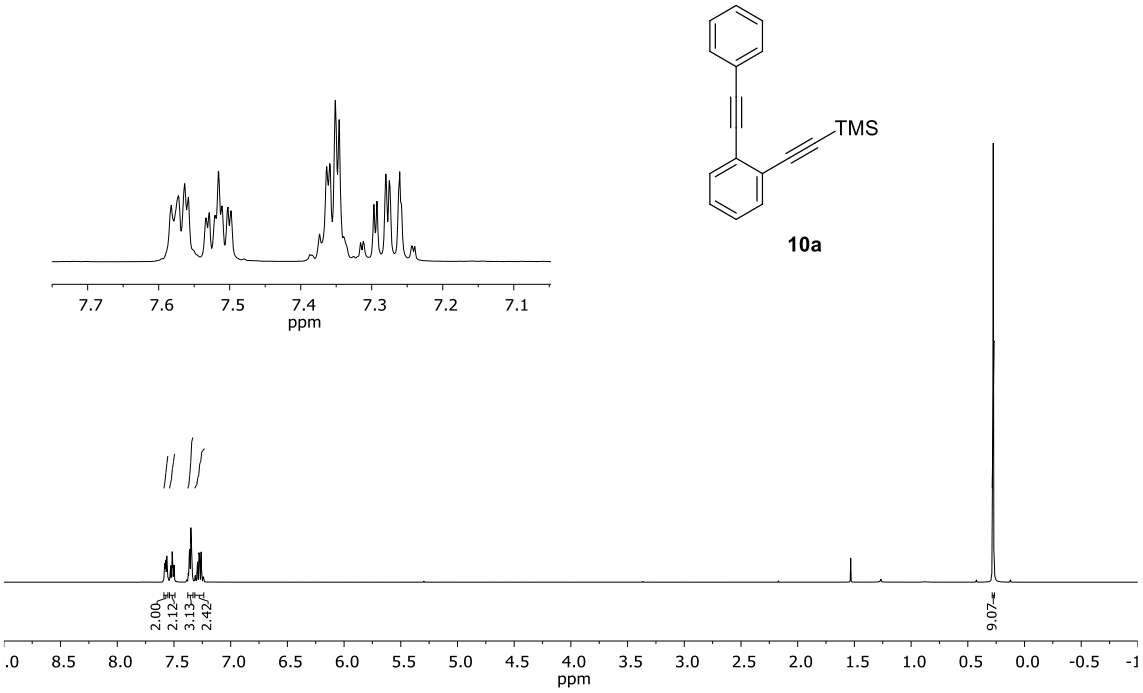


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10a**.

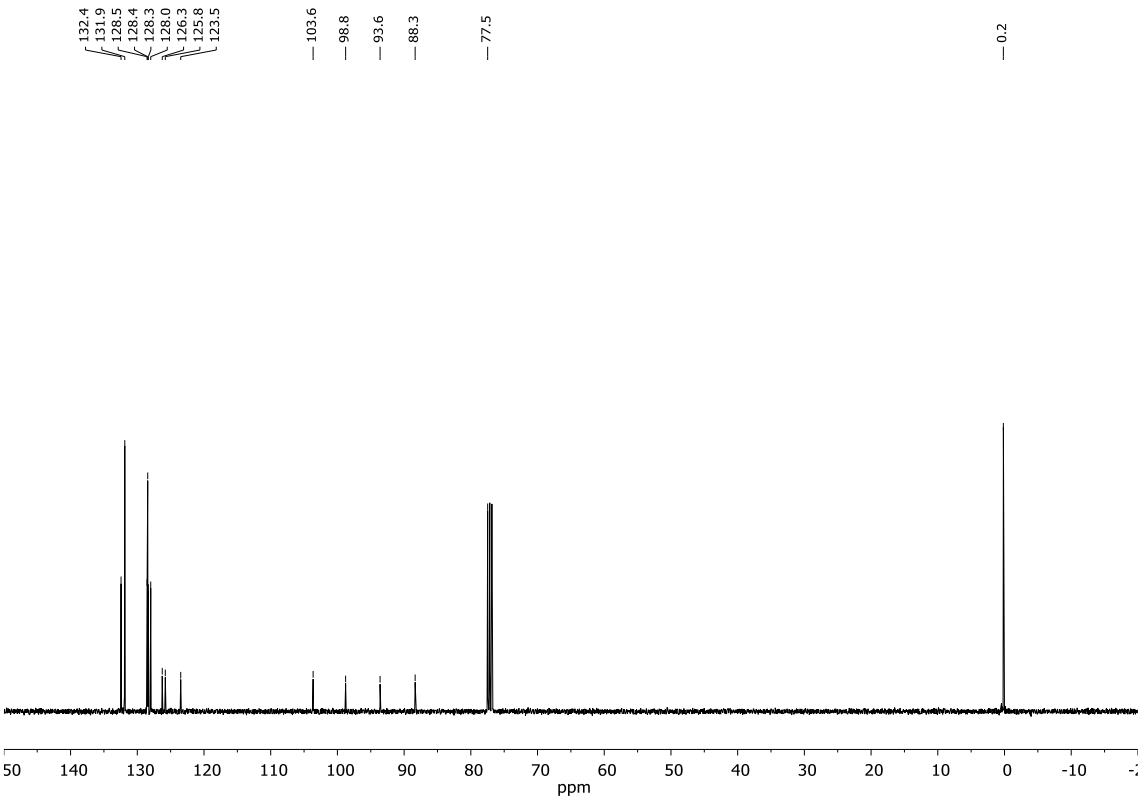


Figure S6. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **10a**.

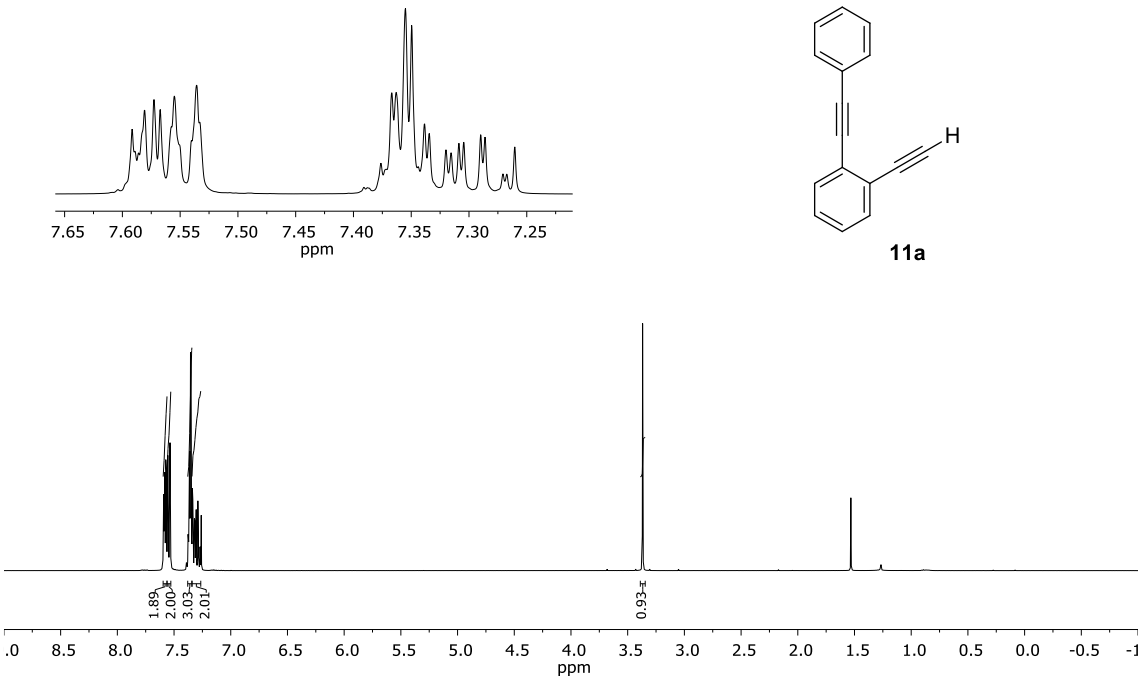


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11a**.

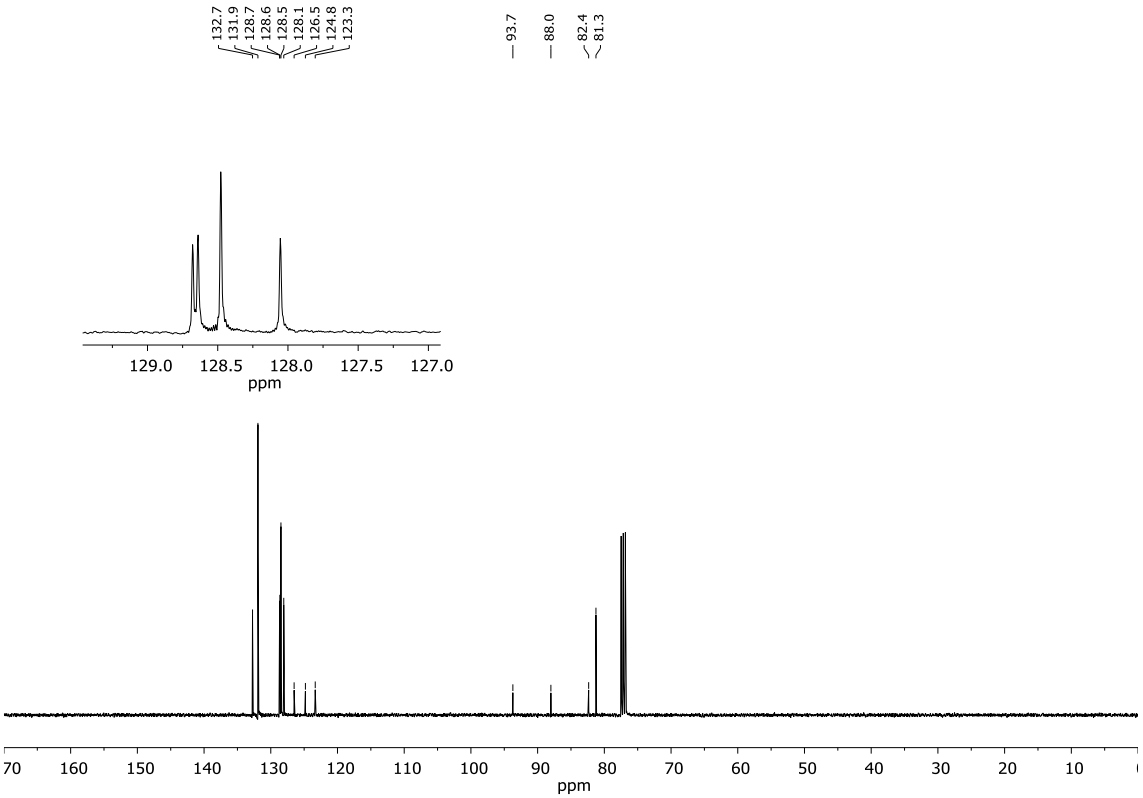


Figure S8. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **11a**.

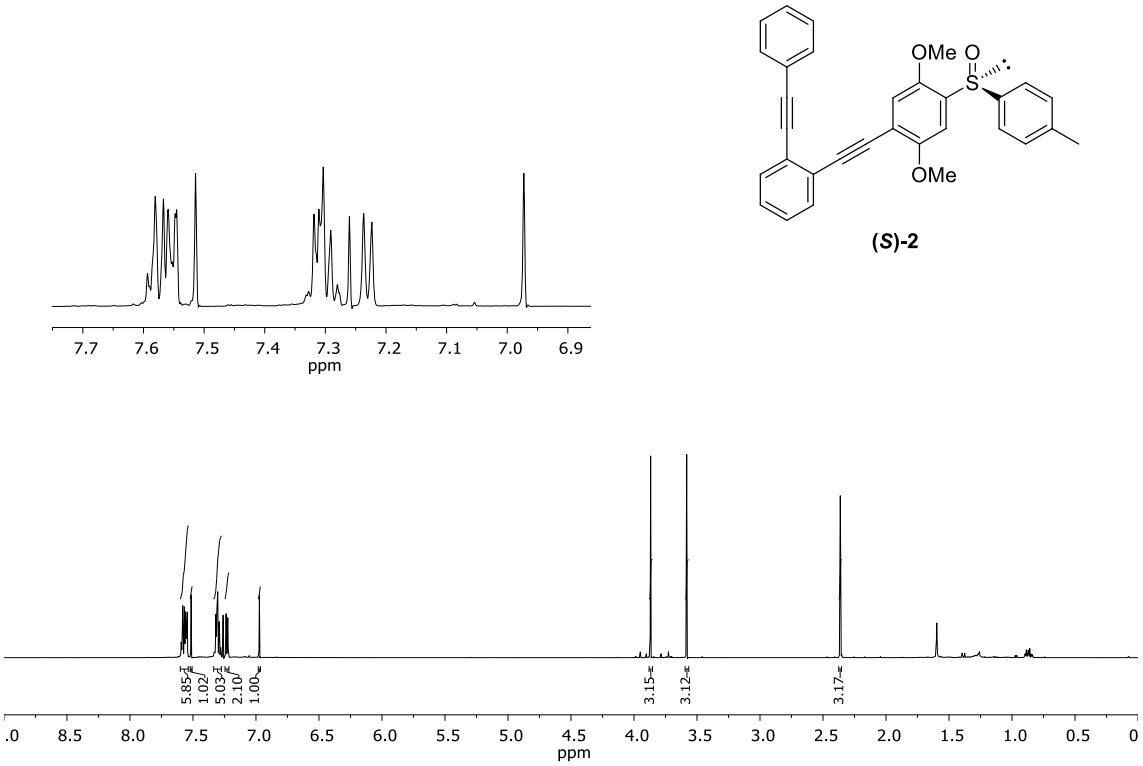


Figure S9. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound (*S*)-**2**.

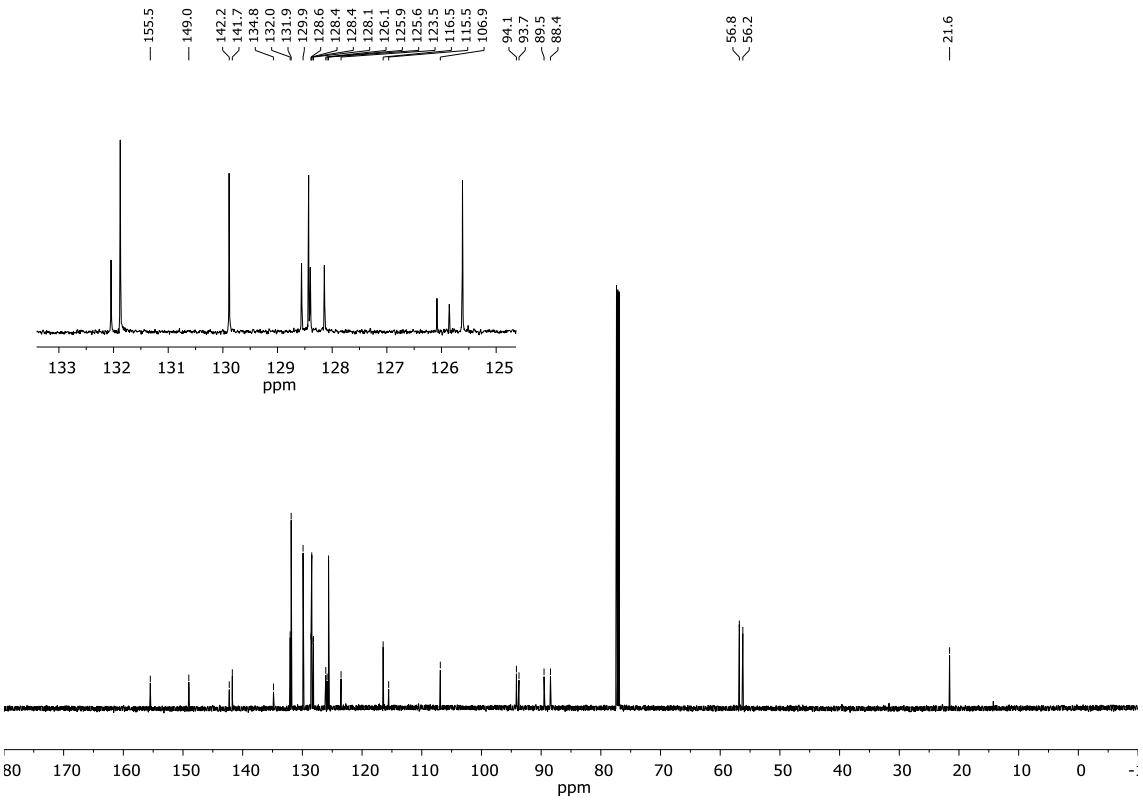


Figure S10. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound (*S*)-**2**.

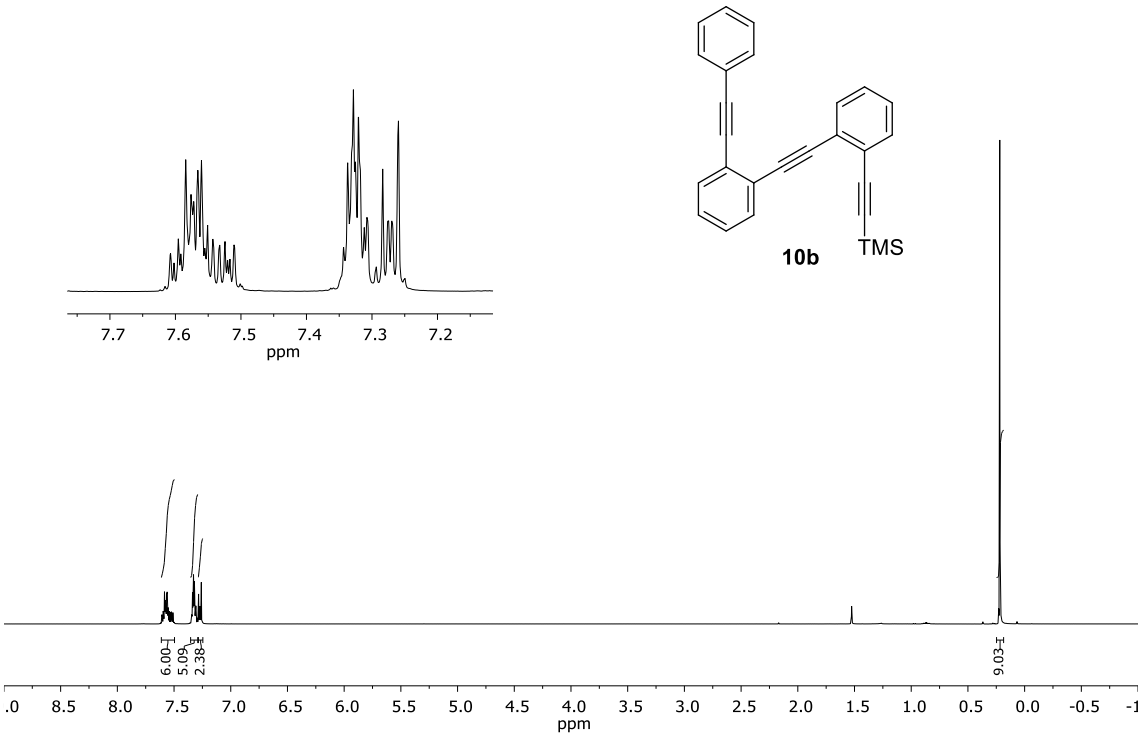
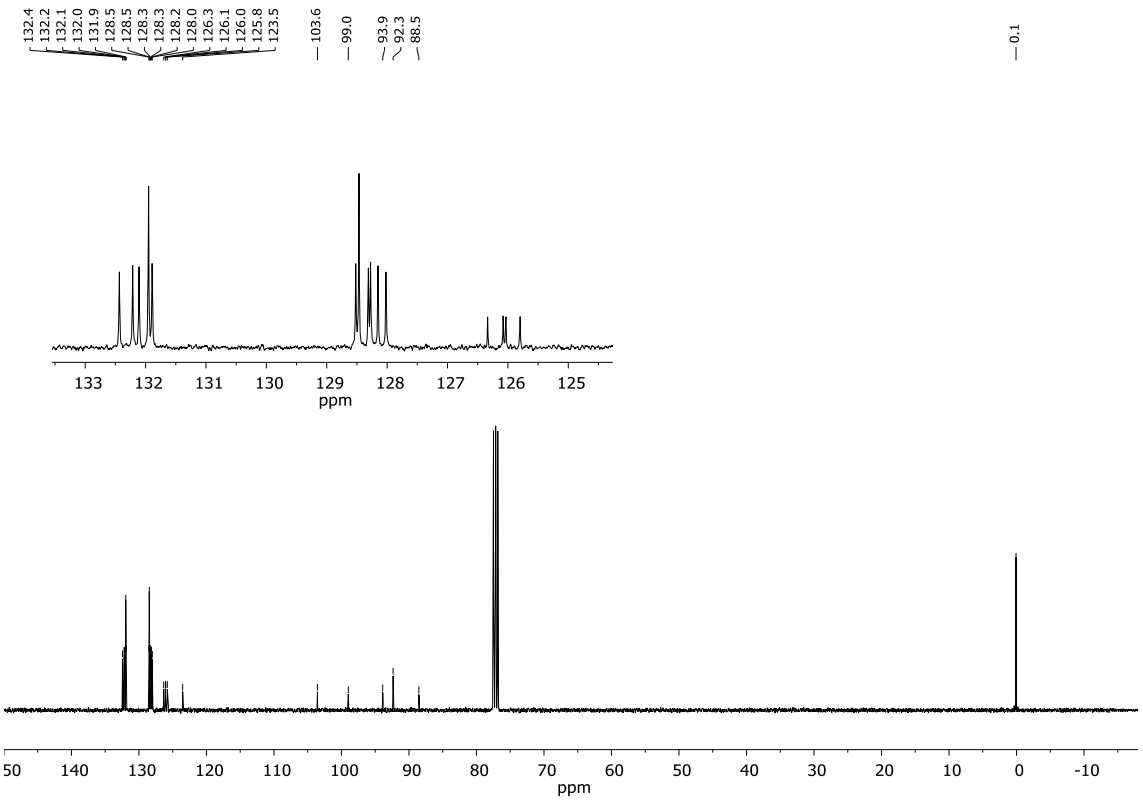


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10b**



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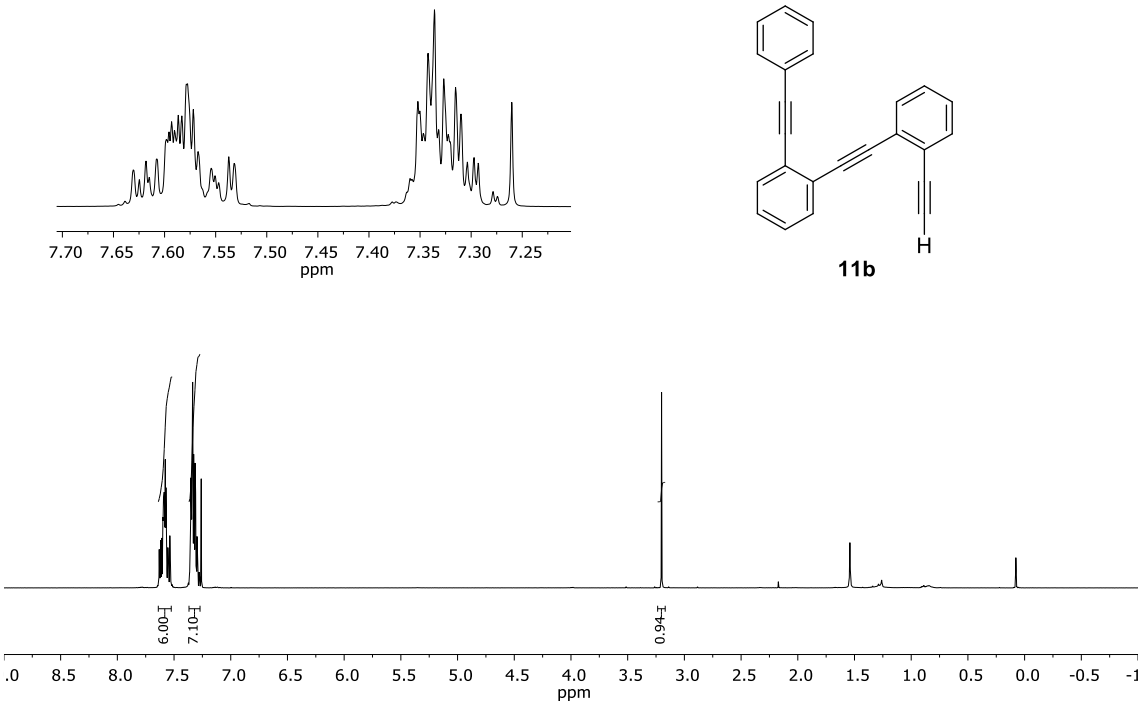


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11b**

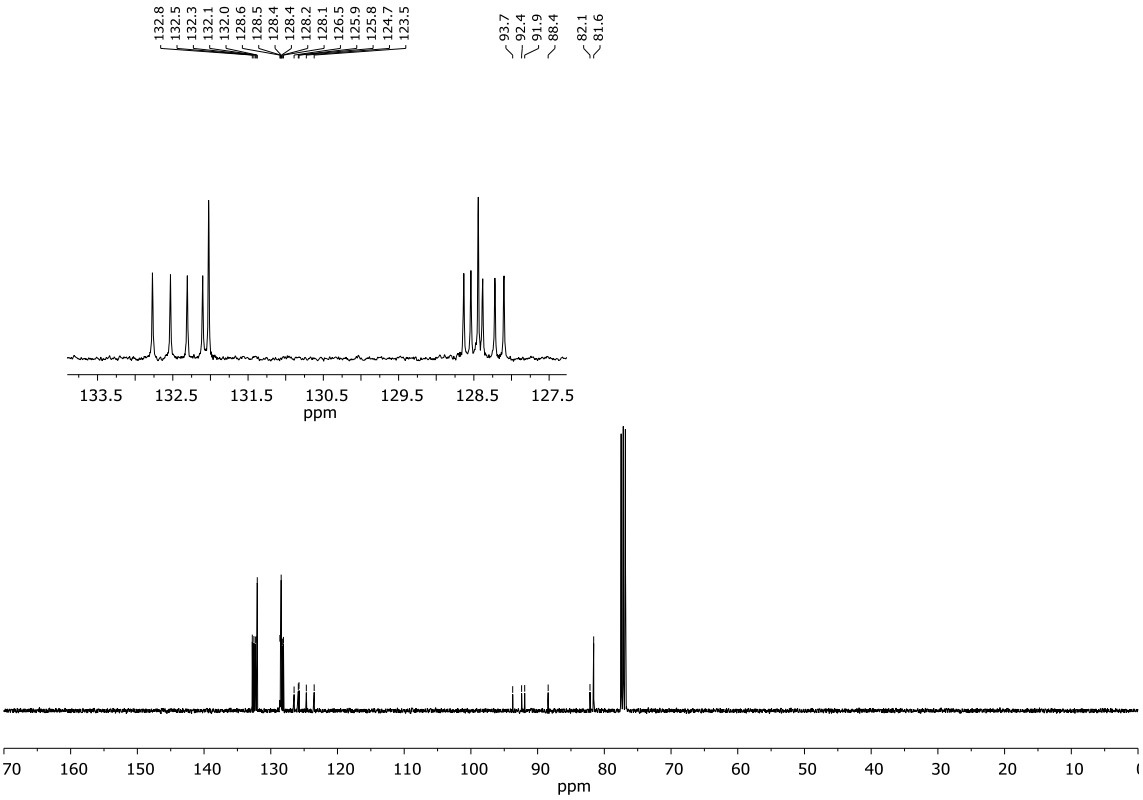


Figure S14. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **11b**.

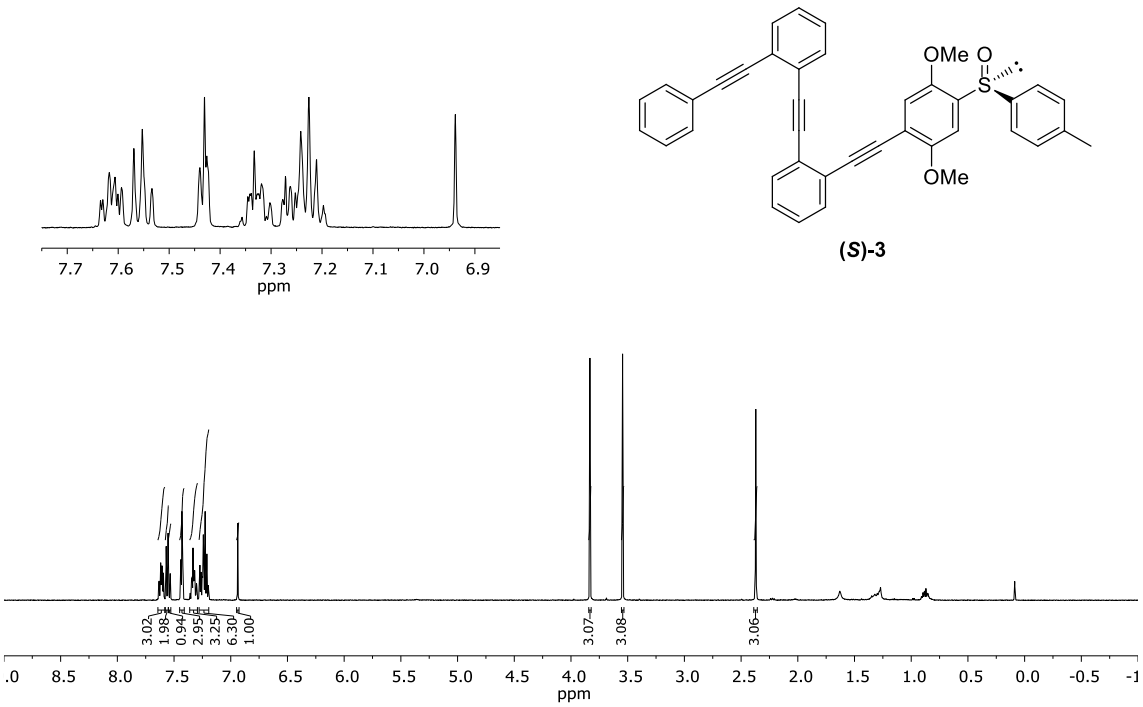


Figure S15. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound (*S*)-**3**.

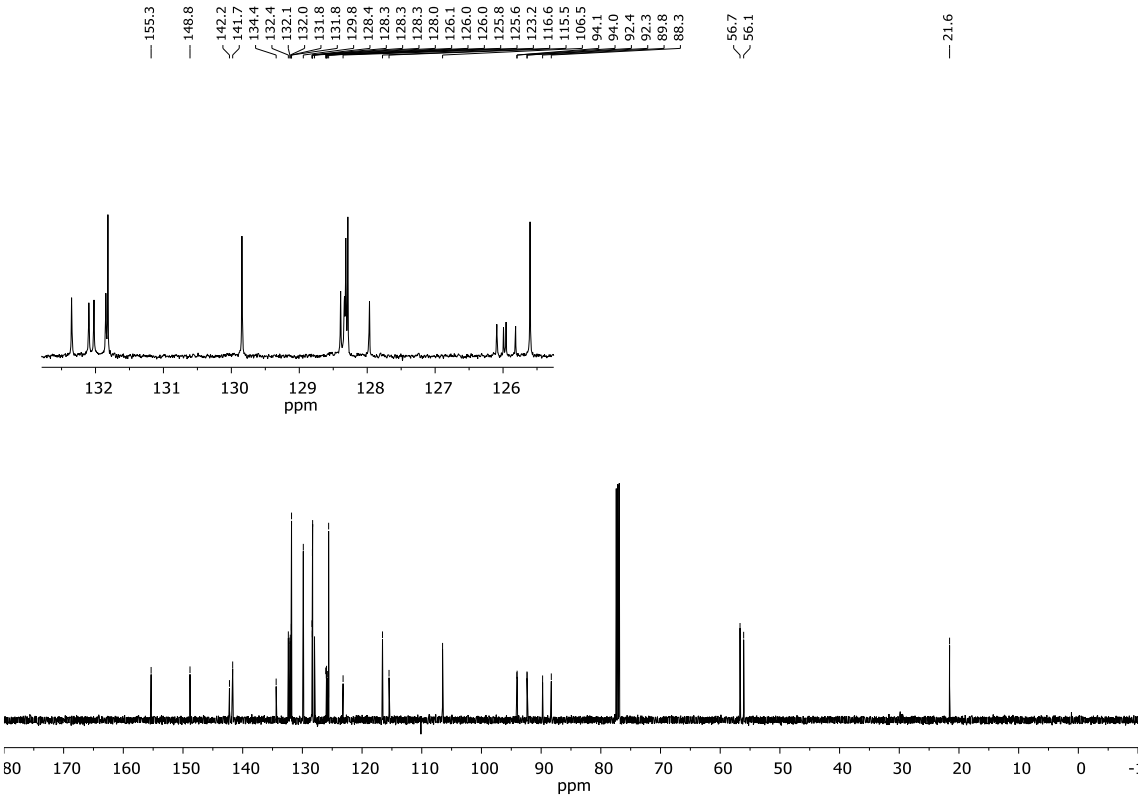


Figure S16. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (*S*)-**3**.

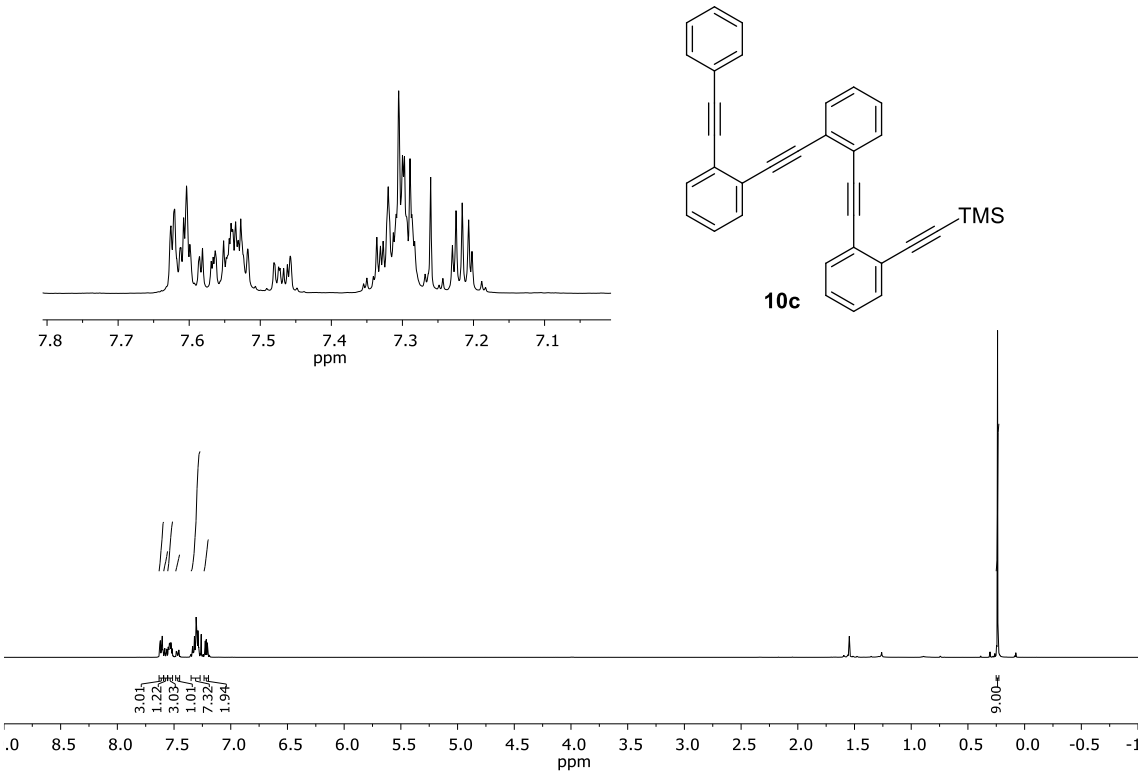
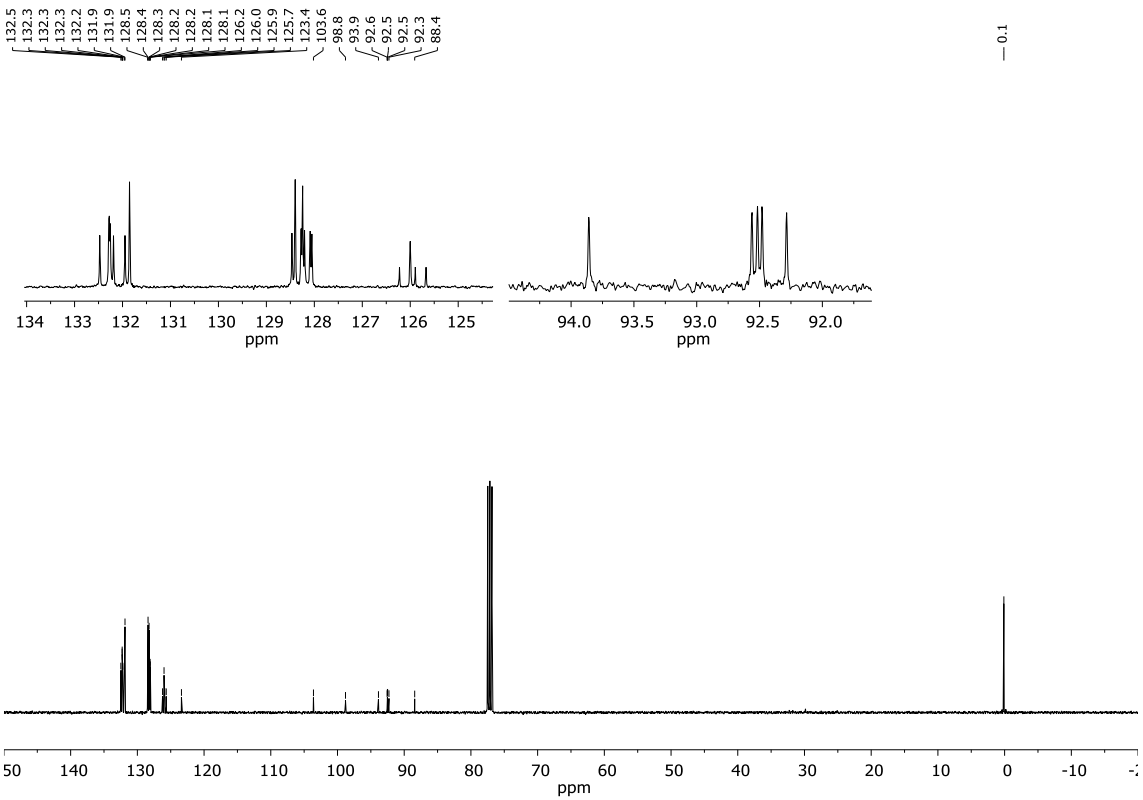


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10c**.



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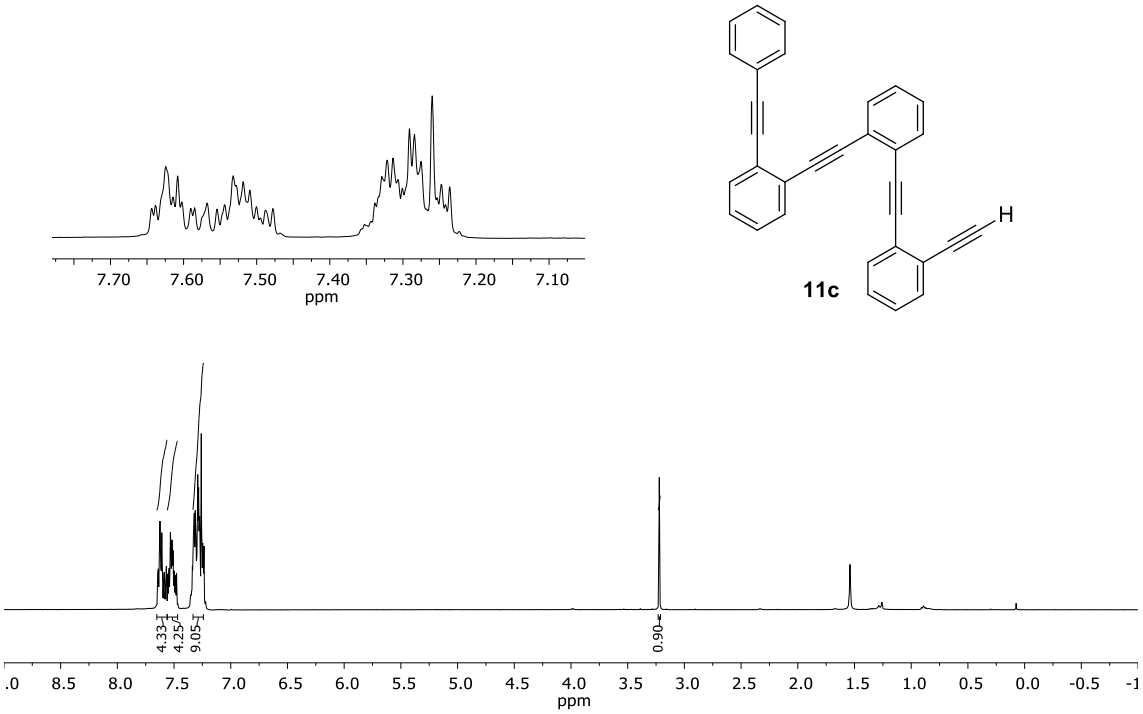


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11c**.

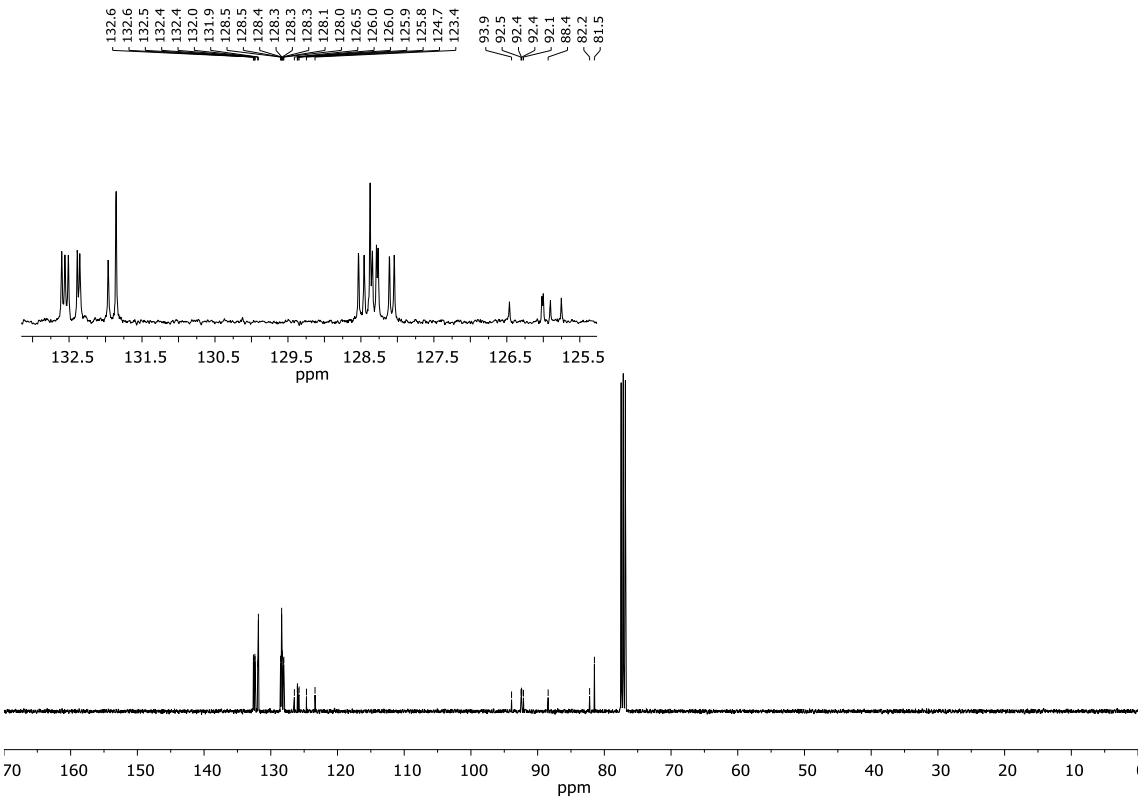


Figure S20. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **11c**.

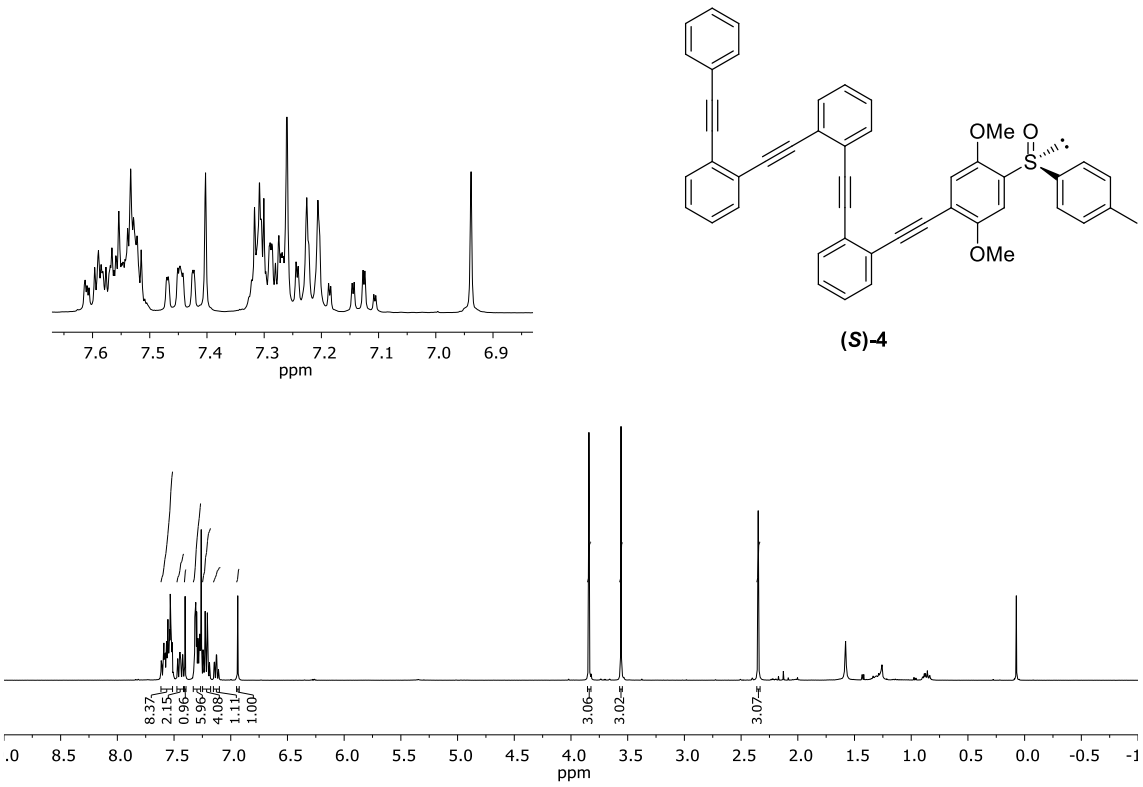


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound (*S*)-**4**.

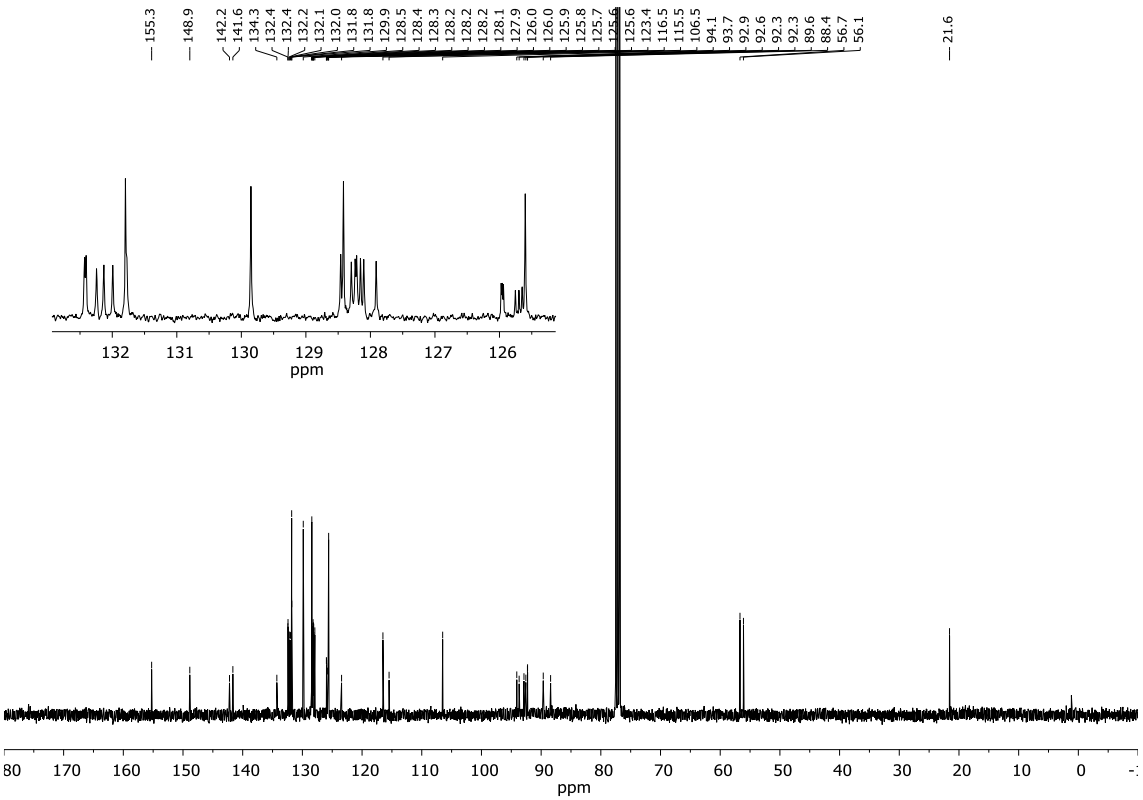


Figure S22. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound (*S*)-**4**.

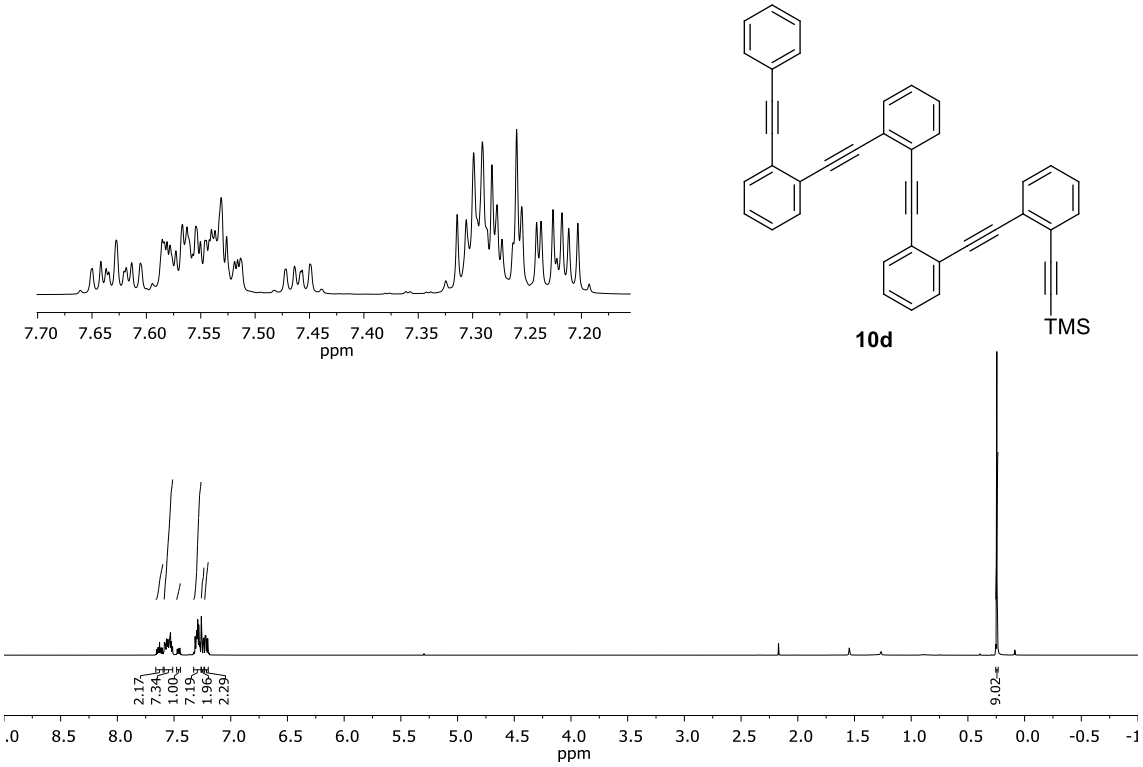


Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10d**.

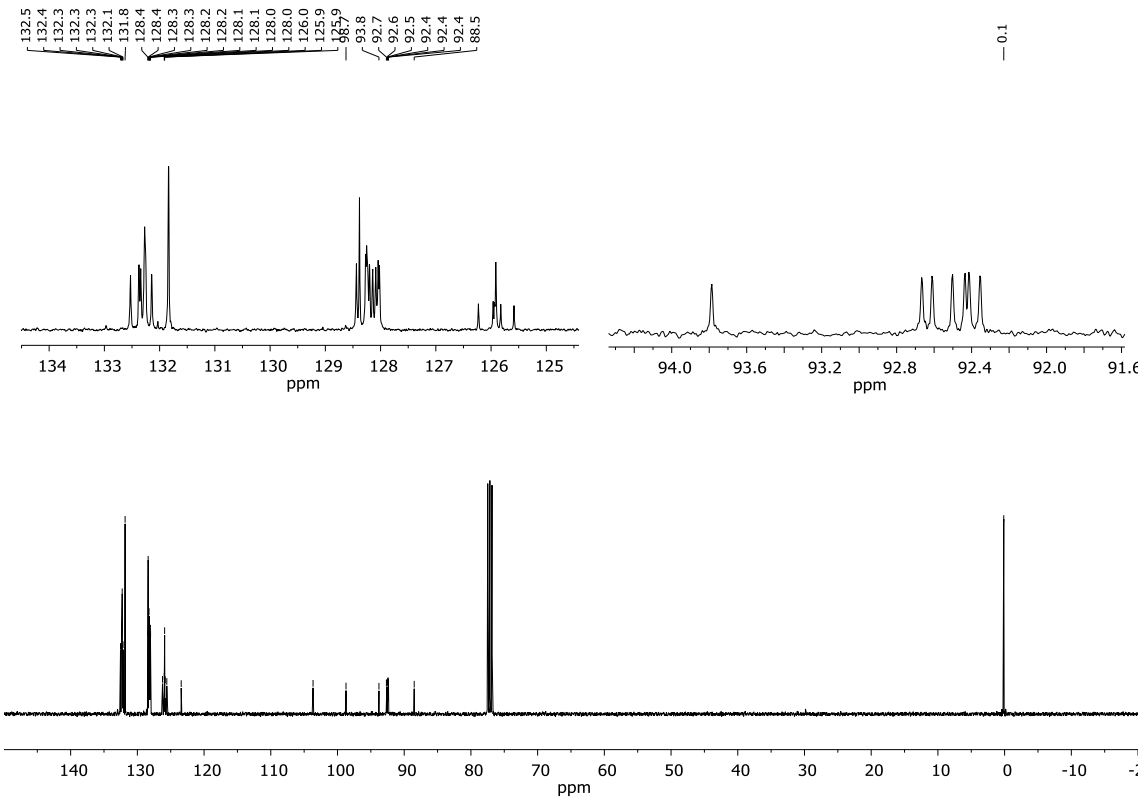


Figure S24. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **10d**.

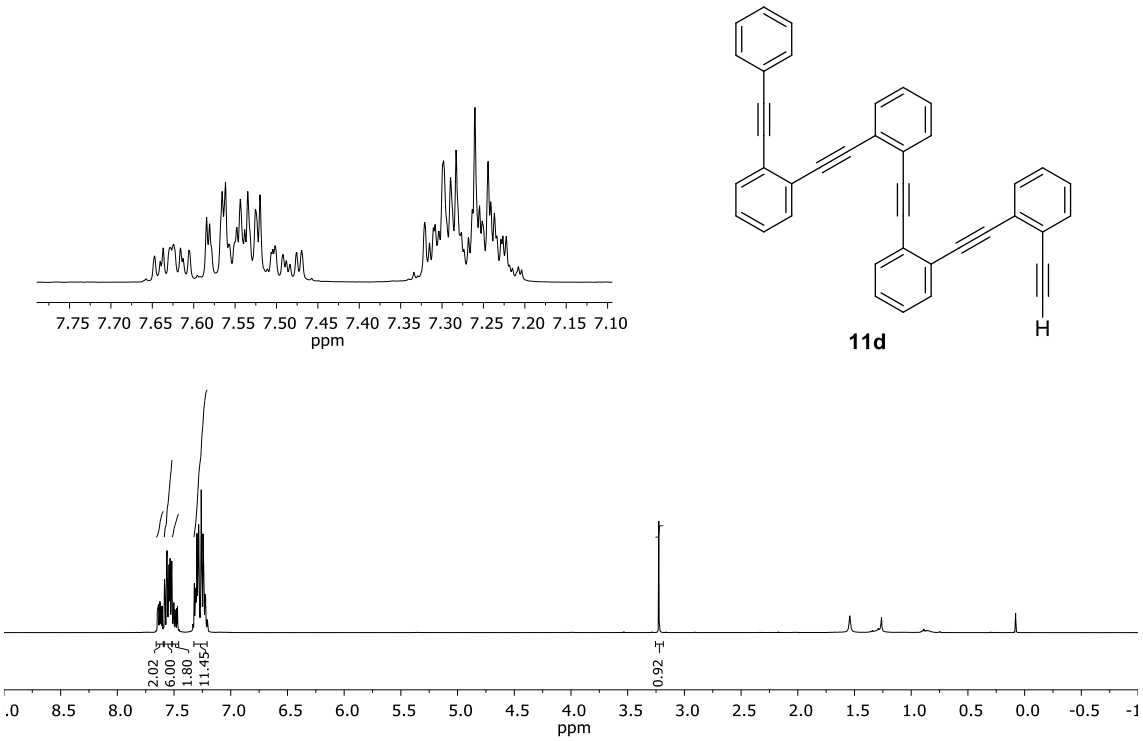


Figure S25. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **11d**.

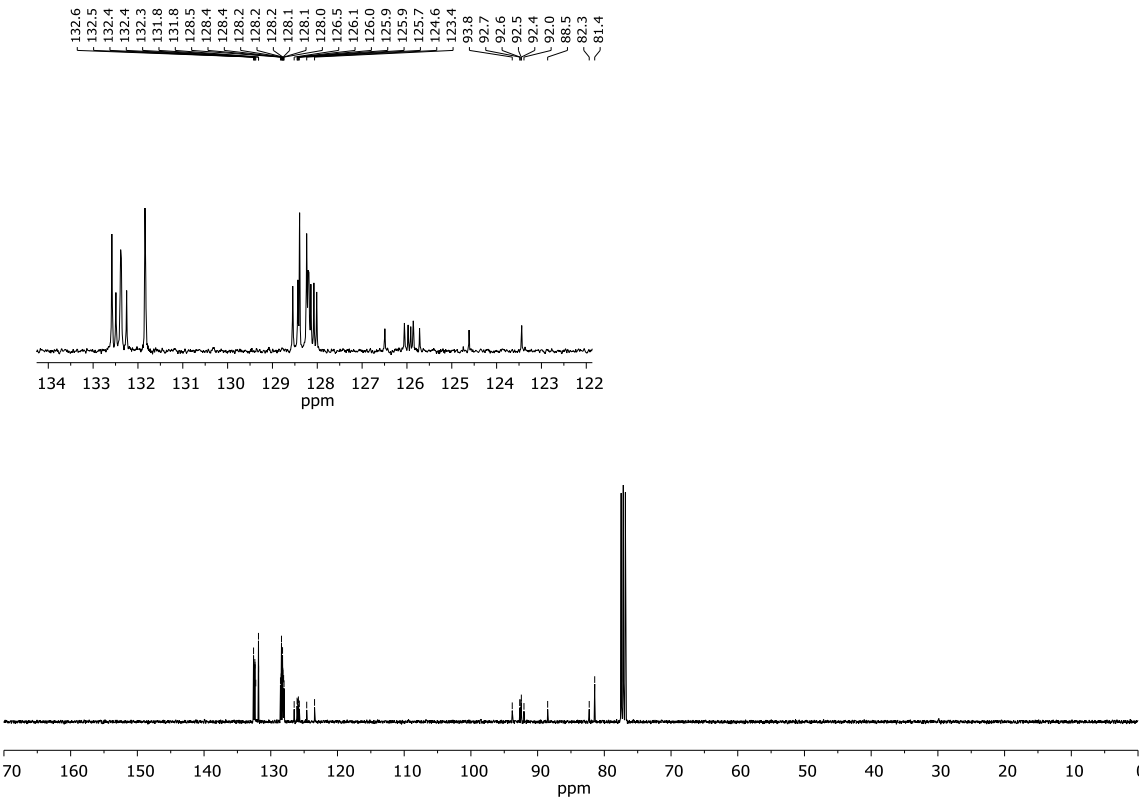


Figure S26. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of compound **11d**.

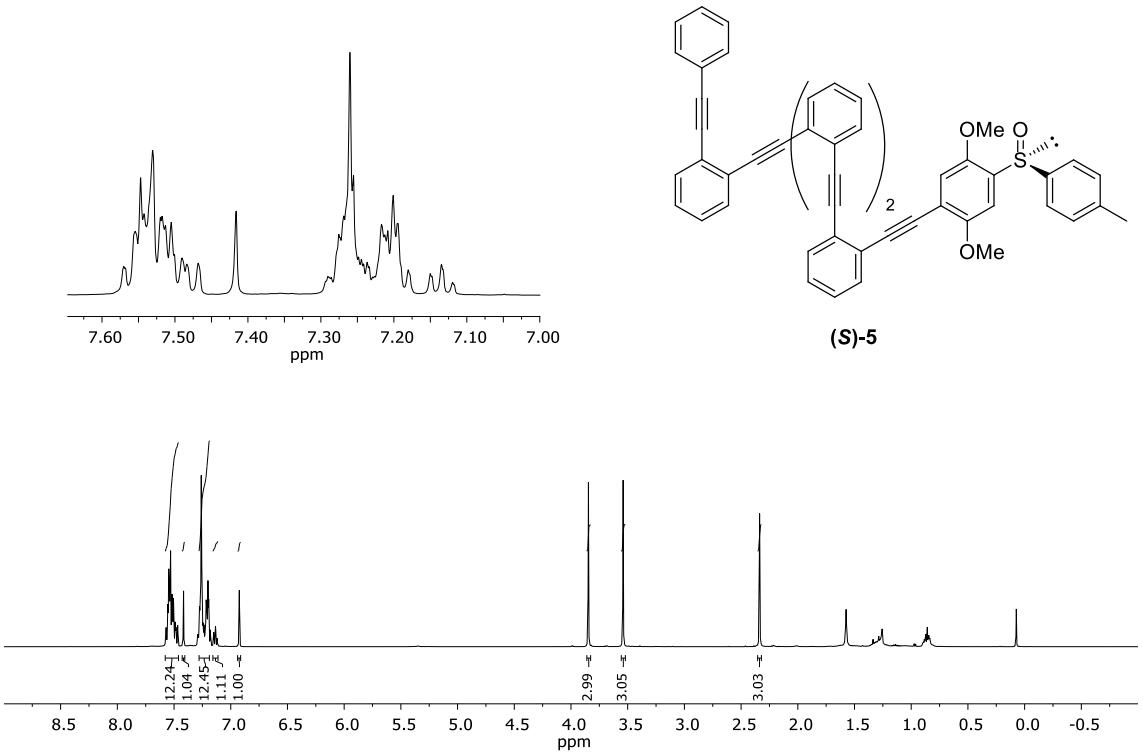


Figure S27. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound (*S*)-**5**.

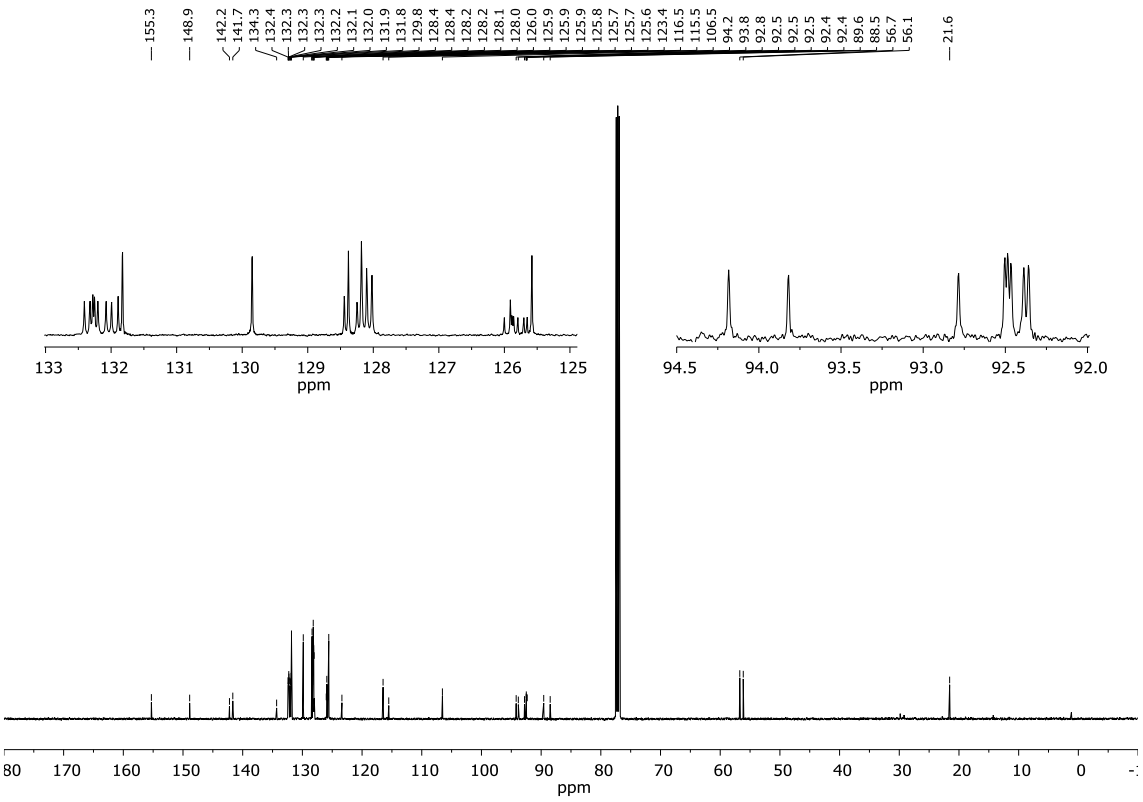


Figure S28. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (*S*)-**5**.

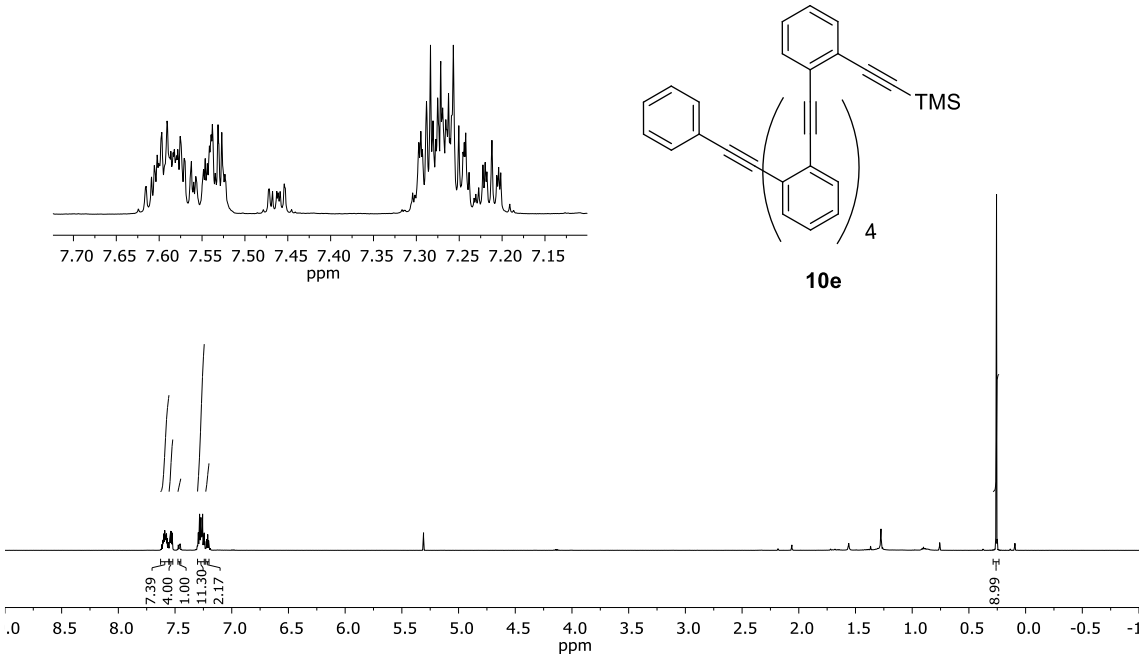


Figure S29. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **10e**.

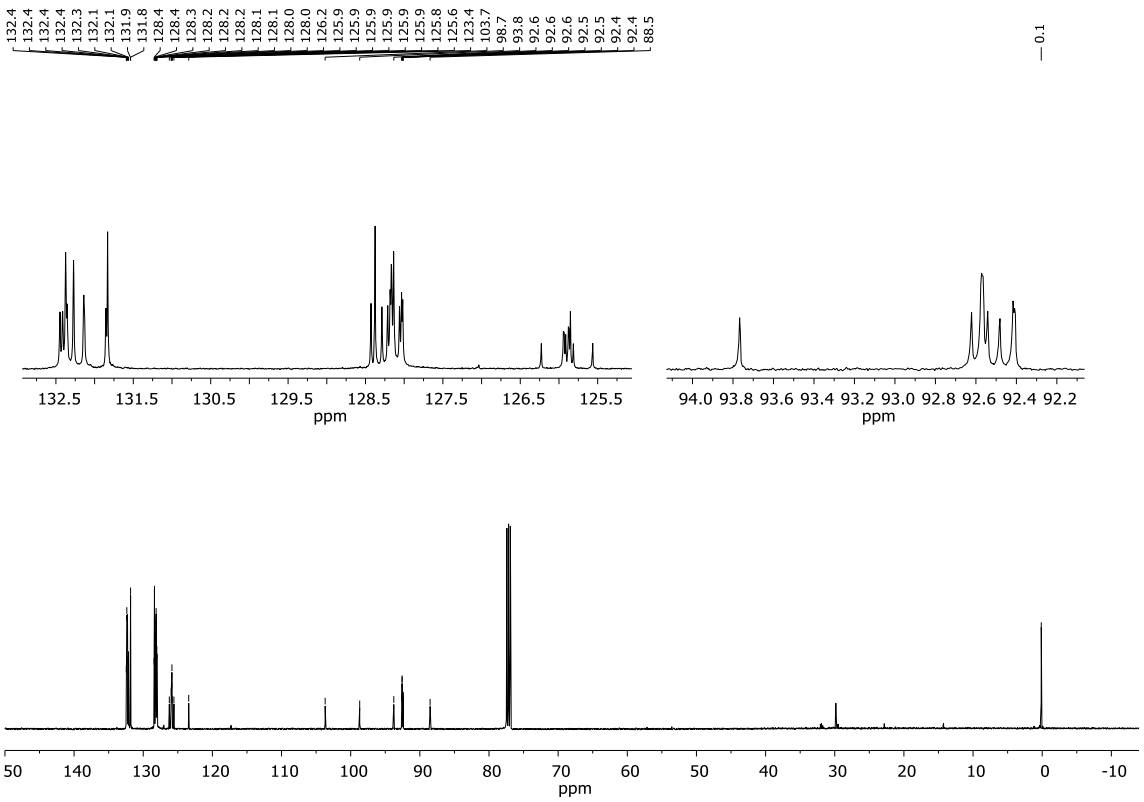


Figure S30. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **10e**.

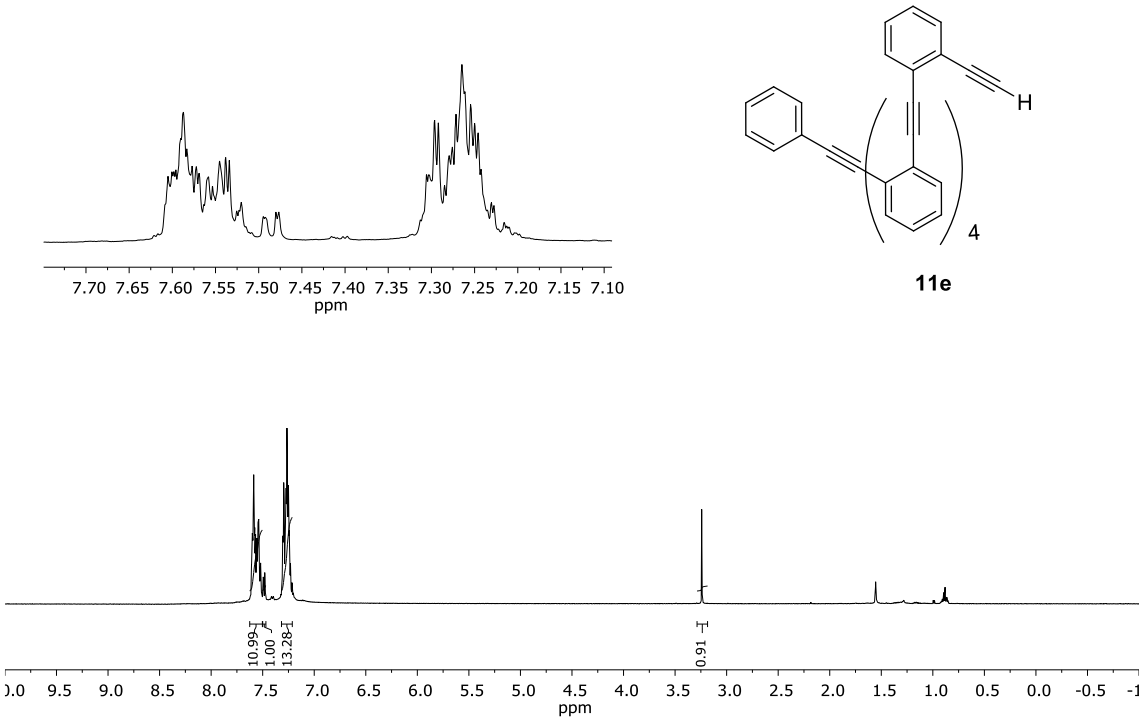


Figure S31. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **11e**.

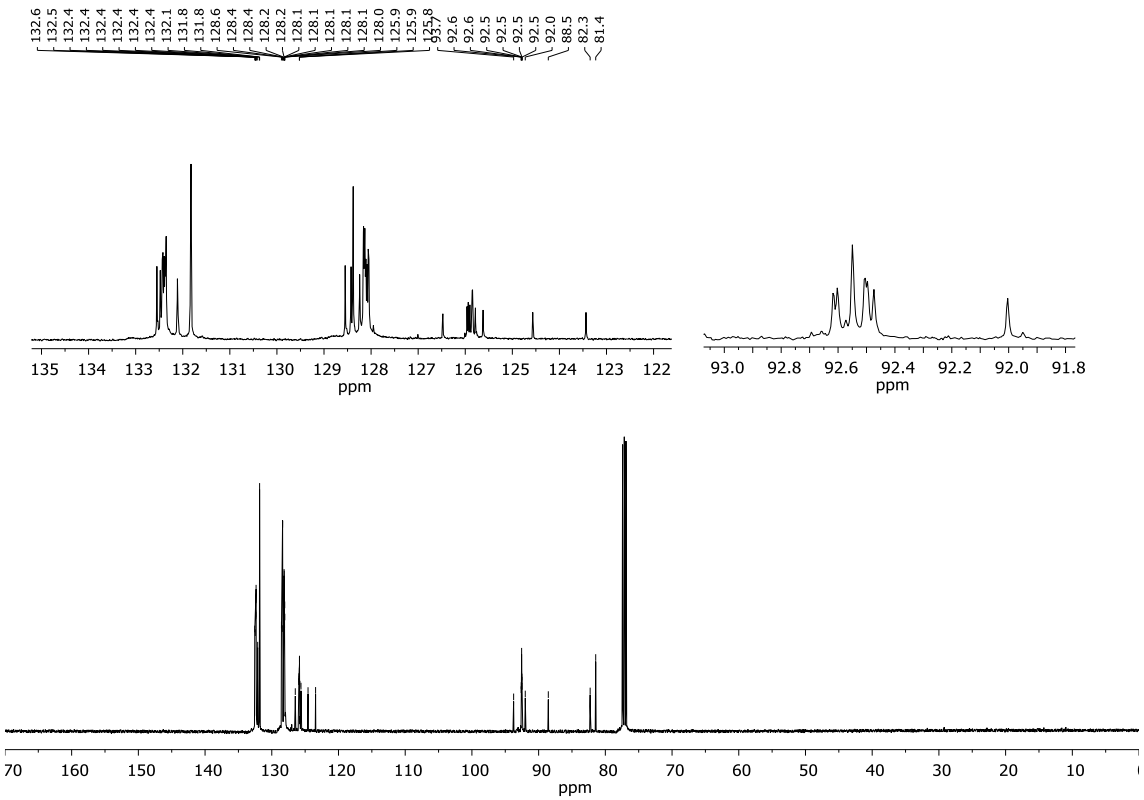


Figure S32. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **11e**.

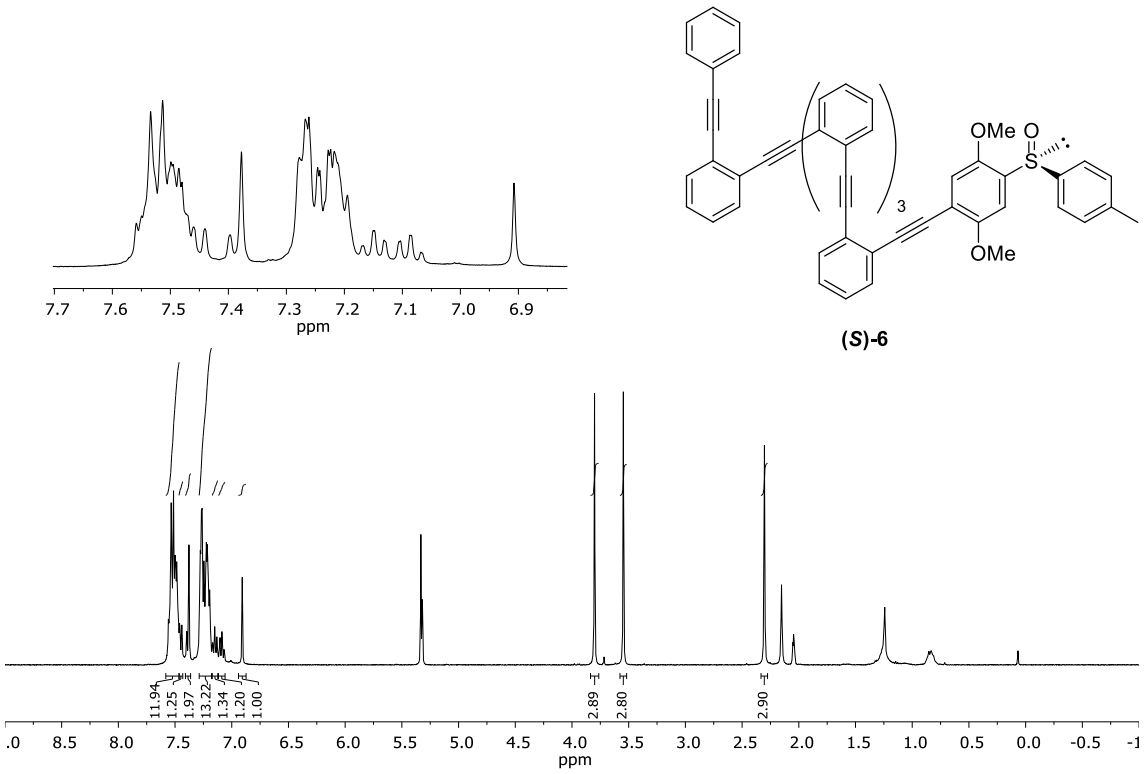


Figure S33. ^{1}H NMR (400 MHz, CD_2Cl_2:Acetone-d_6) spectrum of compound (*S*)-**6**.

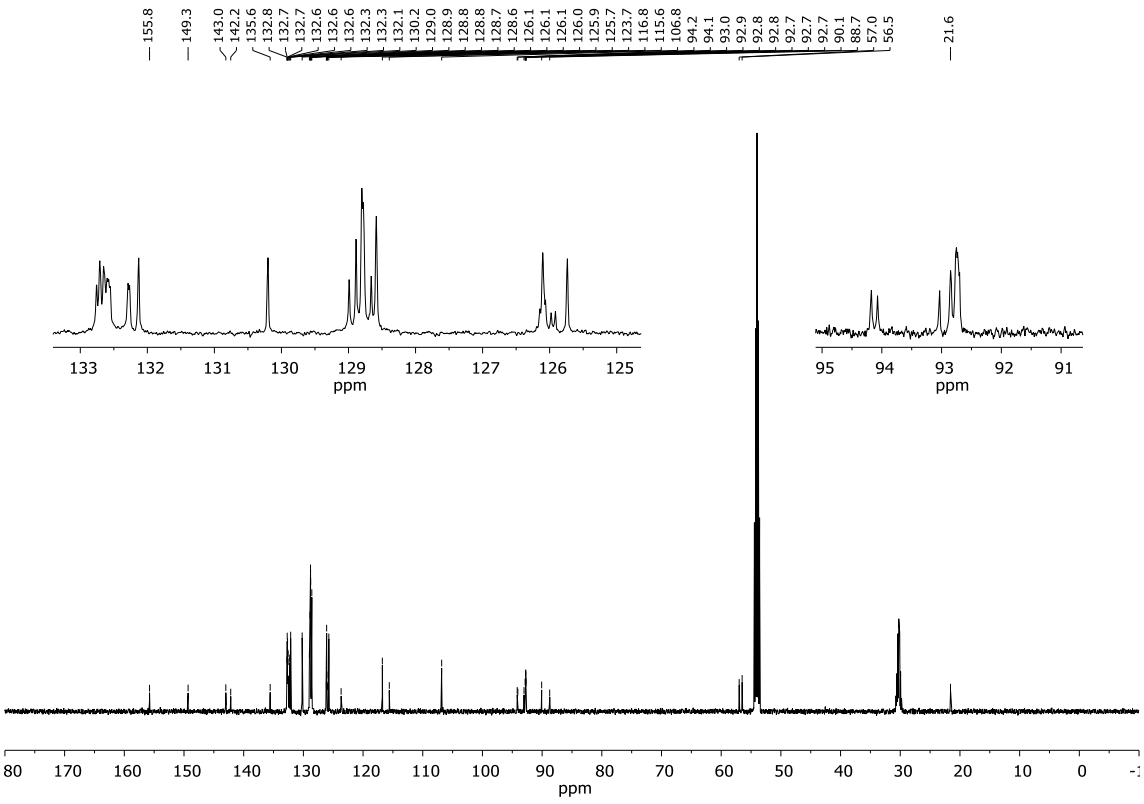


Figure S34. ^{13}C NMR (126 MHz, CD_2Cl_2:Acetone-d_6) spectrum of compound (*S*)-**6**.

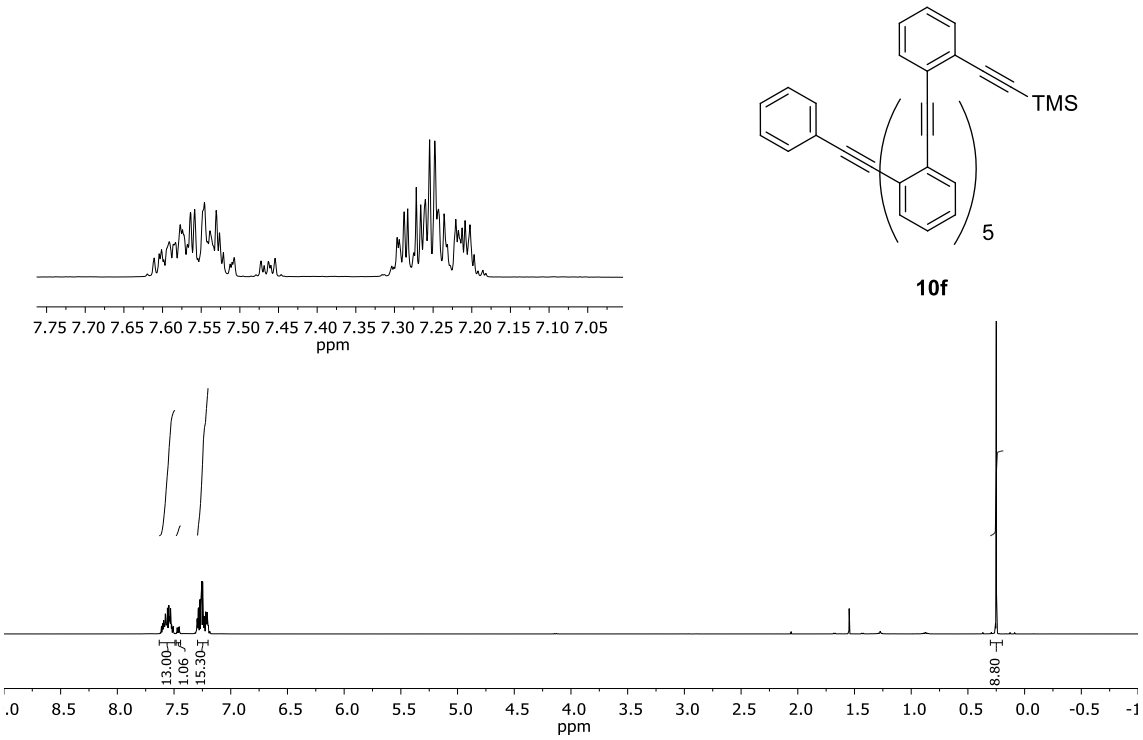


Figure S35. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **10f**.

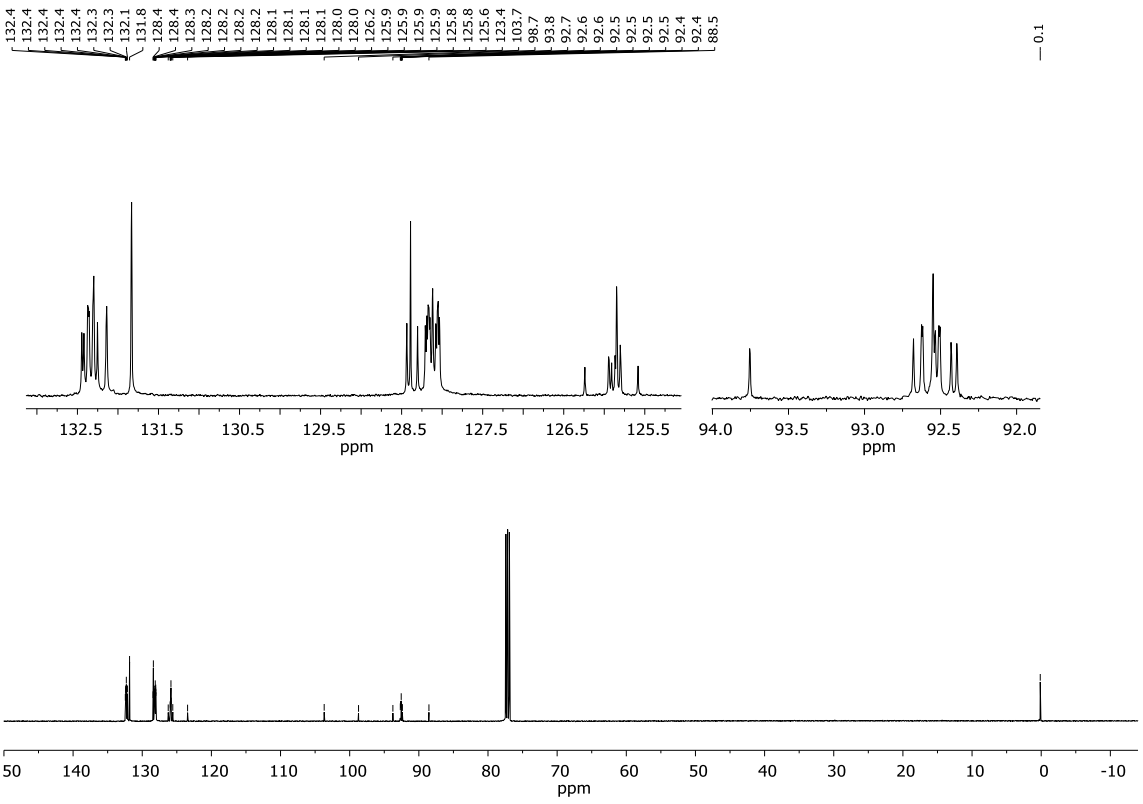


Figure S36. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **10f**.

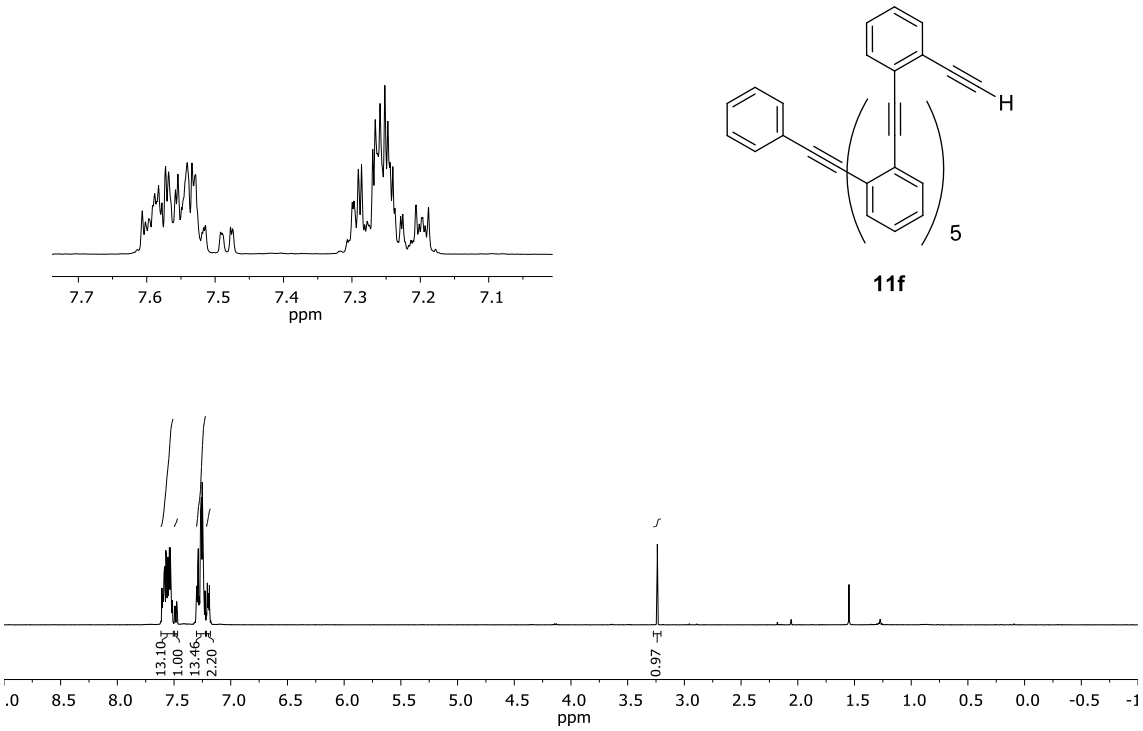


Figure S37. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **11f**.

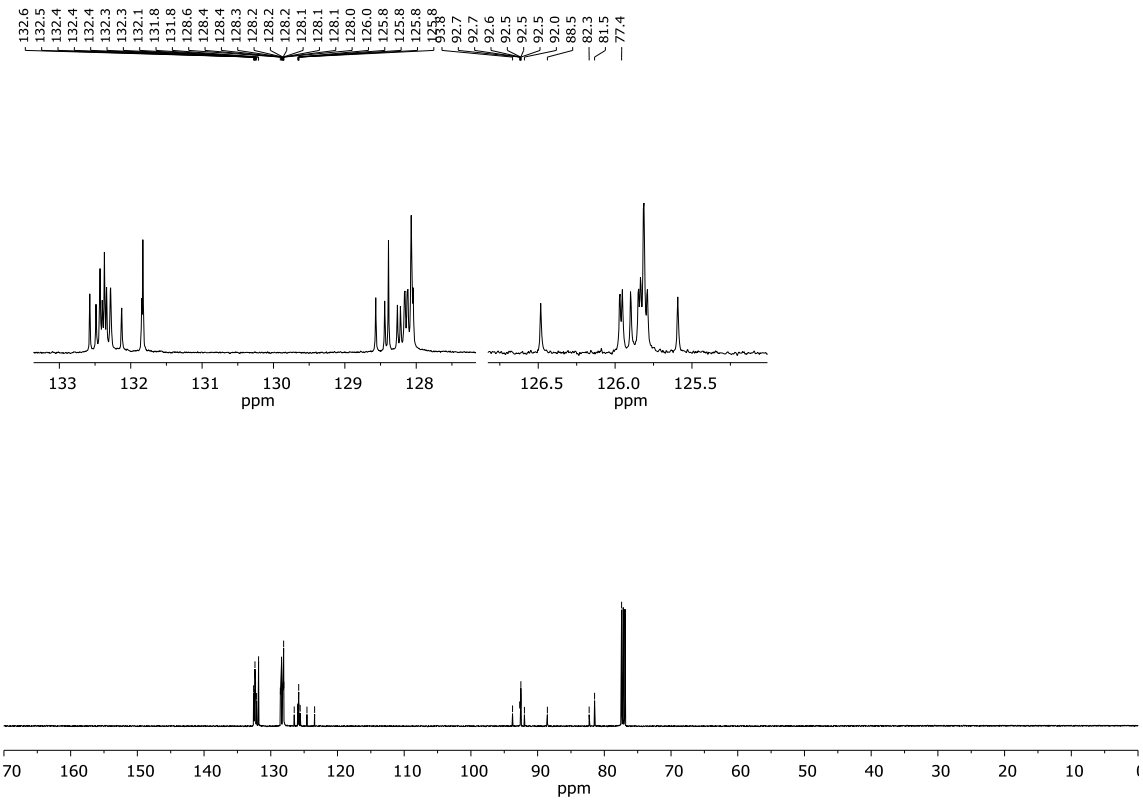


Figure S38. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **11f**.

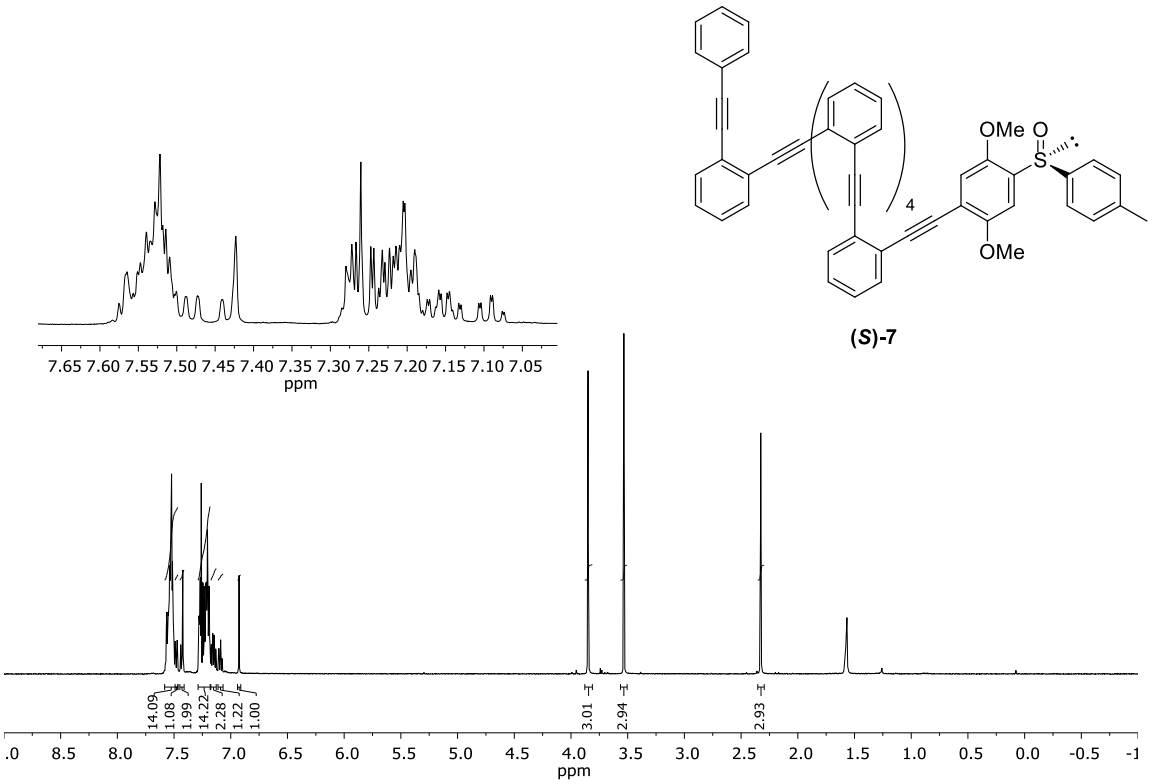


Figure S39. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound (*S*)**-7.**

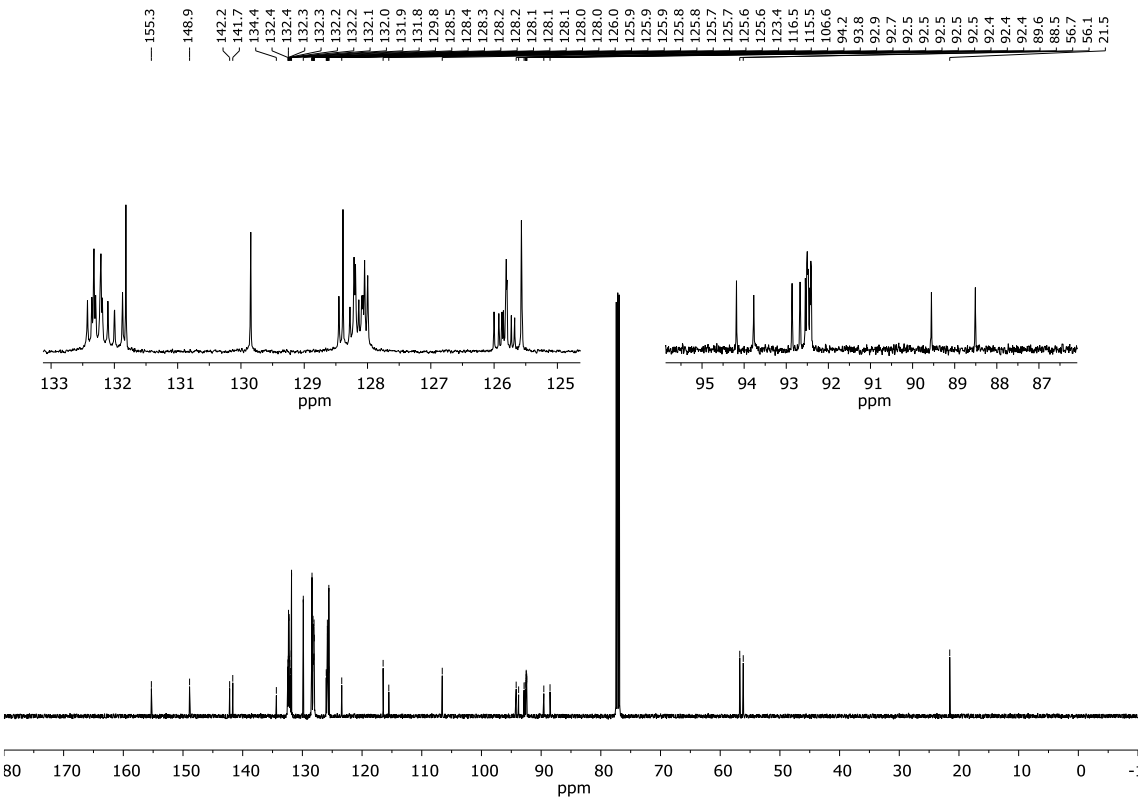


Figure S40. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound (*S*)**-7.**

^{1}H and ^{13}C NMR spectra of the Ag(I) complexes

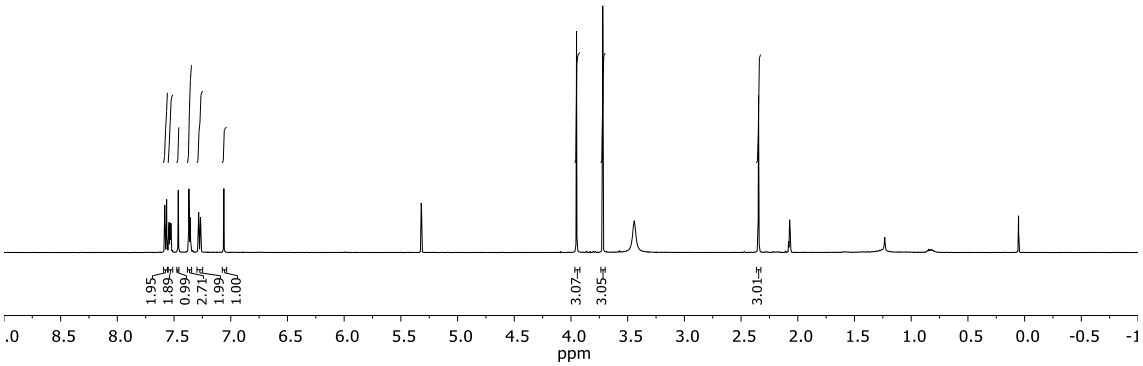


Figure S41. ^{1}H NMR (500 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-1.**

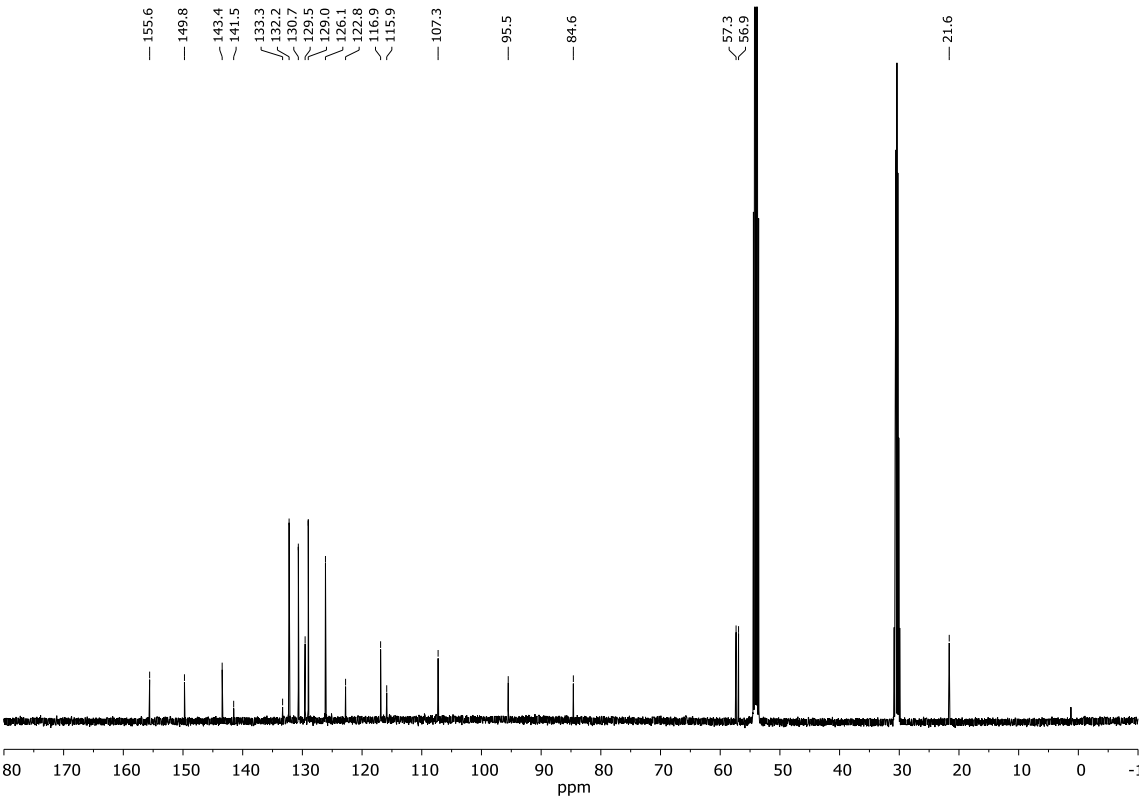


Figure S42. ^{13}C NMR (126 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-1.**

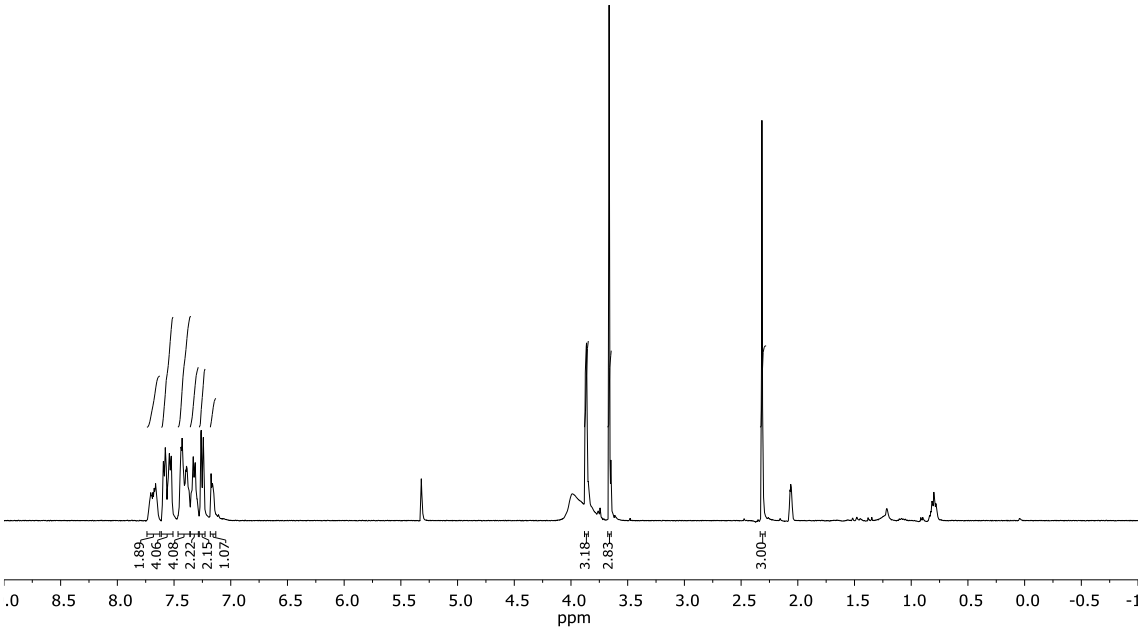


Figure S43. ^{1}H NMR (400 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)-**2.**

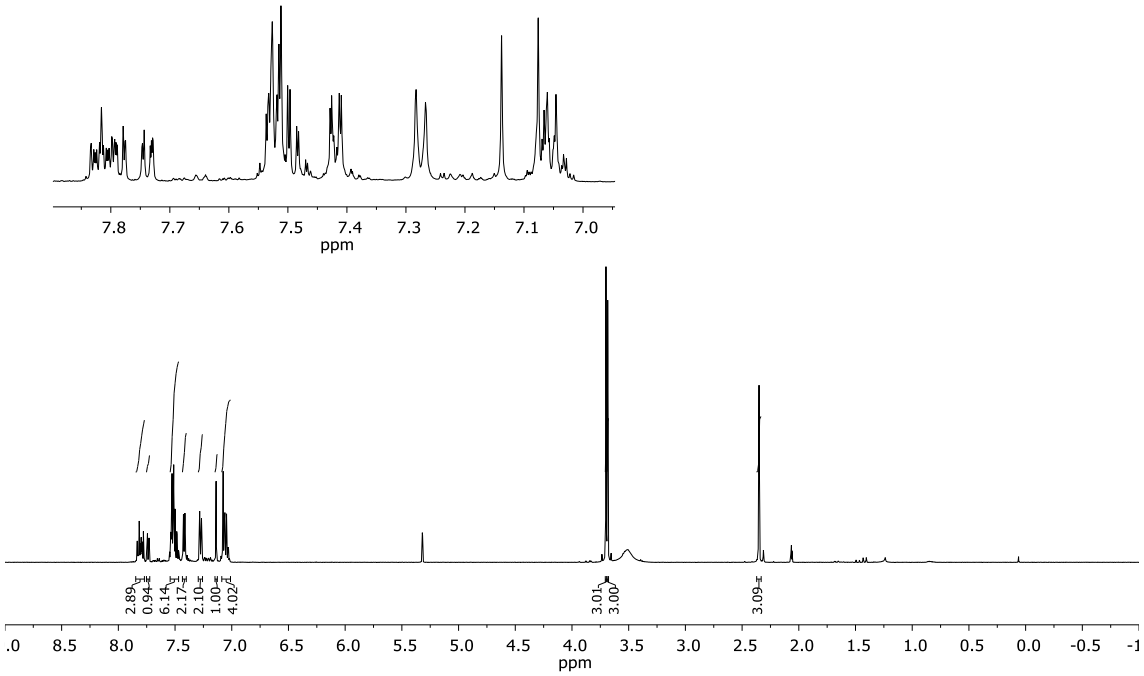


Figure S44. ^{1}H NMR (500 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-3.**

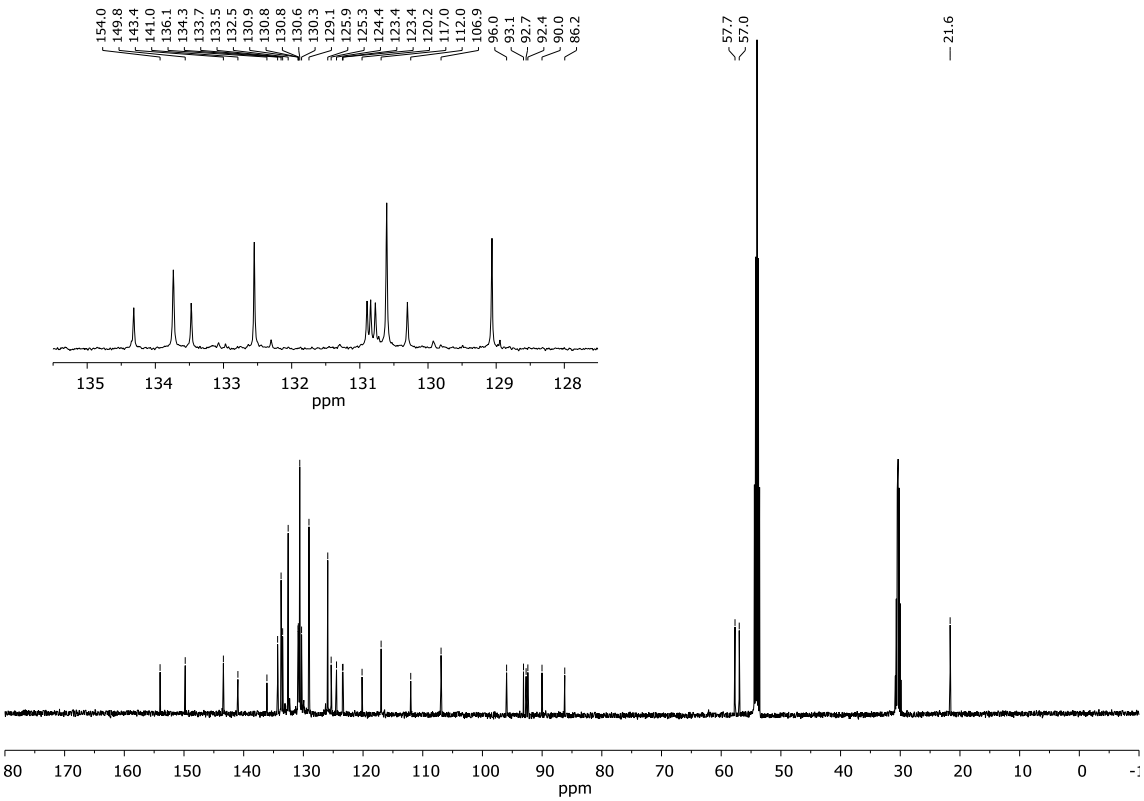


Figure S45. ^{13}C NMR (126 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-3.**

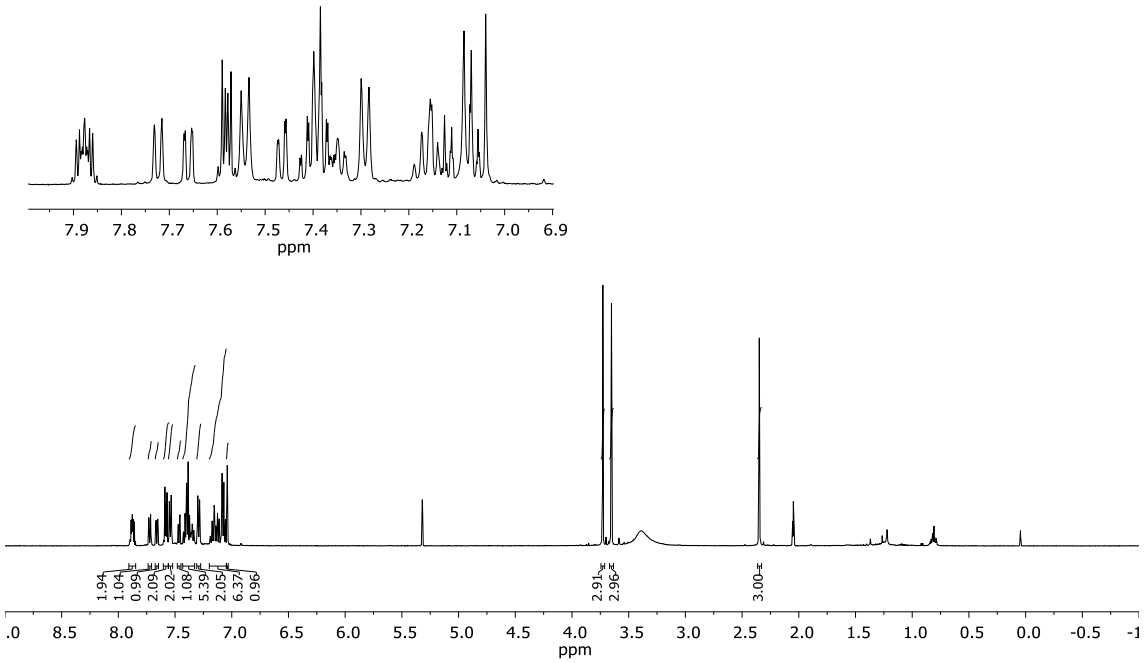


Figure S46. ^{1}H NMR (500 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-4.**

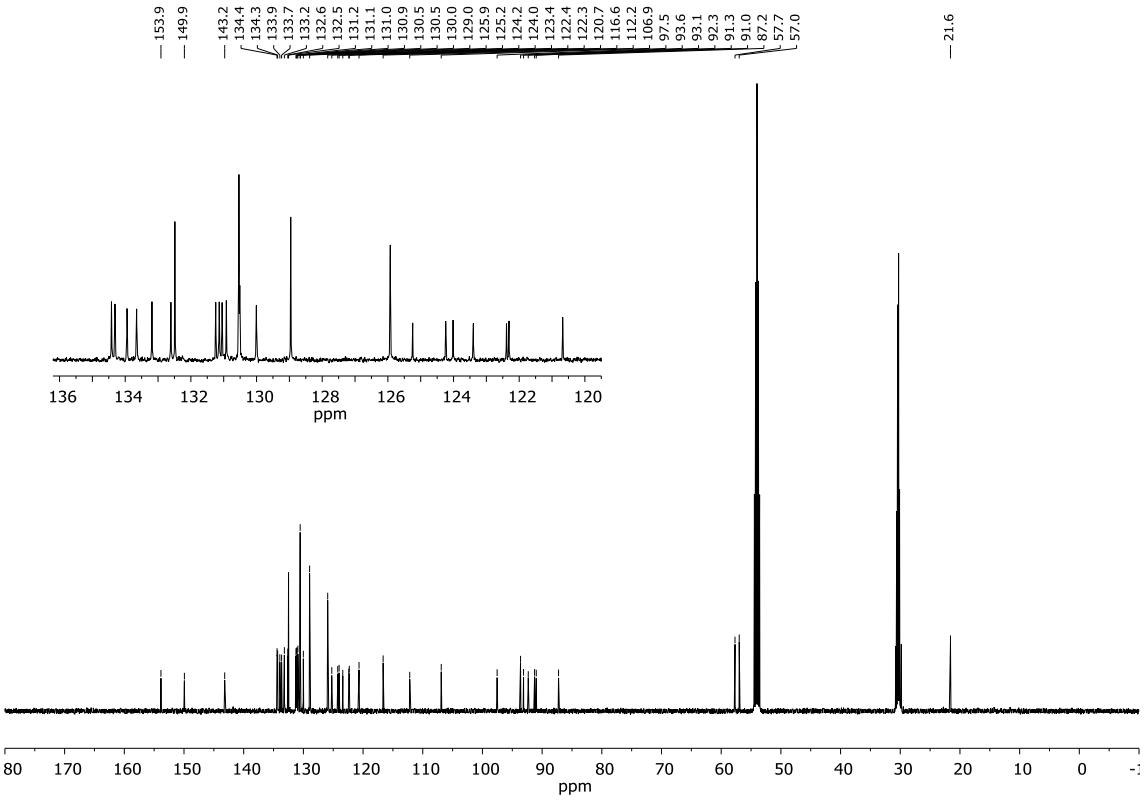


Figure S47. ^{13}C NMR (126 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-4.**

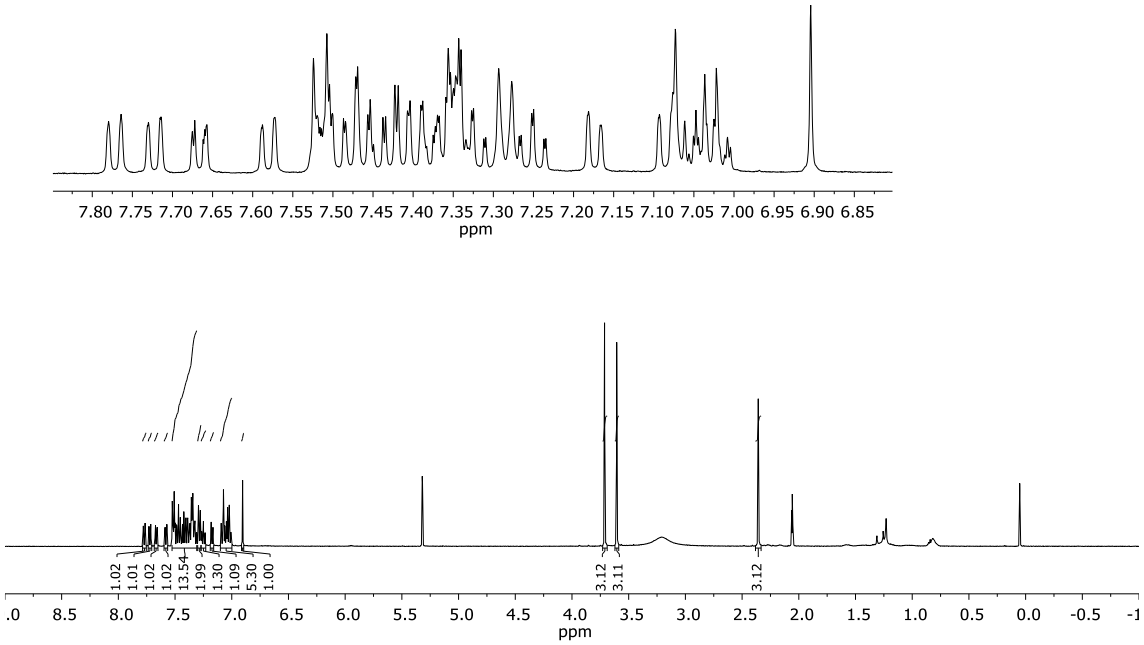


Figure S48. ^{1}H NMR (500 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)-**5**.

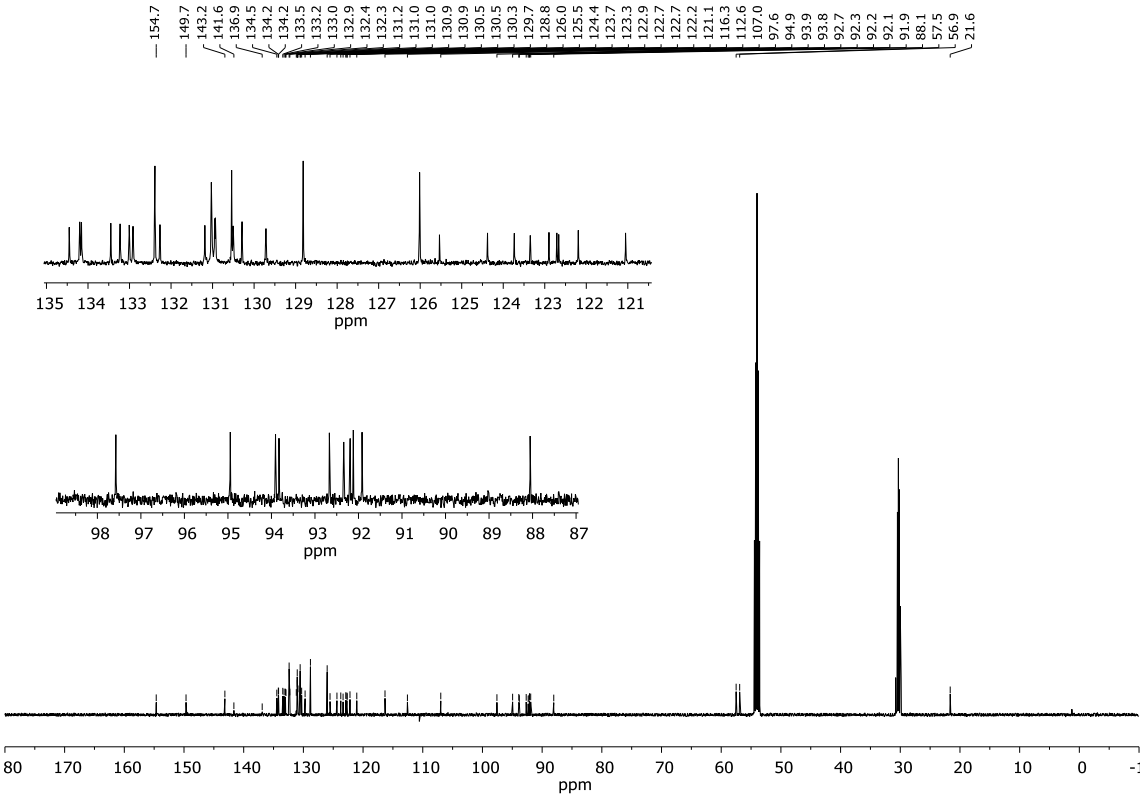


Figure S49. ^{13}C NMR (126 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)-**5**.

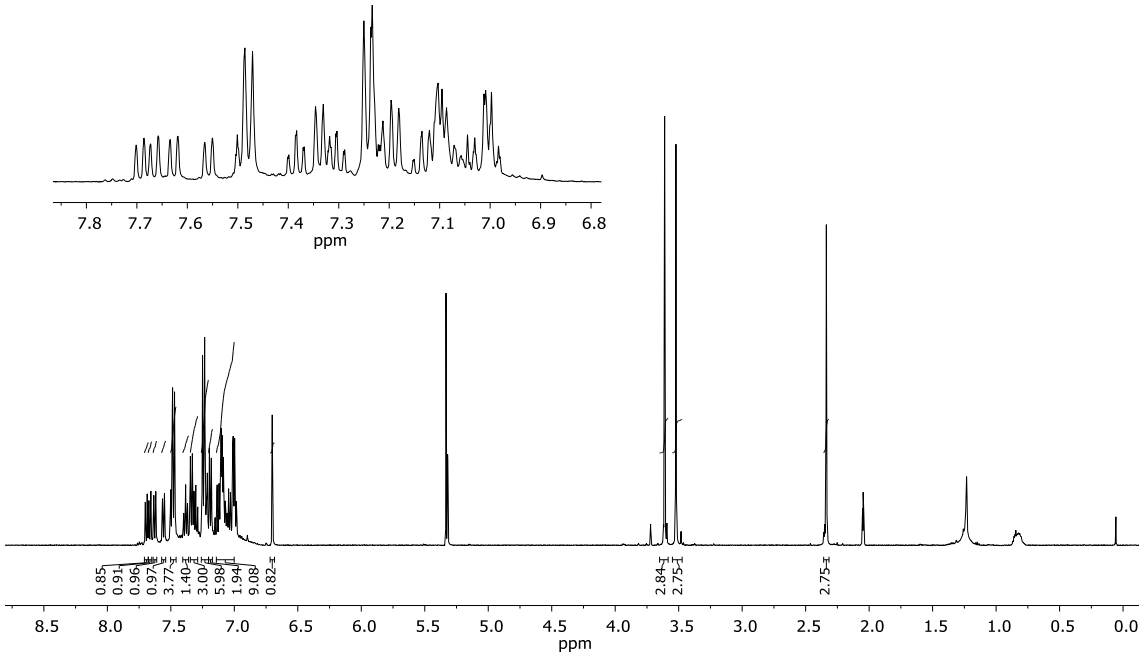


Figure S50. ^{1}H NMR (500 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-6.**

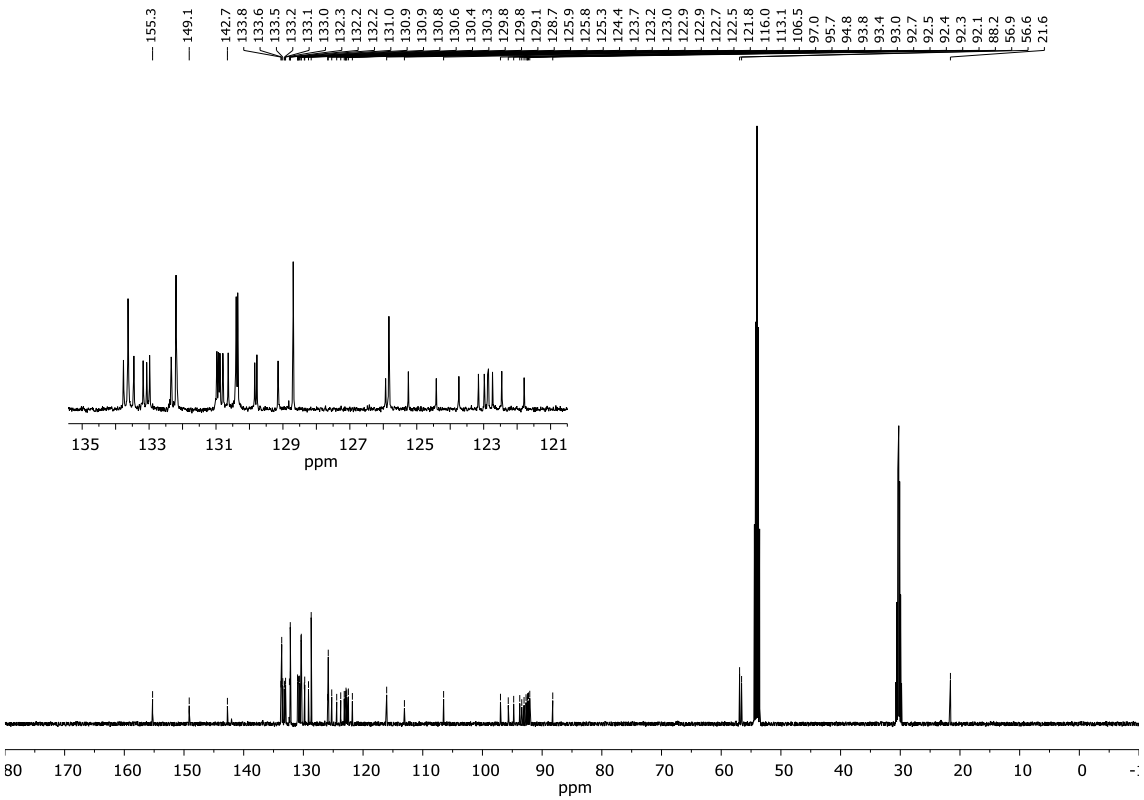


Figure S51. ^{13}C NMR (126 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-6.**

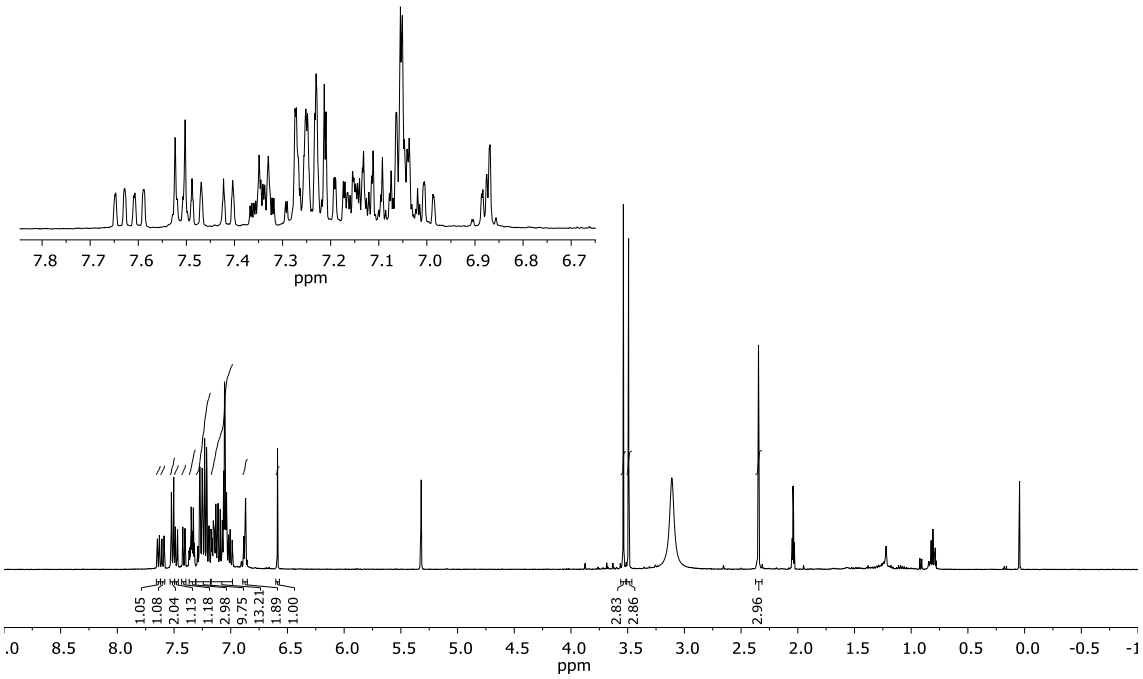


Figure S52. ^{1}H NMR (400 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-7.**

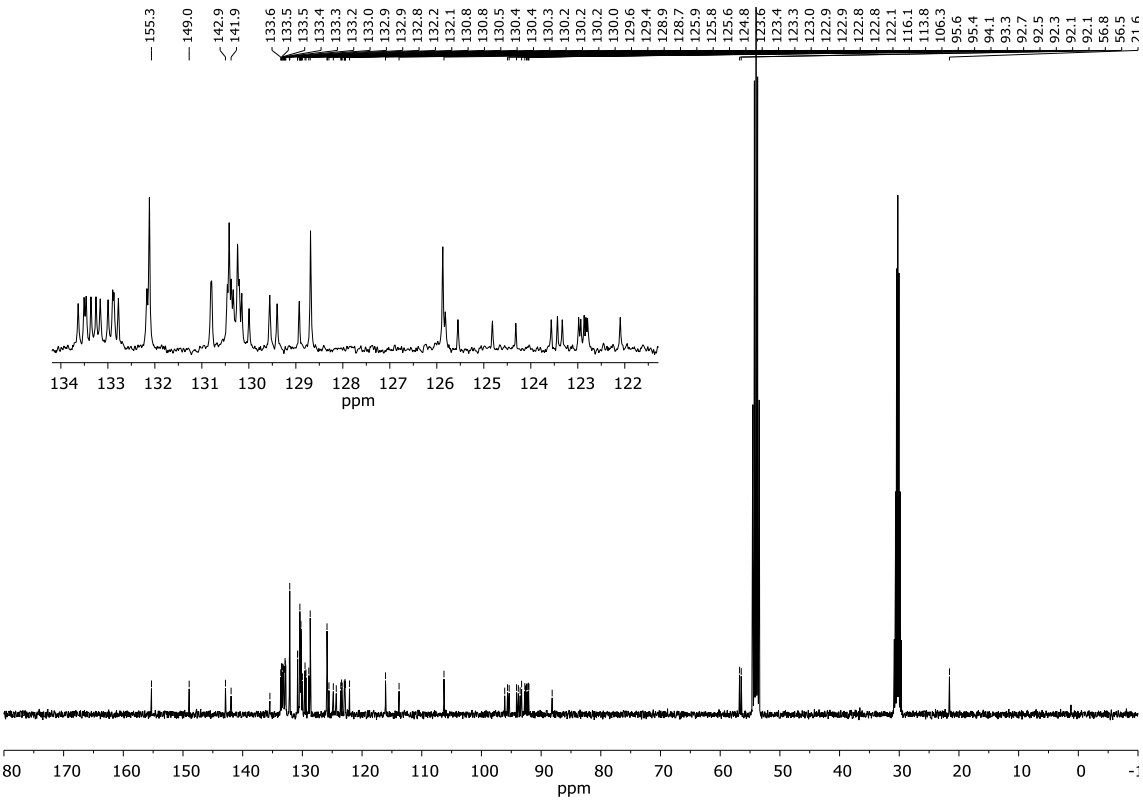


Figure S53. ^{13}C NMR (101 MHz, 9:1CD_2Cl_2:Acetone-d_6) spectrum of Ag(I) complex of compound (*S*)**-7.**

ECD titrations of compounds (S)-3 to (S)-7 with $AgBF_4$

Experimental

CD titrations were performed in a JASCO J-15 Spectropolarimeter with a 1.0 cm path-length quartz cell. Temperature was set at 10ºC using a Peltier JASCO PTC-348 WI to avoid evaporation of the solvent.

General procedures for the CD titration of compounds (S)-3 to (S)-7

Titrations of compounds (*S*)-**3**to (*S*)-**7** were carried out by addition of progressive quantities of a $2.5x10^{-4}$M solution of $AgBF_4$ salt, which was commercially available, to a $2.5x10^{-5}$M solution of the corresponding compound. First, $5x10^{-4}$M stock solutions were prepared by solving 1 mmol of compound in 2 mL of a 9:1 mixture of CH_2Cl_2:acetone. To carry out titrations stock solutions were diluted 20 times to get a $2.5x10^{-5}$M final concentration. To make the fitting of the kinetic constant easier, concentration of ligands (*S*)-**3**to (*S*)-**7** were kept constant during the titration. To ensure this, the $2.5x10^{-5}$M solution of compounds (*S*)-**3**to (*S*)-**7** was used as solvent to prepare the $AgBF_4$ solution.

The fitting was carried out with DynaFit program (v. 4.06019), which has been previously used to study guest-host complexation equilibria.[S1]Input script files contained Ag(I) concentration and CD signal obtained at 380 nm, corresponding to the maxima of absorption of complexes. An example is given beyond.

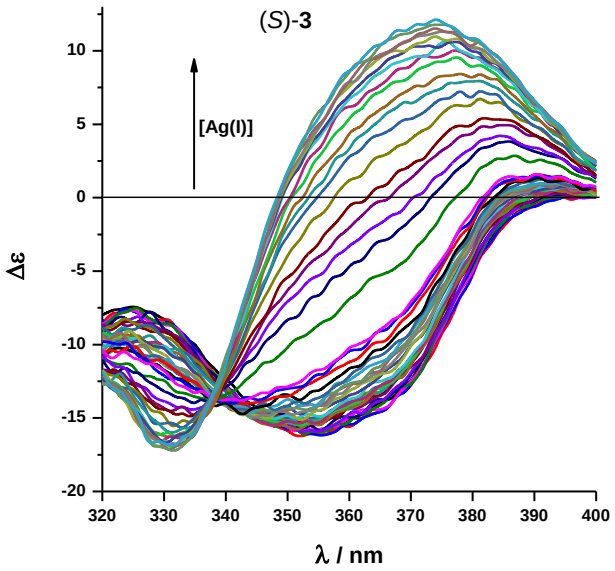
General input file for dynafit fitting

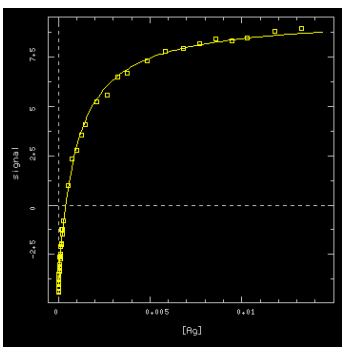
```
[task]

  data = equilibria
  task = fit

[mechanism]

   L + Ag <==> LAg : K1 assoc

[constants]

  K1 = 2400000??

[concentrations]

L = 0.0000286

[responses]

LAg = 1540000??

[data]
variable Ag
  set complex

[output]

  directory ./examples/chemistry/cryptand/output/models

;_____

[set:complex]

[Ag],M   CD
```

0.00E+00	-1.949081
6.14E-06	-1.916077
1.23E-05	-0.52949
1.83E-05	1.902313
2.44E-05	3.892489
3.04E-05	5.828279
3.64E-05	8.144073
4.24E-05	9.705623
4.83E-05	11.10436
5.42E-05	12.80866
6.01E-05	14.217359
6.59E-05	15.69406
7.18E-05	16.680793
7.75E-05	17.84756
8.33E-05	19.107793
8.90E-05	19.893525
9.48E-05	20.836326
1.00E-04	21.400127
1.12E-04	22.942725
1.23E-04	24.198726
1.34E-04	26.219093
1.45E-04	27.216693
1.56E-04	27.875159
1.83E-04	29.728793
2.09E-04	30.887592
2.34E-04	31.560394
3.46E-04	34.300025
4.58E-04	35.310023
5.69E-04	35.911025
6.80E-04	36.151195
8.99E-04	36.773193
1.12E-03	37.161891
1.33E-03	37.206161
1.86E-03	37.241862
2.38E-03	37.798461
2.89E-03	37.827228

3.39E-03	37.796325
3.88E-03	37.801894
4.36E-03	38.119426
5.28E-03	37.953658
6.17E-03	37.982127
7.03E-03	38.156093
7.85E-03	38.28886
8.65E-03	38.541026
9.41E-03	38.455795
1.01E-02	38.731792
4.36E-03	38.119426
5.28E-03	37.953658
6.17E-03	37.982127
7.03E-03	38.156093
7.85E-03	38.28886

Figure S54. ECD titration of compound (*S*)-**3** with $AgBF_4$ and DynaFit fitting





(*S*)-**3**:Ag fitting

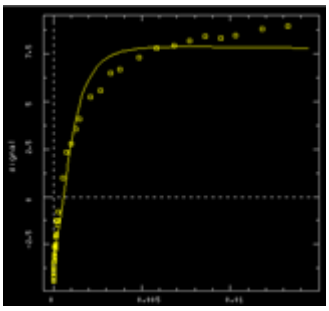
Parameters

Marquardt Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low[a]	High[a]	Note
#1	K	1082.59	1083	39	3.6	1003	1167	
#2	r(L)	-164612	-164600	2300	1.4	-169500	-159800	
#3	r(LAg)	383711	383700	4100	1.1	375400	392300	

[a] Confidence intervals at **95 %** probability level.



(*S*)-**3**:Ag_2 fitting

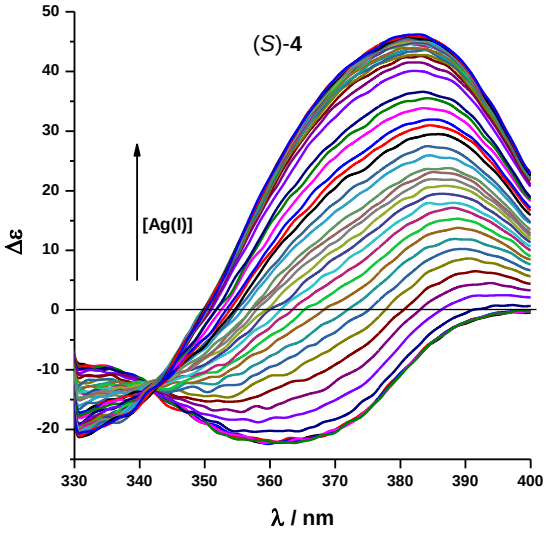
Parameters

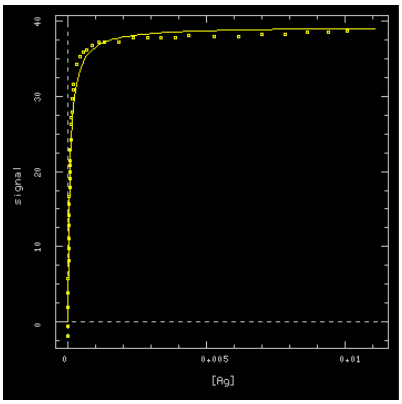
Marquardt Minimization Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low	Low P (%)	High	High P (%)	Note
#1	K1	24000	0.632809	233.805	36947.20	< 0.024	(14.1)	80.0318	95	
#2	K2	100	1.04346e+006	3.90137e+008	37388.95	8589.01	95	> 1.50477e+007	(13.9)	
#3	r(L)	-40000	-129492	10369.3	8.01	-945518	100.0	> -129492	(38.3)	
#4	r(LAg)	1e+006	1.84961e+008	6.79969e+010	36762.75	1.93756e+006	95	> 2.66733e+009	(13.9)	
#5	r(LAg2)	881200	303275	28797.1	9.50	0.8812	100.0	705528	100.0	

Figure S55. ECD titration of compound (*S*)-**4** with $AgBF_4$ and DynaFit fitting





(*S*)-**4**:Ag fitting

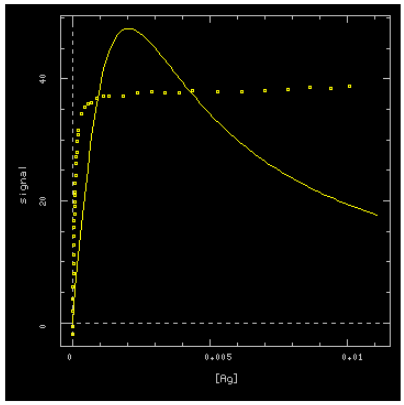
Parameters

Marquardt Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low[a]	High[a]	Note
#1	K1	13499	13500	780	5.8	12100	15100	
#2	r(LAg)	1.37328e+006	1.373e+006	15000	1.1	1.344e+006	1.403e+006	

[a] Confidence intervals at **95 %** probability level.



(*S*)-**4**:Ag_2 fitting

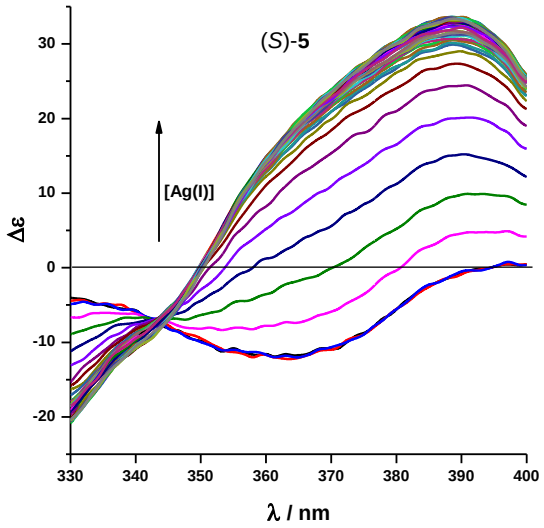
Parameters

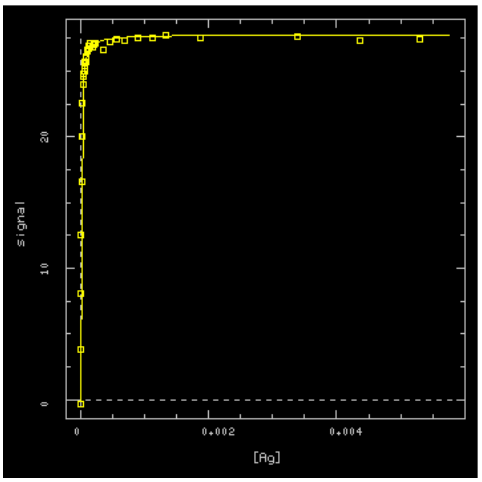
Marquardt Minimization Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low	Low P (%)	High	High P (%)	Note
#1	K1	2.4e+006	56.9879	401.423	704.40					
#2	K2	100	4298.43	23286.4	541.74					
#3	r(L)	-78000	-0.078	132529	169908833.80					MAX
#4	r(LAg)	1.48e+006	3.54752e+007	2.29682e+008	647.45					

Figure S56. ECD titration of compound (*S*)-**5** with $AgBF_4$ and DynaFit fitting





(*S*)-**5**:Ag fitting

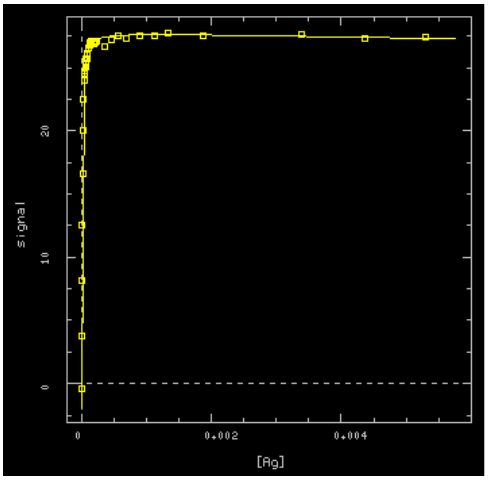
Parameters

Marquardt Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low[a]	High[a]	Note
#1	K1	203504	204000	18000	8.7	173000	244000	
#2	r(LAg)	1.11154e+006	1.1115e+006	7400	0.7	1.0968e+006	1.1264e+006	

[a] Confidence intervals at **95 %** probability level.



(*S*)-**5**:Ag_2 fitting

Parameters

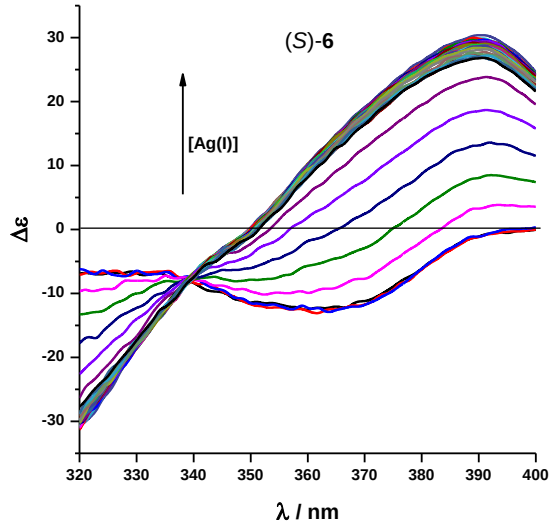
Marquardt Minimization Algorithm

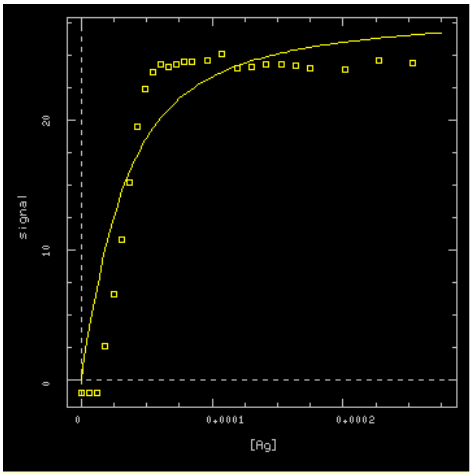
Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low	Low P (%)	High	High P (%)	Note
#1	K1	240000	232258	20374.3	8.77	196035	95	277872	95	
#2	K2	100	3.35798	3.43906	102.41	< 0.0001	(67.2)	10.5433	95	
#3	r(L)	-16000	-78088.9	17430	22.32	-113511	95	-42868.1	95	
#4	r(LAg)	1.108e+006	1.11305e+006	7577.19	0.68	1.09823e+006	95	1.12845e+006	95	

In this case, although the graphic does not seem bad, there is a Std error in the K2 of the 102.4%.

Figure S57. ECD titration of compound (*S*)-**6** with $AgBF_4$ and DynaFit fitting





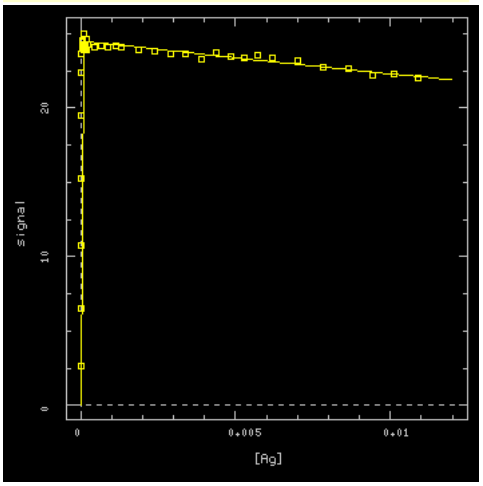
(*S*)-**6**:Ag fitting

Parameters

Marquardt Minimization Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low	Low P (%)	High	High P (%)	Note
#1	K	150000	**54935**	20963.1	38.16	28758.8	95	118760	95	
#2	r(LAg)	984400	**1.14557e+006**	87119.2	7.60	1.00153e+006	95	1.33449e+006	95	



(*S*)-**6**:Ag_2 fitting

Parameters

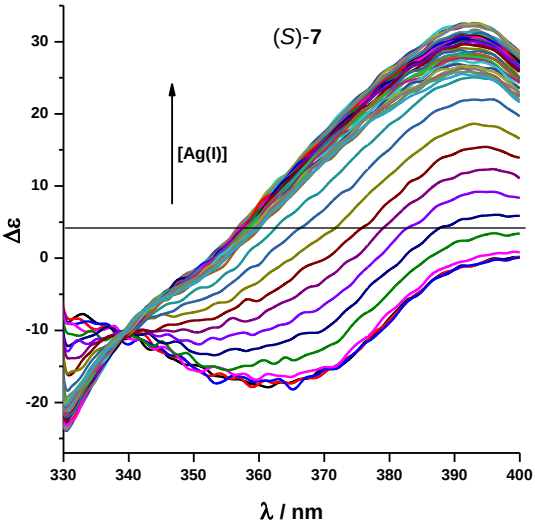
Marquardt Algorithm

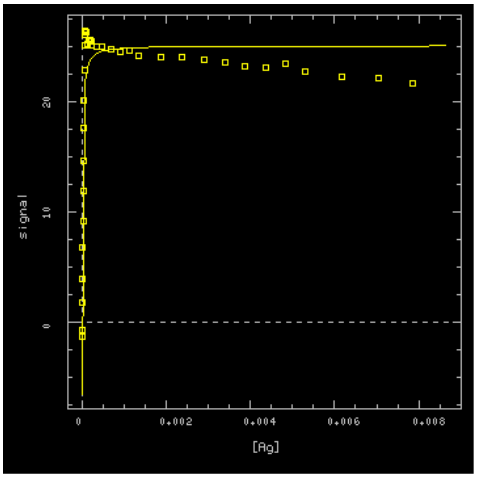
Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low[a]	High[a]	Note
#1	K1	1.17878e+006	1.18e+006	250000	21.5	835000	1.86e+006	
#2	K2	10.1523	10.2	1.5	14.4	7.36	13	
#3	r(L)	-0.04	-0.04	17000	43327567.3	< -0.04	> -0.04	MAX
#4	r(LAg)	982711	982700	6100	0.6	971200	994400	

[a] Confidence intervals at **95 %** probability level.

Figure S58. ECD titration of compound (*S*)-**7** with $AgBF_4$ and DynaFit fitting





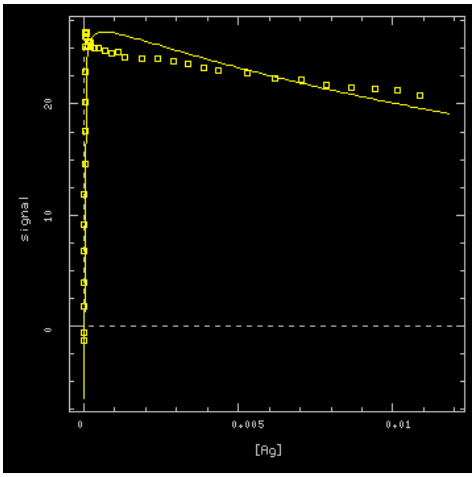
(*S*)-**7**:Ag fitting

Parameters

Marquardt Minimization Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low	Low P (%)	High	High P (%)	Note
#1	K1	1e+006	132439	38626	29.17	82652.9	95	224584	95	
#2	r(L)	-48000	-262214	87978.2	33.55	-432997	95	-94157.9	95	
#3	r(LAg)	1.06e+006	1.00465e+006	27832.3	2.77	951551	95	1.0588e+006	95	



(*S*)-**7**:Ag_2 fitting

Parameters

Marquardt Algorithm

Optimized Parameters

No.	Par#Set	Initial	Final	Std. Error	CV (%)	Low[a]	High[a]	Note
#1	K1	89514	90000	21000	23.3	60000	140000	
#2	K2	36.8838	36.9	9.1	24.8	20	57.1	
#3	r(L)	-255254	-255000	71000	27.8	-393000	-120000	
#4	r(LAg)	1.1042e+006	1.104e+006	37000	3.4	1.035e+006	1.178e+006	

[a] Confidence intervals at **95 %** probability level.

Calculated ECD spectra

Technical Details

All calculations have been performed with Gaussian09 package.[S2]

All structures have been optimized at the M06/6-31g* level using the polarizable continuum model approximation (PCM) in dichloromethane. Cationic structures incorporating Ag(I) were calculated using the SSDAll pseudopotential for Ag(I).

The time-dependent DFT (TD-DFT) method has been used to calculate absorption and CD spectra at the same level of theory (also with the PCM in the same solvent) for Ag(I) non-containing and Ag(I) containing structures.

The nature of the optimized structures was assessed through a frequency calculation, and enthalpies (H) and Gibbs free energies (G) were obtained by taking into account zero-point energies, thermal motion, and entropy contribution at standard conditions (temperature of 298.15 K, pressure of 1 atm).

Figure S59. Comparison of calculated and experimental ECD spectra for Ag(I) complexes of compounds (*S*)-**3**-**5.**

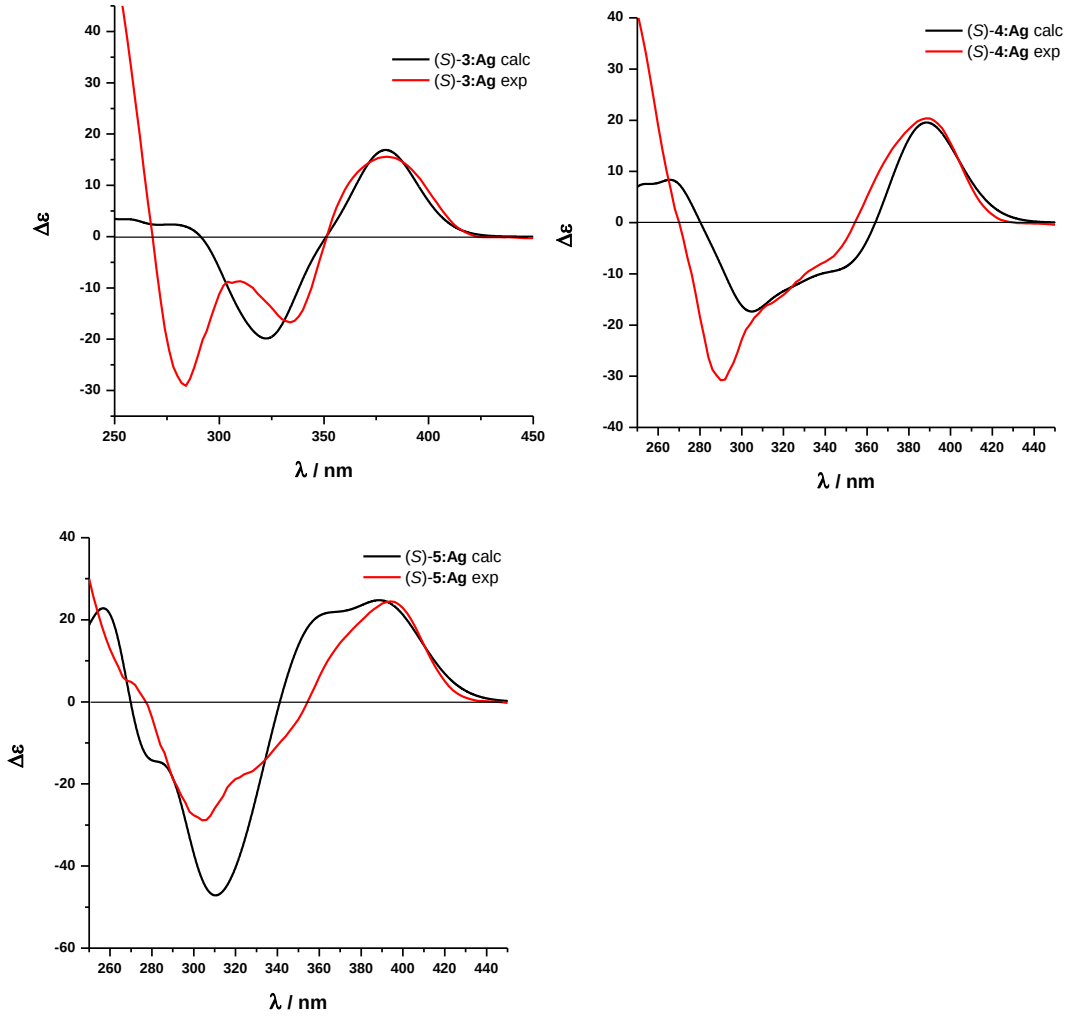
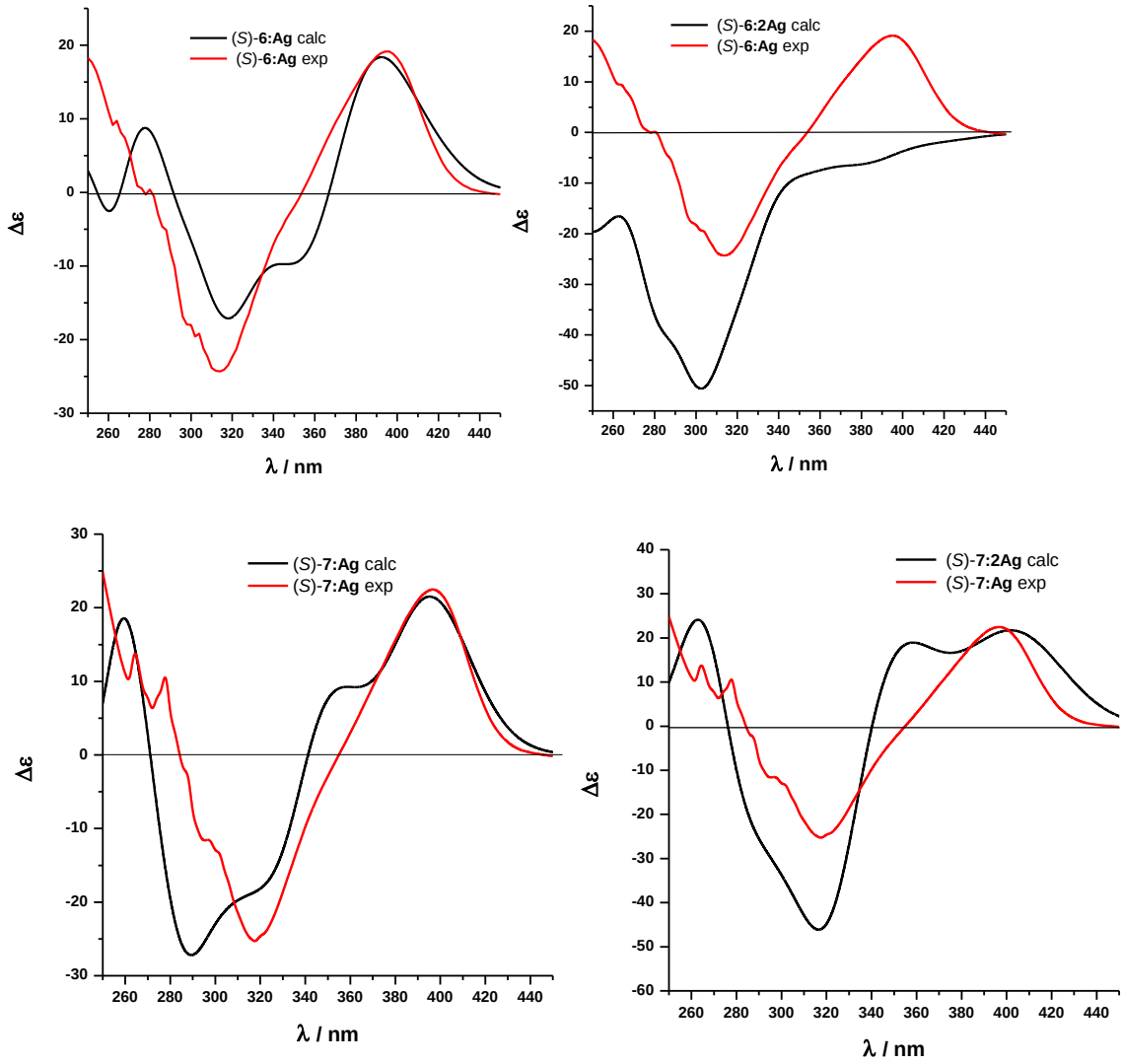


Figure S60. Comparison of calculated and experimental ECD spectra for Ag(I) complexes of compounds (*S*)-**6**-**7.**



Taking into account the much lower second binding constant and the potential overlapping of ECD signals for mono and bimetallic complexes a perfect match between the calculated and experimental ECDs both (*S)*-**6** an (*S*)-**7** could not be obtained.

Experimental VCD and IR spectra

Figure S61.VCD spectra ofmonosulfoxides of the present work (left), and disulfoxides of previous work[S2] (right). The number of the compounds indicates also the number of triple bonds.

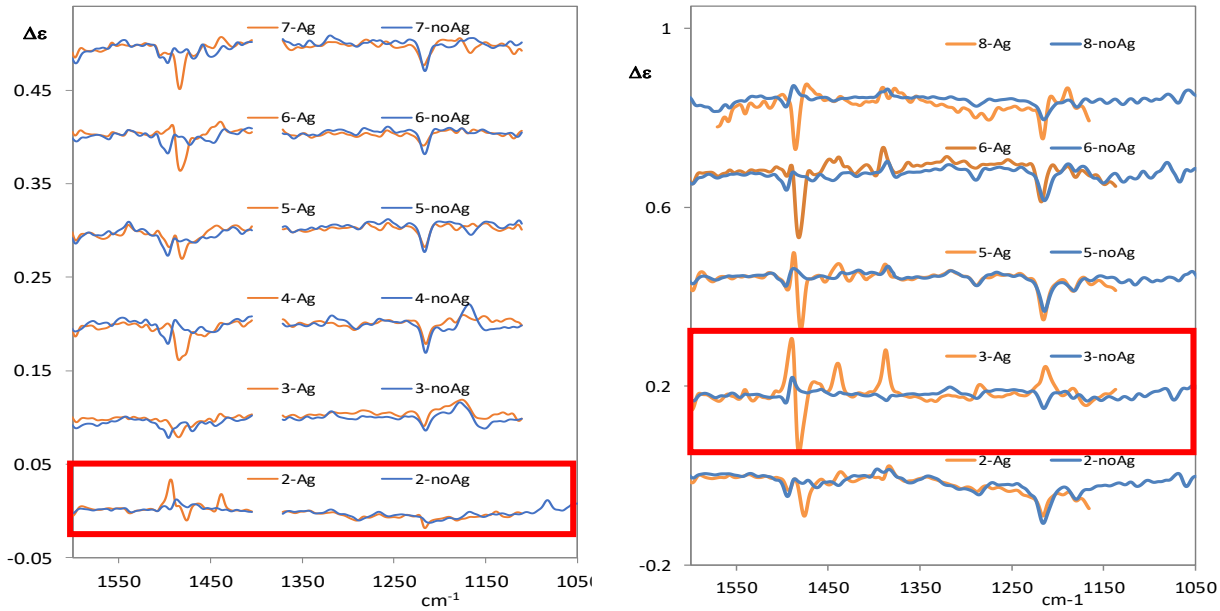


Figure S62.IR spectra ofmonosulfoxides of the present work (left), and disulfoxides of previous work[S2] (right). The number of the compounds indicates also the number of triple bonds.

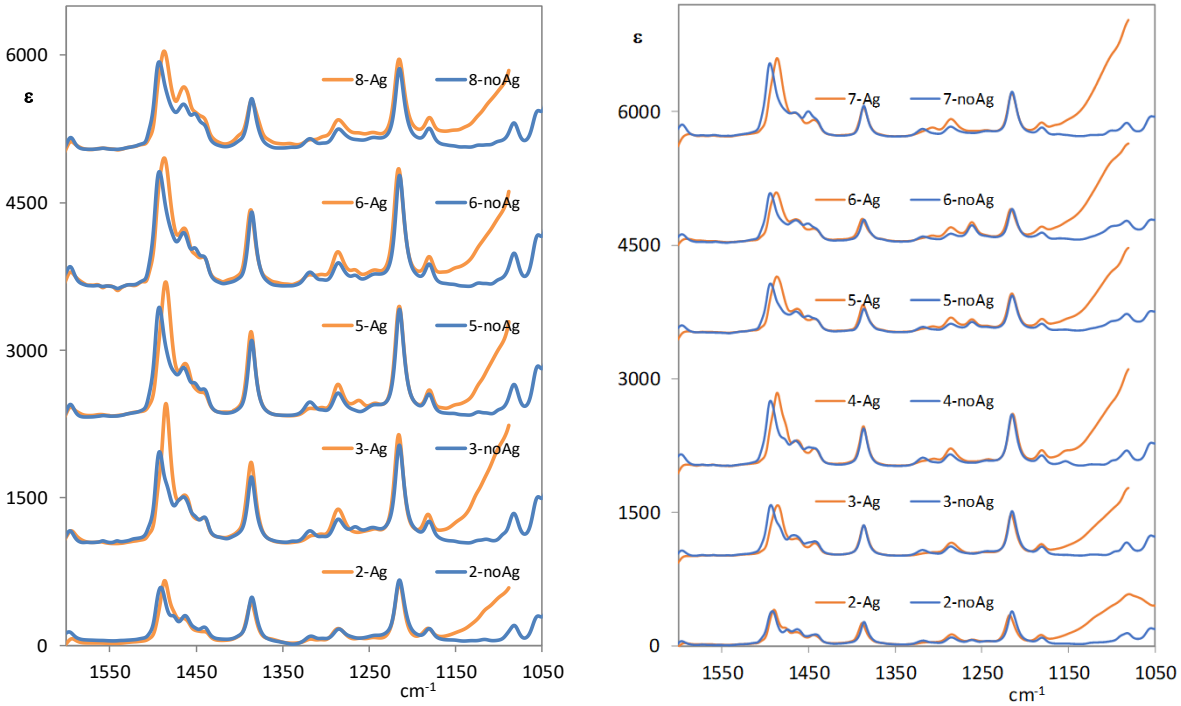
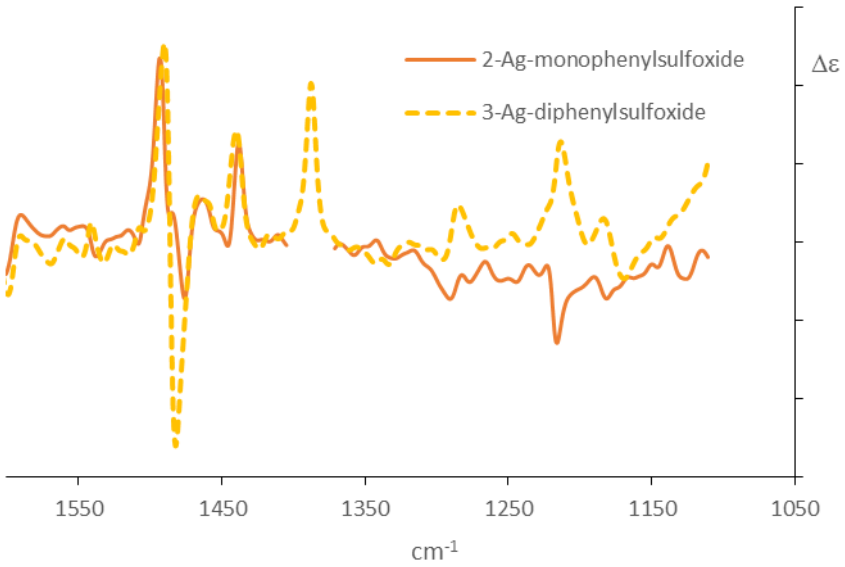


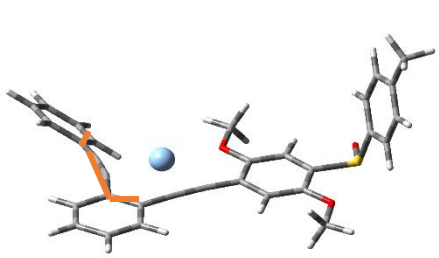
Figure S63. Superposition of VCD spectra of monosulfoxide (*S*)-**2**(two CC triple bonds) and disulfoxide (*S,S*)-**3**(three CC triple bonds)[S2] after normalization of the corresponding absorption spectra



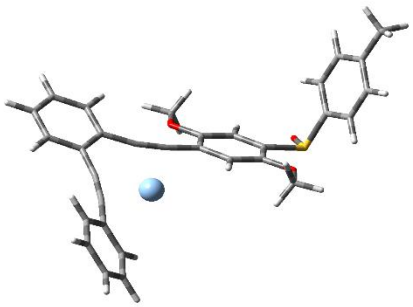
Analysis of (S)-2 structure in presence of Ag(I) cation

In order to calculate VCD spectra, DFT calculation, iefpcm solvent model, at B3LYP/6-31G** level have been performed. To describe Ag, we adopted the Stuttgart/Cologne energy-consistent pseudopotentials ECP28MDF and the associated basis sets ECP28MDF_VDZ. The Gaussian code has been used[S3]. Spectra have been simulated with Lorentzian functions centered at the computed normal mode wavenumbers. Linewidth was assumed equal to 12 cm-1. To further facilitate comparison of observed and calculated spectra, 0.973 scaling factor was applied to the calculated wavenumbers.[S3]

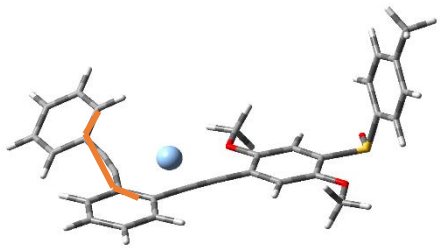
Figure S64. Four different structures are possible, as represented below. Conformer-c and conformer-d are by far at higher energy (more than 6 Kcal/mol) and thus they are not populated. The diphenylacetylene moiety presents high mobility.



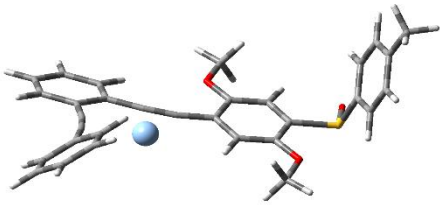
conformer-a



conformer-c



conformer-b



conformer-d

Figure S65. Libration energy curve describing interconversion from conformer-a to -b (energy in Kcal/mol), as function of torsion within the diphenylacetylene moiety: energy values obtained through a relaxed scan with respect to the dihedral angle indicated in the previous figure.

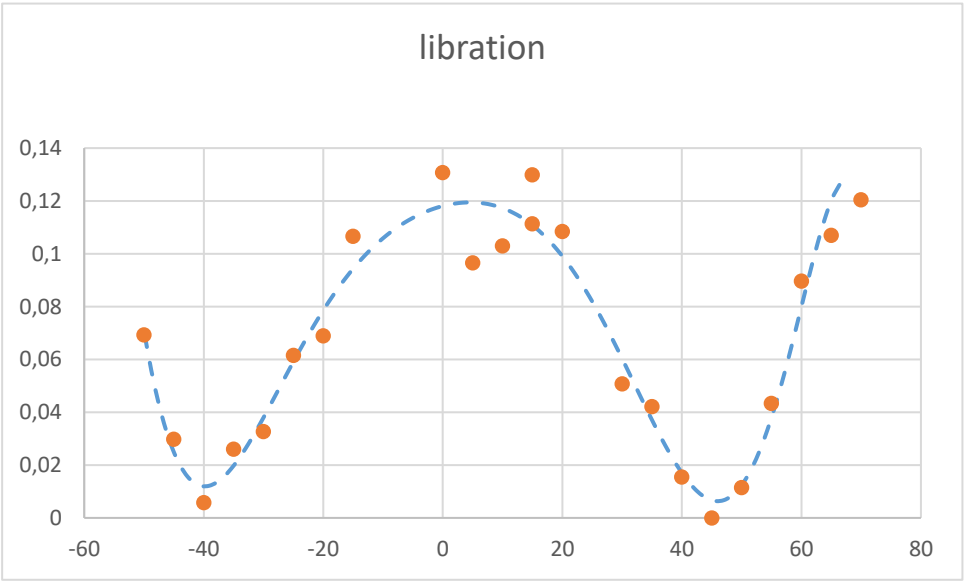
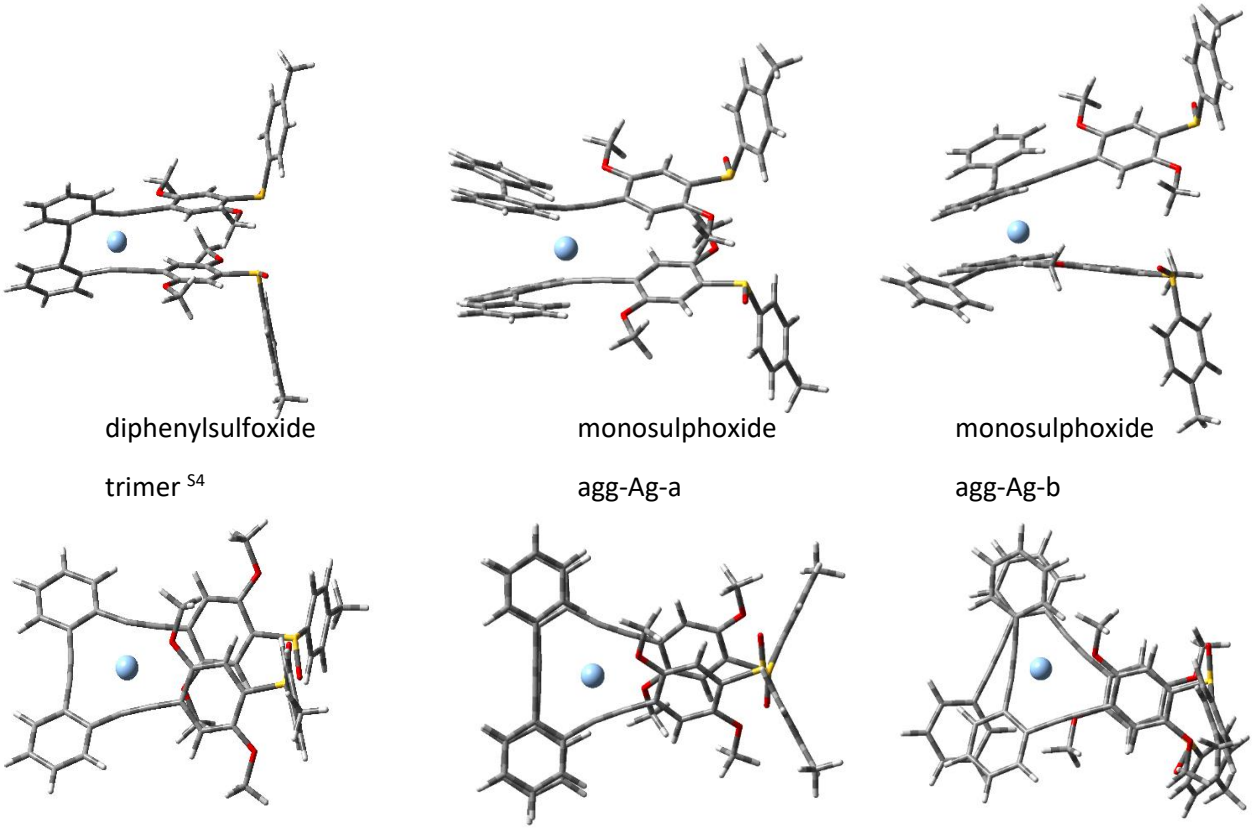


Figure S66. Examples of aggregates of two (*S*)-**2** molecules hosting an Ag(I) cation(agg-Ag-a and agg-Ag-b) , first and second row show the same structures from different points of view. The structure represented in the middle (agg-Ag-a) is particularly similar to the structure of the trimer-diphenylsulfoxide[S2]represented on the right.

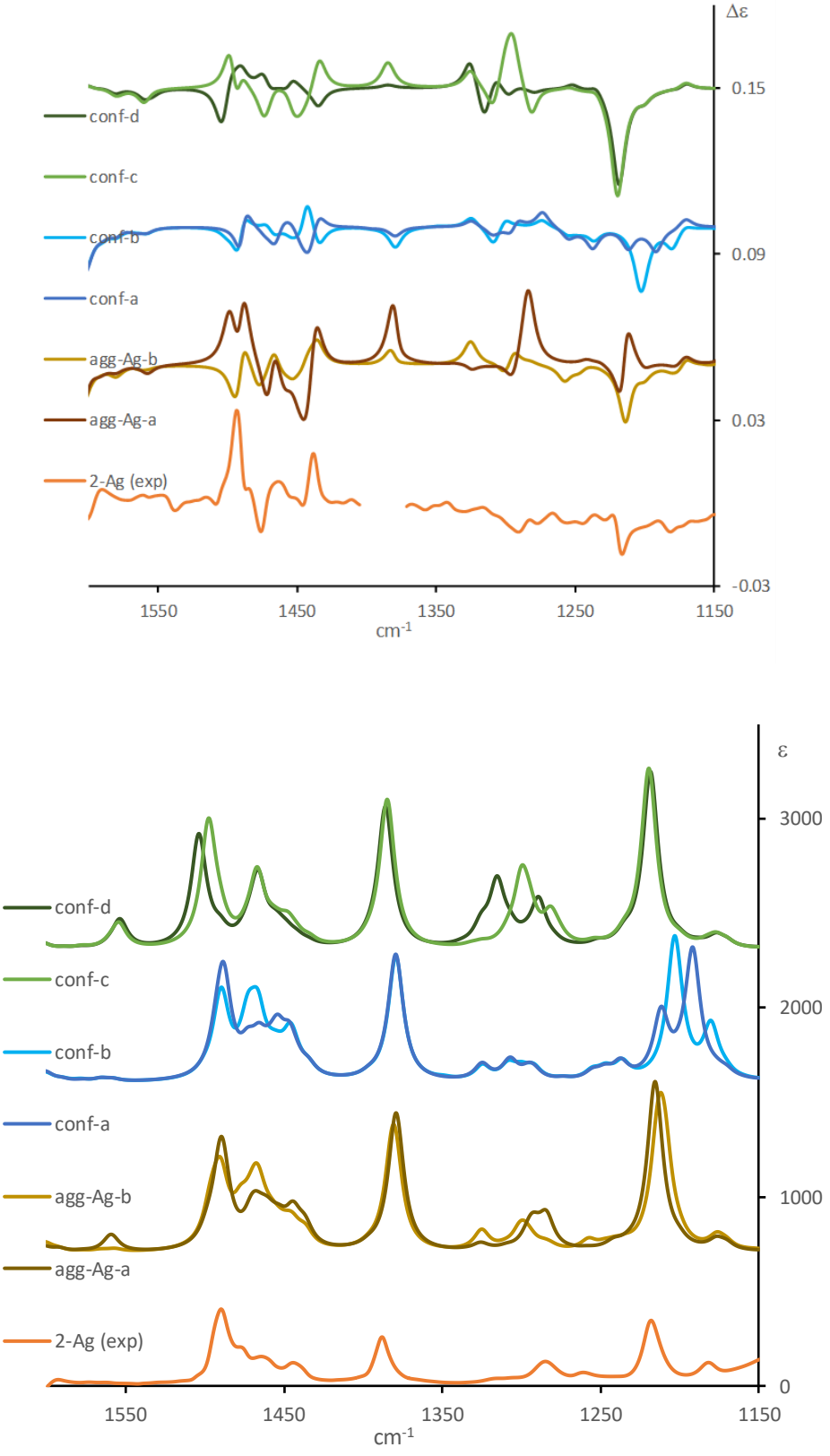


diphenylsulfoxide trimer [S4]

monosulphoxide agg-Ag-a

monosulphoxide agg-Ag-b

Figure S67. Calculated VCD (up) and IR (down) spectra considering the four monomers of monosulphoxide (*S*)-**2** compound previously discussed and the two aggregated structures agg-Ag-a and agg-Ag-b. The analysis does not pretend to be exhaustive but still suggests that some aggregation mediated by silver for these molecules may be responsible of the VCD observations.



Atomic coordinates of DFT optimized structures of Ag(I) complexes of compounds (S)-3 to (S)-7, the four conformers of Ag(I) complex of (S)-2and aggregates of two (S)-2 molecules and Ag(I)

Table S2. Atomic coordinates of (*S*)-**3**:Ag(I) complex

S	4.582478	-1.407831	0.653305
O	4.286732	-2.604509	-0.216142
O	0.005594	-0.232986	-1.447757
C	0.181524	-1.306696	-2.362586
H	0.326915	-2.256336	-1.829598
H	1.034583	-1.113905	-3.02486
H	-0.738131	-1.351432	-2.950175
O	3.920983	0.963323	2.246859
C	-5.462959	-0.7912	-0.463029
C	-4.798893	-2.02911	-0.275612
C	-3.946087	2.955078	-0.050403
C	1.005763	-4.121547	0.696329
H	1.539295	-4.936378	0.211743
C	-4.331283	1.591896	-0.213176
C	-2.607192	3.357478	0.182161
C	-3.415754	-2.112919	0.080257
C	-0.280934	-3.799444	0.286018
C	-6.826396	-0.786324	-0.788338
H	-7.327923	0.16898	-0.927787
C	6.669076	0.250473	-2.401102
H	6.727578	0.130199	-3.483045
C	1.004819	0.036401	-0.567983
C	1.616949	-3.397528	1.717803
C	-0.964571	-2.735473	0.896714
C	1.738973	1.446104	1.283223
H	1.531021	2.271936	1.958643
C	2.187635	-0.687515	-0.477679
H	2.401096	-1.558099	-1.097367
C	-7.522811	-1.97667	-0.934964
H	-8.579312	-1.954637	-1.191332
C	6.536242	0.55405	0.366829
H	6.483256	0.664507	1.448914
C	7.498376	1.184137	-1.77199
C	5.780087	-0.525799	-1.668012
H	5.144657	-1.269782	-2.147475
C	-1.516421	2.435008	0.225893
C	0.773156	1.102878	0.324149
C	-2.328669	4.718161	0.370922
H	-1.299418	5.020414	0.55164
C	-4.798854	0.463184	-0.325295

C	-0.344111	-2.011291	1.928082
H	-0.876271	-1.184482	2.399408
C	3.123913	-0.337249	0.478733
C	0.939676	-2.347379	2.334465
C	2.927024	0.728025	1.363621
C	-2.28028	-2.391324	0.457005
C	-4.656524	5.269069	0.082178
H	-5.452315	6.008857	0.038949
C	5.717022	-0.357952	-0.29059
C	-4.954862	3.927797	-0.101614
H	-5.97917	3.609901	-0.283607
C	-5.520341	-3.219415	-0.429655
H	-5.005298	-4.1667	-0.285444
C	7.416811	1.325071	-0.383031
H	8.063268	2.045839	0.118082
C	-3.341849	5.664352	0.322748
H	-3.103926	6.715154	0.470473
C	-0.457334	1.817615	0.269894
C	8.479527	1.996341	-2.562065
H	9.491197	1.5739	-2.486263
H	8.535985	3.028532	-2.194715
H	8.215713	2.024242	-3.625735
C	-6.868456	-3.194128	-0.757368
H	-7.410344	-4.129795	-0.873517
C	3.723966	1.982203	3.209312
H	4.62071	1.992034	3.831711
H	2.846866	1.767946	3.835362
H	3.602895	2.962676	2.729089
Ag	-2.291105	0.067616	-0.239492
H	-0.767445	-4.358639	-0.511789
H	1.4234	-1.774895	3.124271
H	2.631183	-3.64749	2.022945

E = -2271.0157617
H = -2270.422304
G = -2270.538564

Table S3. Atomic coordinates of (*S*)-**4**:Ag(I) complex

C	-1.960592000	2.744001000	2.448153000
C	-2.837799000	3.817666000	2.376636000
C	-4.203182000	3.597059000	2.202544000
C	-4.694898000	2.297137000	2.099038000
C	-3.826663000	1.216738000	2.172123000
C	-2.449258000	1.433432000	2.340115000
C	-1.557632000	0.321305000	2.318291000
C	-0.822606000	-0.647438000	2.239622000
C	-0.016893000	-1.809610000	2.090896000

C	-0.474394000	-2.878366000	1.275418000
C	0.328650000	-4.014987000	1.115011000
C	1.573571000	-4.088540000	1.725710000
C	2.030189000	-3.031694000	2.512174000
C	1.238955000	-1.906304000	2.700204000
H	-0.890356000	2.905025000	2.572720000
H	-5.760560000	2.125058000	1.959769000
H	-0.031661000	-4.832045000	0.492324000
H	2.194043000	-4.969625000	1.580820000
H	3.014879000	-3.083437000	2.971998000
H	1.588373000	-1.078711000	3.314861000
C	-1.724271000	-2.785446000	0.595002000
C	-2.794295000	-2.683769000	0.003325000
C	1.118514000	0.959002000	-0.317864000
C	2.017581000	1.674981000	0.488395000
C	3.230700000	1.105332000	0.858301000
C	3.526213000	-0.187786000	0.410838000
C	2.648377000	-0.914093000	-0.373961000
C	1.438047000	-0.343374000	-0.751168000
H	2.928316000	-1.934634000	-0.634579000
O	0.487148000	-0.980059000	-1.483219000
C	0.795756000	-2.251652000	-2.036014000
H	1.666745000	-2.183426000	-2.699706000
H	0.985474000	-2.990662000	-1.245560000
H	-0.083949000	-2.549011000	-2.611720000
O	4.164011000	1.697774000	1.633143000
C	3.887151000	2.989842000	2.138812000
H	3.749845000	3.713885000	1.324254000
H	4.755549000	3.276276000	2.735267000
S	5.039368000	-1.027020000	0.967402000
C	6.927055000	0.859252000	0.191218000
H	6.843866000	1.253036000	1.203175000
C	6.160077000	-0.227745000	-0.208065000
C	6.269602000	-0.759525000	-1.489265000
C	7.148744000	-0.174050000	-2.388051000
C	7.923096000	0.934643000	-2.021794000
C	8.865773000	1.554929000	-3.008123000
C	7.800792000	1.437734000	-0.725508000
H	8.407486000	2.292241000	-0.425885000
H	9.576268000	0.815179000	-3.399982000
H	8.324389000	1.963049000	-3.872282000
H	7.246229000	-0.582323000	-3.394604000
H	5.678591000	-1.634520000	-1.759426000
H	9.441673000	2.370978000	-2.557083000
O	4.877750000	-2.452777000	0.500698000
H	2.993032000	2.981666000	2.777574000
C	-3.902249000	0.792277000	-1.318372000
C	-4.238978000	-0.385666000	-1.231743000
C	-4.771428000	-1.709988000	-1.188240000
C	-4.085301000	-2.803732000	-0.600560000
C	-4.690682000	-4.067857000	-0.600392000
H	-4.158293000	-4.900832000	-0.146317000
H	-6.395726000	-5.245285000	-1.152276000
C	-5.944126000	-4.256124000	-1.163079000

C	-6.619070000	-3.181633000	-1.738912000
H	-7.601388000	-3.325321000	-2.182843000
C	-6.038741000	-1.922248000	-1.750393000
H	-6.558531000	-1.079779000	-2.201640000
C	-3.675560000	2.199534000	-1.399878000
C	-4.776490000	3.021601000	-1.680264000
C	-4.638070000	4.400735000	-1.730646000
C	-3.394948000	4.985428000	-1.497889000
C	-2.292028000	4.189188000	-1.227428000
C	-2.406315000	2.793256000	-1.183831000
C	-1.230073000	2.034404000	-0.903281000
C	-0.138166000	1.537190000	-0.654054000
H	-1.316831000	4.638439000	-1.050020000
H	-3.283211000	6.066714000	-1.530083000
H	-5.504415000	5.020913000	-1.948462000
H	-5.746710000	2.557676000	-1.846201000
H	1.737504000	2.672328000	0.817880000
Ag	-1.861029000	-0.395973000	-0.449693000
H	-2.454570000	4.833351000	2.453471000
H	-4.886267000	4.442190000	2.141434000
H	-4.197366000	0.194906000	2.086995000

E = -2577.9981848
H = -2577.305838
G = -2577.433301

Table S4. Atomic coordinates of (*S*)-**5**:Ag(I) complex

S	-5.048091	-1.292467	-0.887305
O	-0.753031	-1.110115	1.98465
C	1.338608	2.97085	-1.79382
C	0.658374	1.747253	-2.063262
C	2.097205	2.51206	2.088561
O	-4.294061	1.517438	-1.329642
O	-4.835214	-2.73257	-0.489548
C	3.132442	-2.348319	1.588508
C	0.595282	-2.012974	-1.072452
C	-0.48913	-1.73374	-1.960275
C	0.072419	0.68744	-2.236732
C	-0.918889	-2.494351	2.230616
H	-0.88268	-3.068398	1.291963
H	-1.865371	-2.695969	2.749956
H	-0.084675	-2.791427	2.87054
C	0.84997	1.963704	1.676931
C	-2.793073	-1.1175	0.664521
H	-3.024274	-2.169204	0.831497
C	2.361089	-3.037966	0.617468
C	-6.473274	-1.259769	1.474837
H	-5.855504	-2.120293	1.73061
C	4.032401	0.680183	-1.331136

C	-1.668117	-0.496411	1.204456
C	3.216652	1.660759	2.287149
C	3.068616	-0.935818	1.783183
C	-7.442467	-0.781124	2.343582
H	-7.58563	-1.259938	3.312961
C	2.708322	2.966434	-1.421068
C	1.429398	-2.400517	-0.258018
C	2.241747	3.890372	2.278504
H	1.381316	4.536011	2.113452
C	-0.740831	-0.451885	-2.512931
C	4.306997	-1.616773	-2.133031
C	-3.645486	-0.398662	-0.15377
C	-1.417288	0.855768	0.892535
C	-6.300795	-0.634889	0.24381
C	5.721115	-0.798993	-0.337002
H	6.014202	0.011094	0.329321
C	-1.367364	-2.788173	-2.250393
H	-1.177219	-3.764364	-1.808042
C	4.911764	-2.862386	-2.035454
H	4.598723	-3.66851	-2.696076
C	-8.247404	0.311092	1.994995
C	0.644894	4.18604	-1.837791
H	-0.404623	4.185101	-2.126255
C	3.379403	-5.130236	1.307566
H	3.469512	-6.208425	1.198267
C	2.495625	-4.429293	0.500924
H	1.897832	-4.949936	-0.244515
C	4.439751	2.218515	2.677838
H	5.29386	1.561674	2.830709
C	-2.71783	-1.332418	-3.61261
H	-3.585956	-1.169714	-4.247431
C	-8.058285	0.911089	0.748895
H	-8.683835	1.757103	0.464141
C	4.705276	-0.576366	-1.278615
C	3.334599	4.173197	-1.093441
H	4.380304	4.157211	-0.791671
C	4.025686	-3.076695	2.386423
H	4.622149	-2.539628	3.121155
C	-2.472035	-2.591003	-3.066213
H	-3.152696	-3.416579	-3.260416
C	4.148599	-4.451373	2.250118
H	4.846389	-4.995055	2.882752
C	4.56111	3.589001	2.868178
H	5.517642	4.007176	3.173231
C	-2.295028	1.567284	0.058995
H	-2.052341	2.600523	-0.176416
C	1.286648	5.375263	-1.517397
H	0.734871	6.311736	-1.555676

C	-1.860403	-0.276682	-3.338361
H	-2.048865	0.709465	-3.75875
C	3.463716	4.424041	2.666279
H	3.56087	5.497938	2.809712
C	3.122777	0.258614	2.043483
C	5.913649	-3.080891	-1.0917
C	-3.41113	0.941755	-0.481312
C	-0.211335	1.462884	1.3397
C	6.318361	-2.048753	-0.246791
C	3.426619	1.739134	-1.359567
C	-7.0917	0.441889	-0.136772
H	-6.95304	0.914692	-1.108284
C	-4.030753	2.840955	-1.75149
H	-4.82298	3.102108	-2.455758
H	-3.055151	2.907924	-2.256409
H	-4.050231	3.540079	-0.904391
C	2.629019	5.368109	-1.142435
H	3.128588	6.299291	-0.883958
C	-9.299269	0.805049	2.94149
H -	10.099989	0.063291	3.065861
H	-9.757852	1.734828	2.586015
H	-8.881641	0.990689	3.939698
Ag	1.602007	0.098303	-0.141474
H	3.517137	-1.434522	-2.861431
H	6.378535	-4.061735	-1.010011
H	7.098706	-2.221694	0.49187

E = =-2884.9814075
H = -2884.193158
G = -2884.335195

Table S5. Atomic coordinates of (*S*)-**6**:Ag(I) complex

S	5.358595	-1.153699	0.189448
O	5.248825	-2.411238	-0.637532
O	1.124994	-0.324069	-2.657798
C	-2.994594	2.079463	-2.295723
C	-2.760584	0.680422	-2.402784
C	-2.587441	2.91949	1.882923
C	-3.410545	1.918444	1.293065
C	1.485968	-1.463403	-3.413997
H	1.522378	-2.364031	-2.782357
H	2.459012	-1.323238	-3.904604
H	0.710781	-1.585734	-4.174313
C	1.001111	-0.689108	2.169129
O	4.404178	1.316088	1.467183

C	-0.65923	-2.14298	-0.78179
C	-1.444455	-2.68365	-1.841768
C	-2.538409	-0.520815	-2.420482
C	-3.987171	-1.644992	0.951276
C	-0.871209	-2.580855	4.589365
H	-0.597108	-2.055681	5.502435
C	1.022113	-1.733138	1.21475
C	0.330461	1.811848	-1.160787
C	-1.827408	-2.036817	3.742435
C	-1.264012	2.661673	2.312799
C	0.069668	0.389416	2.126505
C	-1.998492	2.912762	-1.722846
C	-5.014819	-1.069357	0.155324
C	0.074349	-1.858048	0.157341
C	-3.111318	4.212619	2.020725
H	-4.12809	4.40028	1.681225
C	7.800634	0.461987	-2.616039
H	8.009122	0.309789	-3.675623
C	-2.350775	-1.918989	-2.617223
C	1.951918	0.043647	-1.657759
C	-4.243942	1.184143	0.783894
C	-0.261362	-3.791619	4.268162
C	-2.181159	-2.707635	2.561327
C	2.381625	1.629373	0.148885
H	2.050642	2.498036	0.714304
C	-5.174876	0.33818	0.120567
C	-1.292219	-4.051035	-2.118283
H	-0.587729	-4.628278	-1.521701
C	3.129179	-0.624297	-1.323984
H	3.449551	-1.532599	-1.832943
C	7.284783	0.848621	0.09558
H	7.082977	0.991576	1.156173
C	-4.222147	2.635267	-2.673808
H	-4.976876	1.991918	-3.122697
C	2.96806	-2.682148	2.312651
H	3.736573	-3.451121	2.356122
C	8.509817	1.444826	-1.914173
C	-6.216807	0.895487	-0.631707
H	-6.335317	1.97769	-0.648341
C	-7.06916	0.079335	-1.362334
H	-7.872116	0.523864	-1.946085
C	6.843604	-0.317477	-1.982805
H	6.299143	-1.097066	-2.515032
C	2.014675	-2.720577	1.306249
H	2.033387	-3.511789	0.558059
C	-0.512911	3.704892	2.87416
H	0.502327	3.496875	3.207546
C	-2.92465	-3.909151	-3.882094

H	-3.501925	-4.381689	-4.673455
C	1.569066	1.171133	-0.899712
C	-2.281752	4.262938	-1.493791
H	-1.520946	4.889824	-1.031414
C	1.963435	-0.677665	3.190736
H	1.930631	0.123021	3.928132
C	-5.875666	-1.874529	-0.59838
H	-5.739974	-2.953979	-0.575858
C	-2.023247	-4.658677	-3.127792
H	-1.891407	-5.720117	-3.324685
C	2.936711	-1.662227	3.264013
H	3.677617	-1.630209	4.059609
C	-1.049381	4.977189	3.003179
H	-0.449945	5.773314	3.438602
C	-1.564677	-3.927738	2.243594
H	-1.836346	-4.437362	1.319776
C	-4.479449	3.981863	-2.452618
H	-5.439485	4.401884	-2.744852
C	-3.084664	-2.55502	-3.628863
H	-3.780322	-1.961261	-4.218333
C	-2.351409	5.231927	2.574393
H	-2.776255	6.228201	2.67379
C	-0.638242	1.386178	2.188778
C	3.908055	-0.164658	-0.277158
C	-0.606373	-4.460426	3.094307
C	-3.14832	-2.138276	1.684777
C	-6.890819	-1.303792	-1.354566
H	-7.552198	-1.941899	-1.936536
C	3.559311	0.965781	0.469107
C	-0.741437	2.348455	-1.378366
C	6.587838	-0.10803	-0.631602
C	8.238677	1.625122	-0.556488
H	8.789612	2.382867	0.000732
C	9.552428	2.265213	-2.61129
H	10.442015	1.663083	-2.842022
H	9.876409	3.113426	-1.997292
H	9.178721	2.65788	-3.565784
C	-3.515555	4.79104	-1.851216
H	-3.725076	5.842499	-1.666204
C	4.036043	2.413112	2.277468
H	4.815614	2.51321	3.035419
H	3.068533	2.233837	2.769972
H	3.977631	3.339483	1.68947
Ag	-1.728144	0.046096	0.172007
H	-2.304251	-1.084906	3.974665
H	0.49436	-4.210763	4.929994
H	-0.123464	-5.402703	2.842359

E = -3191.9605476

H = -3191.073227

G = -3191.227681

Table S6. Atomic coordinates of (*S*)-**6**:Ag_2(I) complex

S	-5.891688	-1.526532	-0.842733
O	-5.518041	-2.77476	-0.081836
O	-1.913895	-0.043667	2.097656
C	1.864738	3.638699	1.313381
C	2.287874	2.32197	1.663949
C	2.044512	2.528689	-2.061565
C	3.161186	1.759851	-1.617963
C	-2.181903	-1.13849	2.968039
H	-2.197863	-2.087035	2.41576
H	-3.139957	-0.991613	3.480955
H	-1.366674	-1.150065	3.694769
C	-0.749966	-1.624434	-1.080321
O	-5.375597	1.116723	-2.039716
C	1.718657	-1.479653	1.523865
C	2.972291	-1.238787	2.171085
C	2.798883	1.241664	1.946701
C	4.575184	-1.737993	-0.862929
C	2.258724	-5.966214	-0.215572
H	2.362834	-6.756598	0.524514
C	-0.33292	-2.33823	0.075896
C	-1.479444	2.253244	0.662606
C	3.117525	-4.875977	-0.179815
C	0.744934	1.981112	-2.207993
C	-0.101396	-0.419184	-1.480059
C	0.537894	3.949747	0.919381
C	5.589604	-0.769466	-0.581939
C	0.759165	-1.877008	0.867617
C	2.250285	3.88203	-2.363185
H	3.245642	4.302576	-2.236292
C	-8.571656	-0.591867	2.051138
H	-8.748695	-0.866373	3.091178
C	3.514651	0.063616	2.313699
C	-2.800949	0.222051	1.09926
C	4.17822	1.181781	-1.24743
C	1.269341	-6.047633	-1.193502
C	2.987768	-3.852197	-1.131287
C	-3.4467	1.741926	-0.692834
H	-3.267365	2.672992	-1.224928
C	5.396749	0.62489	-0.758153
C	3.720643	-2.343703	2.597389
H	3.284928	-3.336629	2.504651
C	-3.828195	-0.636695	0.728673
H	-3.998501	-1.598728	1.212203
C	-8.146277	0.089409	-0.618339
H	-7.984489	0.338842	-1.666102

C	2.825846	4.659403	1.35061
H	3.841279	4.411805	1.653477
C	-2.078448	-3.967834	-0.324337
H	-2.598922	-4.876201	-0.030831
C	-9.44502	0.301357	1.422743
C	6.43705	1.506342	-0.432449
H	6.28291	2.573874	-0.574601
C	7.641865	1.028593	0.061916
H	8.437052	1.727515	0.309774
C	-7.491193	-1.136516	1.368599
H	-6.81806	-1.849122	1.843963
C	-1.000579	-3.517068	0.428139
H	-0.668218	-4.068945	1.305547
C	-0.291842	2.791922	-2.690443
H	-1.282204	2.355665	-2.813437
C	5.543	-0.898878	3.226022
H	6.544924	-0.764706	3.627312
C	-2.591716	1.410642	0.372156
C	0.223104	5.271526	0.575845
H	-0.795248	5.502809	0.26977
C	-1.838023	-2.094497	-1.824111
H	-2.155808	-1.53656	-2.702643
C	6.815333	-1.230415	-0.084818
H	6.956116	-2.301132	0.048804
C	4.994278	-2.176063	3.121918
H	5.562674	-3.045143	3.44433
C	-2.50144	-3.253823	-1.44338
H	-3.35489	-3.601203	-2.019896
C	-0.063112	4.124986	-2.997626
H	-0.878966	4.740193	-3.369396
C	2.000719	-3.949458	-2.125006
H	1.91165	-3.160128	-2.872711
C	2.490517	5.96147	1.009923
H	3.248222	6.740289	1.050129
C	4.808106	0.210427	2.833002
H	5.225482	1.210823	2.927584
C	1.206463	4.673023	-2.820412
H	1.387223	5.721011	-3.048243
C	0.421064	0.638678	-1.830983
C	-4.652121	-0.297859	-0.328859
C	1.144677	-5.041179	-2.14914
C	3.836194	-2.70458	-1.042266
C	7.831655	-0.341164	0.234183
H	8.775839	-0.71985	0.618674
C	-4.49132	0.893822	-1.04624
C	-0.498959	2.971401	0.826985
C	-7.283898	-0.780046	0.042258
C	-9.21928	0.627981	0.081508

H	-9.905665	1.307879	-0.423474
C	-10.596663	0.906484	2.166631
H	-11.501876	0.938367	1.547473
H	-10.374823	1.941554	2.461651
H	-10.826729	0.346468	3.080381
C	1.187054	6.268129	0.623952
H	0.9203	7.288407	0.35851
C	-5.243184	2.303403	-2.80084
H	-6.067098	2.299076	-3.516596
H	-4.288408	2.320257	-3.345312
H	-5.3192	3.193594	-2.162253
Ag	2.447379	-0.656995	-1.374979
Ag	0.404365	0.687043	1.487174
H	0.378086	-5.11029	-2.917894
H	0.595168	-6.901375	-1.213523
H	3.897343	-4.806555	0.576822

E = -3337.6096998
H = -3336.719142
G = -3336.878189

Table S7. Atomic coordinates of (*S*)-**7**:Ag(I) complex

S	-5.782771	0.129771	1.03941
O	-5.958753	1.610074	1.275948
O	-2.030937	2.238865	-1.822585
C	2.313482	1.022844	-3.431275
C	1.942476	2.046003	-2.515557
C	2.615573	-2.513835	-0.967243
C	3.210341	-1.235742	-0.76184
C	-2.587263	3.502115	-1.514906
H	-2.610469	3.669748	-0.42725
H	-3.60296	3.601241	-1.921999
H	-1.936163	4.244805	-1.981976
C	-1.222478	-0.779388	1.890816
O	-4.371948	-2.313343	0.239946
C	-0.117513	2.537098	0.716047
C	0.439767	3.787163	0.315784
C	1.62441	2.869755	-1.672263
C	3.460335	1.613047	1.492931
C	0.879243	-0.791633	4.875029
H	0.827136	-1.836576	5.175017
C	-1.46035	0.614664	1.935433
C	-0.797326	-0.152964	-2.264344
C	1.779506	-0.424435	3.866238
C	1.371622	-2.883516	-0.400731
C	-0.211393	-1.370816	1.079032

C	1.503782	-0.136295	-3.551414
C	4.38467	1.923574	0.458561
C	-0.678073	1.575505	1.229721
C	3.29935	-3.433481	-1.773963
H	4.25659	-3.137897	-2.199997
C	-8.518179	0.276355	-1.952179
H	-8.907177	1.024647	-2.643504
C	1.285968	3.949567	-0.808707
C	-2.645798	1.148299	-1.320158
C	3.879584	-0.217333	-0.660971
C	0.070781	0.158383	5.483337
C	1.844928	0.935794	3.468032
C	-2.609448	-1.282789	-1.084928
H	-2.100151	-2.221192	-1.293697
C	4.62943	0.988165	-0.578207
C	0.112608	4.908801	1.093289
H	-0.54826	4.775787	1.948316
C	-3.817529	1.18235	-0.564969
H	-4.315875	2.112989	-0.295368
C	-7.539275	-1.641306	-0.18258
H	-7.157566	-2.383889	0.516903
C	3.509018	1.104927	-4.154028
H	4.118924	2.002177	-4.064789
C	-3.336058	0.239095	3.42953
H	-4.16101	0.63884	4.015472
C	-9.033078	-1.025488	-1.994529
C	5.582252	1.284199	-1.561837
H	5.772505	0.552485	-2.345002
C	6.258356	2.496111	-1.544297
H	6.994227	2.714062	-2.315144
C	-7.528053	0.623491	-1.044659
H	-7.135741	1.6388	-0.990503
C	-2.520979	1.102764	2.714021
H	-2.702632	2.176718	2.731384
C	0.857988	-4.163133	-0.657935
H	-0.10019	-4.438963	-0.22067
C	1.467561	6.318082	-0.31163
H	1.872128	7.297731	-0.555583
C	-2.034061	-0.098657	-1.571069
C	1.944147	-1.202814	-4.341944
H	1.331314	-2.100648	-4.403581
C	-2.049378	-1.635729	2.635496
H	-1.854462	-2.706588	2.60297
C	5.065929	3.146209	0.450583
H	4.865364	3.864453	1.243079
C	0.618107	6.161979	0.782701
H	0.352156	7.018539	1.397866
C	-3.095083	-1.134672	3.39519

H	-3.729374	-1.816562	3.957099
C	1.552853	-5.061179	-1.455084
H	1.136267	-6.048165	-1.643366
C	1.026033	1.882382	4.096632
H	1.084871	2.922438	3.779105
C	3.921349	0.043129	-4.948425
H	4.855963	0.113867	-5.50067
C	1.796167	5.22358	-1.097397
H	2.452876	5.337458	-1.957479
C	2.775465	-4.69485	-2.014909
H	3.323465	-5.395118	-2.641508
C	0.589393	-2.006549	0.406616
C	-4.355915	0.005251	-0.076294
C	0.143228	1.496586	5.095236
C	2.712912	1.321241	2.409784
C	5.990883	3.431242	-0.544919
H	6.514592	4.38461	-0.536078
C	-3.767364	-1.240307	-0.320002
C	0.271667	-0.191997	-2.84757
C	-7.040141	-0.344891	-0.17314
C	-8.529972	-1.974165	-1.101912
H	-8.927841	-2.988852	-1.122043
C -	10.124039	-1.377848	-2.959798
H -	11.097345	-1.011072	-2.60501
H -	10.210773	-2.462466	-3.092522
H	-9.951779	-0.923942	-3.943835
C	3.14776	-1.114723	-5.028853
H	3.480982	-1.951554	-5.638971
C	-3.782045	-3.579994	0.03266
H	-4.399036	-4.299457	0.574811
H	-2.754725	-3.609847	0.427262
H	-3.766462	-3.842134	-1.03437
Ag	1.247825	0.502021	-0.169098
H	-0.627698	-0.146505	6.260043
H	-0.494503	2.238889	5.570663
C	2.609421	-1.392251	3.239346
C	6.116592	-3.518941	0.602074
H	7.031909	-3.158325	0.136119
C	5.330559	-2.645826	1.341952
C	5.735422	-4.851822	0.456843
C	4.148673	-3.101689	1.947027
C	3.777172	-4.447461	1.804299
H	2.855668	-4.796496	2.268303
C	4.567448	-5.313329	1.060717
C	3.320108	-2.191798	2.662001
H	5.614598	-1.600669	1.460043
H	6.351459	-5.5325	-0.128182
H	4.267685	-6.35358	0.946275

E = -3498.9364434
H = -3497.952886
G = -3498.121677

Table S8. Atomic coordinates of (*S*)-**7**:Ag_2(I) complex

S	5.908031	-1.535723	0.462714
O	5.566865	-2.796304	-0.29257
O	1.912717	-0.15368	-2.508471
C	-1.782198	3.569072	-1.941028
C	-2.159806	2.253279	-2.344805
C	-1.623754	2.600361	1.608784
C	-2.729102	1.870311	1.077849
C	2.081242	-1.36434	-3.237553
H	2.023636	-2.236949	-2.572054
H	3.04106	-1.362189	-3.767725
H	1.260319	-1.396922	-3.95703
C	0.863143	-1.70938	0.715328
O	5.492978	1.194485	1.464893
C	-1.690454	-1.557313	-1.86818
C	-2.855129	-1.330882	-2.66659
C	-2.633075	1.161823	-2.647632
C	-4.545064	-1.518647	0.281197
C	-1.474432	-4.979442	1.993415
H	-0.701593	-5.010552	2.759061
C	0.277402	-2.466204	-0.333677
C	1.568178	2.238741	-1.228014
C	-2.227641	-3.809839	1.843486
C	-0.33753	2.031145	1.791931
C	0.383689	-0.407289	1.046844
C	-0.480219	3.896422	-1.481773
C	-5.349047	-0.420958	-0.15351
C	-0.788175	-1.94898	-1.129379
C	-1.831026	3.941408	1.956653
H	-2.81414	4.38013	1.796835
C	8.725378	-0.641514	-2.307378
H	8.926844	-0.889548	-3.349943
C	-3.310156	-0.036433	-3.028303
C	2.832872	0.155797	-1.554839
C	-3.747414	1.345416	0.634435
C	-1.704937	-6.077685	1.175522
C	-3.220222	-3.748741	0.830567
C	3.570396	1.790499	0.096437
H	3.431094	2.764135	0.560212
C	-4.968732	0.935325	0.017022
C	-3.593101	-2.454515	-3.063568

H	-3.230153	-3.442561	-2.785032
C	3.840508	-0.707301	-1.138538
H	3.971892	-1.708016	-1.55141
C	8.228684	-0.011895	0.362691
H	8.030938	0.225825	1.407209
C	-2.769774	4.564377	-1.965755
H	-3.766509	4.304045	-2.317551
C	1.801494	-4.285023	0.144046
H	2.16116	-5.287957	-0.072209
C	9.621096	0.184588	-1.616485
C	-5.806991	1.94854	-0.469027
H	-5.504579	2.984525	-0.328743
C	-6.994354	1.63904	-1.115852
H	-7.631037	2.438891	-1.486263
C	7.59509	-1.148809	-1.683597
H	6.903967	-1.809744	-2.20618
C	0.74844	-3.759263	-0.593297
H	0.274747	-4.34201	-1.381604
C	0.681388	2.809029	2.357495
H	1.66005	2.355476	2.509703
C	-5.218904	-1.040612	-4.137347
H	-6.139924	-0.92327	-4.703553
C	2.681236	1.404611	-0.9216
C	-0.219129	5.204533	-1.051935
H	0.778053	5.445094	-0.688648
C	1.92383	-2.256701	1.445062
H	2.372321	-1.666833	2.242657
C	-6.552267	-0.710446	-0.812181
H	-6.840047	-1.751854	-0.940083
C	-4.764488	-2.311931	-3.792951
H	-5.324696	-3.194755	-4.091351
C	2.394874	-3.531368	1.155034
H	3.22687	-3.939334	1.723335
C	0.45092	4.131209	2.710897
H	1.25335	4.719586	3.149482
C	-3.443817	-4.870156	0.02148
H	-4.212275	-4.818564	-0.747906
C	-2.48744	5.854386	-1.540387
H	-3.266721	6.612283	-1.566084
C	-4.49854	0.084269	-3.760654
H	-4.84805	1.078172	-4.031956
C	-0.803231	4.700201	2.499746
H	-0.985114	5.739766	2.762522
C	-0.021653	0.694721	1.401877
C	4.700023	-0.312949	-0.129656
C	-2.693097	-6.02555	0.194073
C	-3.948967	-2.548346	0.576577
C	-7.366071	0.307285	-1.288742

H	-8.294328	0.059214	-1.798148
C	4.589666	0.934199	0.497795
C	0.577576	2.941874	-1.391498
C	7.354302	-0.819561	-0.35379
C	9.35603	0.491059	-0.280096
H	10.049943	1.127117	0.269212
C	10.850504	0.703986	-2.297854
H	11.596467	-0.092211	-2.427558
H	11.323077	1.507513	-1.721363
H	10.620401	1.090234	-3.298954
C	-1.211077	6.174002	-1.080978
H	-0.987595	7.182905	-0.742192
C	5.461636	2.465836	2.086515
H	6.299348	2.483269	2.786314
H	4.523337	2.615306	2.638759
H	5.585652	3.267828	1.346468
Ag	-2.264215	-0.611782	1.015259
H	-1.109572	-6.978697	1.304038
H	-2.87843	-6.887114	-0.44292
C	-1.959968	-2.686381	2.677279
C	-1.892252	1.593299	5.052067
H	-2.601207	2.410731	5.169138
C	-2.274908	0.443886	4.374036
C	-0.604769	1.701158	5.573247
C	-1.358694	-0.60653	4.201388
C	-0.068552	-0.499377	4.744244
H	0.636064	-1.31849	4.61003
C	0.300125	0.649742	5.429379
C	-1.705333	-1.742559	3.410331
H	-3.277946	0.353323	3.95609
H	-0.30631	2.606495	6.098379
H	1.301598	0.7317	5.846888
Ag	-0.401877	0.585792	-1.656361

E = -3644.5947705
H = -3643.605848
G = -3643.774334

Table S9. Atomic coordinates of compound -(*S*)-**2**with AgConf-a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.868446	-0.869536	1.690821
2	8	0	4.565373	-2.342250	1.928554

3	8	0	-0.174686	-1.322529	0.576745
4	6	0	0.003430	-2.749338	0.701002
5	1	0	0.345290	-3.004263	1.707344
6	1	0	0.715014	-3.109685	-0.046107
7	1	0	-0.976480	-3.185958	0.520213
8	8	0	4.213668	2.003252	1.306439
9	6	0	-5.454119	-1.538518	-0.294455
10	6	0	-5.227277	-2.566545	0.641932
11	6	0	-4.016965	2.243015	-0.402368
12	6	0	-4.232460	0.825586	-0.320074
13	6	0	-2.735294	2.831398	-0.206500
14	6	0	-6.451930	-1.700904	-1.278021
15	1	0	-6.626735	-0.909798	-1.999477
16	6	0	6.288812	-1.814353	-2.010973
17	1	0	6.215880	-2.658110	-2.692365
18	6	0	0.924993	-0.511360	0.750330
19	6	0	1.836282	1.754279	0.807285
20	1	0	1.667514	2.819037	0.713222
21	6	0	2.192089	-1.010913	1.048482
22	1	0	2.390683	-2.068425	1.181165
23	6	0	-7.203731	-2.872181	-1.316671
24	1	0	-7.970461	-2.991576	-2.075576
25	6	0	6.484759	0.342808	-0.245287
26	1	0	6.563003	1.178010	0.442336
27	6	0	7.069304	-0.703651	-2.368862
28	6	0	5.610402	-1.856193	-0.794279
29	1	0	5.024822	-2.722726	-0.503630
30	6	0	-1.580247	2.044467	0.080332
31	6	0	0.739053	0.885092	0.625041
32	6	0	-2.600706	4.229945	-0.301027
33	1	0	-1.623511	4.674999	-0.149391
34	6	0	-4.715379	-0.311453	-0.259235
35	6	0	3.260405	-0.139929	1.208047
36	6	0	3.101618	1.251510	1.104266
37	6	0	-4.959754	4.450509	-0.784234
38	1	0	-5.819321	5.073645	-1.007900
39	6	0	5.703591	-0.768528	0.073237
40	6	0	-5.116632	3.071319	-0.692071
41	1	0	-6.090708	2.618661	-0.841443
42	6	0	-5.984149	-3.733560	0.590576
43	1	0	-5.804987	-4.521520	1.315122
44	6	0	7.154400	0.369220	-1.469403
45	1	0	7.759564	1.234805	-1.725459
46	6	0	-3.701680	5.029826	-0.587246
47	1	0	-3.579209	6.105549	-0.658017
48	6	0	-0.533633	1.451699	0.328113
49	6	0	7.828319	-0.681648	-3.673759
50	1	0	8.817649	-1.141124	-3.557719
51	1	0	7.983873	0.340841	-4.028985
52	1	0	7.300799	-1.240501	-4.452082

53	6	0	-6.971920	-3.889359	-0.386494
54	1	0	-7.559506	-4.801375	-0.422607
55	6	0	4.094166	3.427458	1.260184
56	1	0	5.089350	3.815195	1.475044
57	1	0	3.389201	3.787898	2.017004
58	1	0	3.776480	3.764565	0.267707
59	1	0	-4.466888	-2.438052	1.405586
60	47	0	-2.299697	-0.373904	0.097910

SCF Done: E(RB3LYP) = -1966.32606128

Low frequencies --- 0.0005 0.0013 0.0017 4.0199 6.5627 10.5009

Low frequencies --- 12.7695 16.7531 21.5044

Table S10. Atomic coordinates of compound -(*S*)-**2**with AgConf-b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	4.891347	-0.699227	1.744346
2	8	0	4.598079	-2.143136	2.126966
3	8	0	-0.188800	-1.242837	0.866170
4	6	0	-0.023494	-2.632001	1.220428
5	1	0	0.356951	-2.720794	2.241096
6	1	0	0.651193	-3.127235	0.517577
7	1	0	-1.015810	-3.073235	1.155960
8	8	0	4.225625	2.121382	1.088037
9	6	0	-5.355466	-1.626450	-0.419669
10	6	0	-4.760159	-2.807227	-0.906227
11	6	0	-4.027724	2.196524	-0.513725
12	6	0	-4.218608	0.779230	-0.386320
13	6	0	-2.760410	2.814355	-0.314253
14	6	0	-6.688694	-1.657503	0.039581
15	1	0	-7.147262	-0.748861	0.415053
16	6	0	6.153176	-1.959340	-1.921868
17	1	0	6.036257	-2.849367	-2.534738
18	6	0	0.916620	-0.422013	0.915419
19	6	0	1.832090	1.832475	0.698165
20	1	0	1.661186	2.881678	0.495521
21	6	0	2.192808	-0.892782	1.221562
22	1	0	2.395960	-1.931724	1.455350
23	6	0	-7.405214	-2.850879	0.008818
24	1	0	-8.430912	-2.868842	0.363279
25	6	0	6.463088	0.317993	-0.332516
26	1	0	6.586126	1.199463	0.287570
27	6	0	6.944017	-0.898269	-2.390323
28	6	0	5.519609	-1.893150	-0.682239
29	1	0	4.926181	-2.721062	-0.307107
30	6	0	-1.600507	2.058249	0.030404
31	6	0	0.728378	0.953775	0.646356

32	6	0	-2.646545	4.210135	-0.460544
33	1	0	-1.679316	4.676765	-0.309947
34	6	0	-4.649998	-0.379808	-0.401487
35	6	0	3.266779	-0.014885	1.250779
36	6	0	3.106066	1.358543	1.005367
37	6	0	-5.002336	4.373363	-0.981074
38	1	0	-5.869007	4.973676	-1.237362
39	6	0	5.669192	-0.746209	0.096551
40	6	0	-5.137267	2.995455	-0.845273
41	1	0	-6.100862	2.521063	-0.995160
42	6	0	-5.486841	-3.994161	-0.929195
43	1	0	-5.023098	-4.900167	-1.306049
44	6	0	7.087215	0.236239	-1.577935
45	1	0	7.701892	1.064608	-1.920032
46	6	0	-3.756472	4.980484	-0.790012
47	1	0	-3.651059	6.055053	-0.896658
48	6	0	-0.551644	1.490782	0.325349
49	6	0	7.653025	-0.991578	-3.719938
50	1	0	8.652583	-1.427230	-3.599771
51	1	0	7.781024	-0.005286	-4.174908
52	1	0	7.104182	-1.626393	-4.421291
53	6	0	-6.808031	-4.019323	-0.472617
54	1	0	-7.370652	-4.947432	-0.492206
55	6	0	4.110075	3.531465	0.881162
56	1	0	5.113496	3.933642	1.016424
57	1	0	3.432785	3.982419	1.614279
58	1	0	3.760472	3.754044	-0.132704
59	1	0	-3.738340	-2.781025	-1.271800
60	47	0	-2.298960	-0.341922	0.249156

SCF Done: E(RB3LYP) = -1966.32605250

Low frequencies --- -0.0008 0.0005 0.0011 3.5139 4.5370 9.2124

Low frequencies --- 13.9742 18.0321 24.2505

Table S11. Atomic coordinates of compound -(*S*)-**2**with AgConf-c

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	5.021238	0.615508	1.741254
2	8	0	5.567603	-0.624646	2.434271
3	8	0	1.190597	-2.849992	1.210279
4	6	0	2.066651	-3.840655	1.755994
5	1	0	2.381366	-3.574463	2.770603
6	1	0	2.948209	-3.981790	1.121669
7	1	0	1.486779	-4.762679	1.784677
8	8	0	2.950898	2.360420	0.535100
9	6	0	-5.750141	1.540045	-0.174779

10	6	0	-5.534665	2.535529	0.798567
11	6	0	-3.997474	-2.079194	-0.709406
12	6	0	-4.388903	-0.724107	-0.454615
13	6	0	-2.658836	-2.527067	-0.530904
14	6	0	-6.814656	1.683870	-1.089703
15	1	0	-6.981443	0.918893	-1.840576
16	6	0	7.077382	-0.403731	-1.628138
17	1	0	7.532213	-1.303880	-2.033575
18	6	0	1.660589	-1.588472	1.059739
19	6	0	1.165727	0.701650	0.337384
20	1	0	0.462070	1.409422	-0.083041
21	6	0	2.955176	-1.177855	1.395345
22	1	0	3.683939	-1.852561	1.830518
23	6	0	-7.641042	2.802139	-1.025088
24	1	0	-8.458131	2.905301	-1.732076
25	6	0	5.920307	1.908888	-0.569797
26	1	0	5.475174	2.807169	-0.155611
27	6	0	7.175455	0.801194	-2.342628
28	6	0	6.411644	-0.464128	-0.405679
29	1	0	6.354507	-1.388761	0.160085
30	6	0	-1.609709	-1.651454	-0.104012
31	6	0	0.755163	-0.634666	0.527734
32	6	0	-2.342659	-3.875163	-0.783224
33	1	0	-1.321074	-4.208492	-0.638239
34	6	0	-4.934856	0.365196	-0.258674
35	6	0	3.341338	0.138450	1.191077
36	6	0	2.458087	1.099970	0.671585
37	6	0	-4.638693	-4.319323	-1.400016
38	1	0	-5.404211	-5.010452	-1.736894
39	6	0	5.825100	0.692885	0.106968
40	6	0	-4.973369	-2.992252	-1.150513
41	1	0	-5.992407	-2.647970	-1.288228
42	6	0	-6.366668	3.650690	0.850460
43	1	0	-6.194469	4.412849	1.603748
44	6	0	6.587849	1.950621	-1.795059
45	1	0	6.659899	2.894276	-2.329324
46	6	0	-3.324557	-4.761524	-1.212781
47	1	0	-3.064812	-5.797454	-1.404106
48	6	0	-0.555582	-1.075900	0.182069
49	6	0	7.927475	0.862484	-3.650354
50	1	0	9.002353	0.996066	-3.476974
51	1	0	7.589394	1.699301	-4.267529
52	1	0	7.805232	-0.060639	-4.224644
53	6	0	-7.419672	3.787184	-0.058414
54	1	0	-8.065885	4.658200	-0.013200
55	6	0	2.092565	3.376322	0.016033
56	1	0	2.686631	4.289619	0.003096
57	1	0	1.216603	3.520726	0.658558
58	1	0	1.768006	3.137450	-1.002898
59	1	0	-4.725878	2.427840	1.514751

60	47	0	-2.503635	0.486976	0.344403

SCF Done: E(RB3LYP) = -1966.31552645

Low frequencies --- -0.0007 0.0009 0.0015 4.5093 7.1441 12.6901

Low frequencies --- 13.7730 18.8039 22.2595

Table S12. Atomic coordinates of compound -(*S*)-**2**with AgConf-d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	5.229137	-0.530042	1.452925
2	8	0	5.801179	-1.908294	1.152992
3	8	0	1.117791	-3.198421	-0.258024
4	6	0	2.005466	-4.270559	-0.588470
5	1	0	2.522085	-4.644590	0.301628
6	1	0	2.740765	-3.957939	-1.337376
7	1	0	1.375592	-5.057407	-1.002233
8	8	0	3.106343	1.476057	1.954363
9	6	0	-5.413553	1.940681	-0.260062
10	6	0	-6.700081	2.071285	0.301809
11	6	0	-4.188313	-1.926994	-0.511518
12	6	0	-4.410336	-0.520840	-0.346246
13	6	0	-2.900165	-2.507113	-0.347026
14	6	0	-4.765532	3.075793	-0.786243
15	1	0	-3.781350	2.971139	-1.232594
16	6	0	6.507639	0.762034	-2.196683
17	1	0	6.799328	0.304981	-3.138810
18	6	0	1.643958	-2.068524	0.273769
19	6	0	1.196729	0.175126	1.153240
20	1	0	0.480697	0.949940	1.397602
21	6	0	3.004537	-1.873424	0.531029
22	1	0	3.748228	-2.637484	0.333788
23	6	0	-5.394092	4.317189	-0.745662
24	1	0	-4.890217	5.187805	-1.153283
25	6	0	5.772437	1.927378	0.234230
26	1	0	5.491307	2.377876	1.180118
27	6	0	6.566748	2.158398	-2.059451
28	6	0	6.087087	-0.047892	-1.143856
29	1	0	6.062642	-1.128972	-1.238922
30	6	0	-1.750442	-1.733185	0.006144
31	6	0	0.729946	-1.027948	0.586070
32	6	0	-2.735670	-3.892316	-0.537640
33	1	0	-1.747991	-4.322570	-0.414266
34	6	0	-4.799444	0.648274	-0.306064
35	6	0	3.444346	-0.674194	1.071622
36	6	0	2.554746	0.360714	1.404514
37	6	0	-5.093471	-4.121974	-1.027578

38	1	0	-5.942340	-4.745366	-1.288283
39	6	0	5.708897	0.544792	0.060855
40	6	0	-5.275209	-2.754247	-0.848650
41	1	0	-6.256876	-2.309875	-0.970396
42	6	0	-7.319194	3.318092	0.333211
43	1	0	-8.309892	3.413223	0.766235
44	6	0	6.193009	2.724162	-0.832062
45	1	0	6.239752	3.802352	-0.704229
46	6	0	-3.823674	-4.689971	-0.875158
47	1	0	-3.682606	-5.756430	-1.016723
48	6	0	-0.650274	-1.264508	0.317191
49	6	0	7.056625	3.024057	-3.195290
50	1	0	8.151999	3.082530	-3.197364
51	1	0	6.675058	4.045490	-3.113695
52	1	0	6.753143	2.618973	-4.165158
53	6	0	-6.669695	4.441225	-0.187012
54	1	0	-7.156766	5.410880	-0.157972
55	6	0	2.242297	2.543451	2.343841
56	1	0	2.889100	3.310404	2.768936
57	1	0	1.521784	2.213206	3.100416
58	1	0	1.708455	2.954725	1.479872
59	1	0	-7.199203	1.197266	0.706555
60	47	0	-2.361986	0.516851	0.321651

SCF Done: E(RB3LYP) = -1966.31576344

Low frequencies --- 0.0013 0.0017 0.0018 5.2585 6.0439 10.6328

Low frequencies --- 13.3880 18.4560 23.3979

Table S13. Atomic coordinates of compound -(*S*)-**2**with AgConf-**agg-Ag-a**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.453705	2.089725	1.075929
2	16	0	-4.900052	-1.640206	-1.059551
3	8	0	-4.811040	-1.672748	-2.579927
4	8	0	0.147463	-2.413254	-1.983119
5	8	0	0.662489	2.250165	1.933155
6	8	0	-3.486365	1.710243	-1.701896
7	8	0	-4.341500	2.123314	2.595177
8	6	0	-0.195695	-2.709641	-3.340828
9	1	0	-0.691170	-1.857852	-3.819303
10	1	0	-0.842369	-3.591204	-3.397995
11	1	0	0.746893	-2.915737	-3.846730
12	8	0	-3.866309	-1.418629	1.709808
13	6	0	4.917713	2.347223	-0.765523
14	6	0	3.756330	2.356724	-1.590001
15	6	0	0.386303	2.589032	3.295650

16	1	0	-0.214026	1.813850	3.784174
17	1	0	-0.131332	3.551570	3.363165
18	1	0	1.357472	2.656608	3.784306
19	6	0	4.455389	-2.707213	0.854979
20	6	0	-1.725765	2.232364	1.443677
21	1	0	-2.036606	2.381352	2.471664
22	6	0	4.810613	1.548445	1.748762
23	6	0	3.244080	-2.809523	1.595282
24	6	0	-4.708208	4.834542	1.433741
25	1	0	-4.252458	4.646137	2.400697
26	6	0	2.482108	1.961270	-1.066082
27	6	0	-0.380893	2.152552	1.071041
28	6	0	6.138360	2.784762	-1.312809
29	1	0	7.022542	2.783241	-0.684601
30	6	0	-5.108168	6.116103	1.059637
31	1	0	-4.944271	6.946924	1.741105
32	6	0	-5.997226	-5.569521	-1.052496
33	1	0	-5.929203	-6.411186	-1.736917
34	6	0	-0.864626	-2.191500	-1.104237
35	6	0	-2.720673	2.093897	0.486191
36	6	0	-0.058194	1.934114	-0.290900
37	6	0	-4.915620	3.773694	0.552625
38	6	0	-1.494322	-1.767567	1.226233
39	1	0	-1.186566	-1.638515	2.255858
40	6	0	-2.212777	-2.101875	-1.461919
41	1	0	-2.551626	-2.201322	-2.487020
42	6	0	-5.723075	6.351710	-0.180347
43	6	0	6.214631	3.211436	-2.635307
44	1	0	7.166225	3.543797	-3.037789
45	6	0	-6.181667	-3.396821	0.694429
46	1	0	-6.256089	-2.551137	1.369757
47	6	0	-6.625375	-5.740858	0.191287
48	6	0	-5.462696	-4.337829	-1.426347
49	1	0	-4.995397	-4.197648	-2.396002
50	6	0	2.012451	-2.330429	1.040818
51	6	0	-5.930327	5.262728	-1.039507
52	1	0	-6.411253	5.423931	-2.000655
53	6	0	-0.503390	-2.026810	0.255575
54	6	0	3.259183	-3.396347	2.871784
55	1	0	2.331935	-3.471240	3.429407
56	6	0	4.851969	1.908521	0.585335
57	6	0	-1.084033	1.788115	-1.248259
58	1	0	-0.807302	1.616925	-2.280566
59	6	0	-3.173335	-1.856043	-0.491228
60	6	0	-2.422857	1.858876	-0.866766
61	6	0	-2.836019	-1.676295	0.860774
62	6	0	1.308637	1.872845	-0.696584
63	6	0	5.639887	-3.780813	2.685004
64	1	0	6.567031	-4.155360	3.106549
65	6	0	-5.547227	-3.263591	-0.541230

66	6	0	5.644726	-3.200635	1.419198
67	1	0	6.566758	-3.122927	0.853553
68	6	0	3.853468	2.785443	-2.925449
69	1	0	2.963023	2.785541	-3.544593
70	6	0	-5.539742	3.972215	-0.679384
71	1	0	-5.710674	3.138130	-1.351542
72	6	0	-6.707966	-4.638165	1.054206
73	1	0	-7.197174	-4.749103	2.018312
74	6	0	4.448602	-3.879597	3.410817
75	1	0	4.446011	-4.332357	4.396898
76	6	0	-3.238800	1.485725	-3.092082
77	1	0	-4.219711	1.396749	-3.556440
78	1	0	-2.682757	0.555702	-3.247657
79	1	0	-2.693987	2.327638	-3.532967
80	6	0	0.857737	-2.145014	0.656827
81	6	0	-7.229167	-7.070207	0.575638
82	1	0	-8.276391	-7.131283	0.254710
83	1	0	-7.212313	-7.218457	1.659092
84	1	0	-6.696261	-7.901647	0.105652
85	6	0	5.072897	3.210635	-3.443696
86	1	0	5.132321	3.542720	-4.474961
87	6	0	-3.580863	-1.243920	3.100659
88	1	0	-4.544888	-1.083540	3.581321
89	1	0	-2.949947	-0.365136	3.262522
90	1	0	-3.104508	-2.137930	3.517166
91	6	0	-6.182780	7.737922	-0.563226
92	1	0	-7.200460	7.926461	-0.199649
93	1	0	-6.195339	7.869394	-1.648792
94	1	0	-5.536290	8.506751	-0.130361
95	47	0	2.380828	-0.266895	-0.197297
96	6	0	4.774588	1.154340	3.117964
97	6	0	5.890545	1.375000	3.951349
98	6	0	3.622140	0.547116	3.658884
99	6	0	5.848424	0.998509	5.291468
100	1	0	6.778625	1.842325	3.538520
101	6	0	3.591564	0.173852	5.000366
102	1	0	2.763438	0.376088	3.017025
103	6	0	4.701727	0.398501	5.820011
104	1	0	6.712172	1.174148	5.925462
105	1	0	2.700740	-0.294546	5.407880
106	1	0	4.673802	0.106444	6.865348
107	6	0	4.462613	-2.125195	-0.446948
108	6	0	4.525859	-1.705956	-1.593794
109	6	0	4.649801	-1.279888	-2.950458
110	6	0	5.928272	-1.084252	-3.511056
111	6	0	3.506323	-1.077440	-3.750390
112	6	0	6.053600	-0.698103	-4.843285
113	1	0	6.809290	-1.239596	-2.897272
114	6	0	3.644134	-0.690139	-5.080505
115	1	0	2.522452	-1.232505	-3.319392

116	6	0	4.915656	-0.500644	-5.630481
117	1	0	7.041754	-0.551552	-5.268236
118	1	0	2.759193	-0.539078	-5.691072
119	1	0	5.018924	-0.200808	-6.668791

SCF Done: E(RB3LYP) = -3785.80117541

Full mass-weighted force constant matrix:

Low frequencies --- -15.6831 -14.9228 -8.7970 -2.9365 0.0008 0.0016

Low frequencies --- 7.2294 11.0009 14.3422

Table S14. Atomic coordinates of compound -(*S*)-**2**with AgConf-a**gg-Ag-b**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	6.170334	1.264285	-1.557996
2	8	0	5.960224	2.129261	-2.794739
3	8	0	1.572657	3.510037	-0.665675
4	6	0	1.896365	4.459501	-1.683365
5	1	0	2.041333	3.973120	-2.654619
6	1	0	2.796344	5.026480	-1.421452
7	1	0	1.043350	5.135445	-1.741247
8	8	0	5.375651	-0.223986	0.875427
9	6	0	-2.930894	3.713342	-1.256442
10	6	0	-1.841629	3.783560	-2.148443
11	6	0	-2.379936	2.510474	2.588917
12	6	0	-2.588998	2.727718	1.189480
13	6	0	-1.083194	2.203913	3.093569
14	6	0	-4.172225	4.268978	-1.623615
15	1	0	-5.008490	4.215733	-0.934463
16	6	0	8.459648	4.229686	0.052400
17	1	0	8.617436	5.290210	-0.126927
18	6	0	2.526658	2.603154	-0.316051
19	6	0	3.198716	0.834697	1.233618
20	1	0	2.964801	0.227765	2.098825
21	6	0	3.732201	2.430250	-1.001609
22	1	0	3.985314	3.002244	-1.887127
23	6	0	-4.314032	4.888679	-2.862867
24	1	0	-5.270865	5.319365	-3.140726
25	6	0	8.057719	1.500621	0.496172
26	1	0	7.901497	0.440885	0.666298
27	6	0	9.192013	3.584021	1.061245
28	6	0	7.536929	3.533226	-0.726055
29	1	0	6.984356	4.023708	-1.521275
30	6	0	0.044891	2.075035	2.235091
31	6	0	2.255291	1.797669	0.817185
32	6	0	-0.929021	2.014382	4.480725
33	1	0	0.057906	1.784686	4.867696
34	6	0	-2.765260	3.098164	0.028485

35	6	0	4.653188	1.487672	-0.563402
36	6	0	4.402883	0.669574	0.549526
37	6	0	-3.286820	2.420209	4.842495
38	1	0	-4.135807	2.500454	5.513186
39	6	0	7.333389	2.174505	-0.487577
40	6	0	-3.467247	2.611368	3.476499
41	1	0	-4.451545	2.835026	3.079949
42	6	0	-1.998191	4.404698	-3.384618
43	1	0	-1.156828	4.459469	-4.068365
44	6	0	8.975532	2.214021	1.268744
45	1	0	9.537372	1.695148	2.040976
46	6	0	-2.015160	2.122356	5.343973
47	1	0	-1.870510	1.973272	6.409265
48	6	0	1.050571	1.957921	1.557934
49	6	0	10.213110	4.339586	1.877596
50	1	0	11.184134	4.360639	1.367550
51	1	0	10.368072	3.873849	2.854770
52	1	0	9.908252	5.378215	2.035730
53	6	0	-3.231529	4.956981	-3.744597
54	1	0	-3.348186	5.440029	-4.709784
55	6	0	5.166843	-1.082564	2.002444
56	1	0	6.075940	-1.678286	2.087916
57	1	0	4.309750	-1.746690	1.846086
58	1	0	5.031227	-0.497865	2.919393
59	1	0	-0.886931	3.360075	-1.854266
60	47	0	-2.865268	0.668878	-0.099166
61	16	0	2.690613	-4.056601	0.051752
62	8	0	2.834423	-3.654853	1.516918
63	8	0	-1.631128	-1.336432	1.001100
64	6	0	-1.323089	-1.430671	2.401444
65	1	0	-0.364289	-0.952339	2.620124
66	1	0	-1.305910	-2.477301	2.718569
67	1	0	-2.123226	-0.901570	2.915872
68	8	0	1.638541	-3.847245	-2.709913
69	6	0	-6.041193	-0.143612	1.936069
70	6	0	-5.369937	-1.130835	2.686683
71	6	0	-5.712481	0.081100	-2.113290
72	6	0	-5.751026	0.020465	-0.690376
73	6	0	-4.543327	-0.299858	-2.832511
74	6	0	-6.912969	0.748689	2.593688
75	1	0	-7.436299	1.504417	2.017102
76	6	0	1.265174	-7.677632	1.265076
77	1	0	0.874467	-8.104117	2.185373
78	6	0	-0.805911	-1.975789	0.115198
79	6	0	-0.360307	-2.528202	-2.224146
80	1	0	-0.657558	-2.457473	-3.262284
81	6	0	0.355166	-2.655104	0.482652
82	1	0	0.700081	-2.710255	1.508790
83	6	0	-7.100562	0.654708	3.970795
84	1	0	-7.775509	1.344095	4.468625

85	6	0	2.285857	-6.577034	-1.092087
86	1	0	2.683985	-6.149421	-2.005971
87	6	0	1.383924	-8.488073	0.124994
88	6	0	1.644024	-6.336630	1.238986
89	1	0	1.573601	-5.712255	2.123989
90	6	0	-3.373954	-0.751782	-2.151549
91	6	0	-1.169467	-1.910078	-1.249012
92	6	0	-4.542429	-0.240135	-4.238333
93	1	0	-3.647714	-0.532092	-4.777367
94	6	0	-5.859185	-0.054317	0.522815
95	6	0	1.129975	-3.272910	-0.489984
96	6	0	0.794236	-3.216319	-1.852334
97	6	0	-6.820069	0.568876	-4.223674
98	1	0	-7.701302	0.905754	-4.760012
99	6	0	2.139779	-5.794422	0.053893
100	6	0	-6.839521	0.517470	-2.832569
101	1	0	-7.729123	0.809113	-2.284975
102	6	0	-5.564546	-1.214622	4.063280
103	1	0	-5.046722	-1.979913	4.633201
104	6	0	1.897615	-7.916800	-1.048452
105	1	0	2.002909	-8.529683	-1.939666
106	6	0	-5.672852	0.187867	-4.927484
107	1	0	-5.658267	0.227247	-6.011714
108	6	0	-2.351376	-1.224963	-1.661223
109	6	0	1.001409	-9.947775	0.172877
110	1	0	1.838715	-10.559386	0.530910
111	1	0	0.724351	-10.321366	-0.816734
112	1	0	0.161920	-10.118209	0.853197
113	6	0	-6.427402	-0.323566	4.708560
114	1	0	-6.578290	-0.394571	5.781339
115	6	0	1.362049	-3.783560	-4.111081
116	1	0	2.168119	-4.332094	-4.597263
117	1	0	1.358865	-2.747156	-4.465436
118	1	0	0.402915	-4.257886	-4.345710
119	1	0	-4.710678	-1.828295	2.180206

SCF Done: E(RB3LYP) = -3785.80154080

Full mass-weighted force constant matrix:

Low frequencies --- -0.0052 -0.0031 -0.0008 2.3354 3.8225 6.1374

Low frequencies --- 7.6674 8.6402 11.1210

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