ELECTRONIC SUPPORTING INFORMATION

OFF/ON switching of Circularly Polarized Luminescence by oxophilic interaction of Homochiral sulfoxyde-containing o-OPEs with metal cations

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SYNTHETIC PART

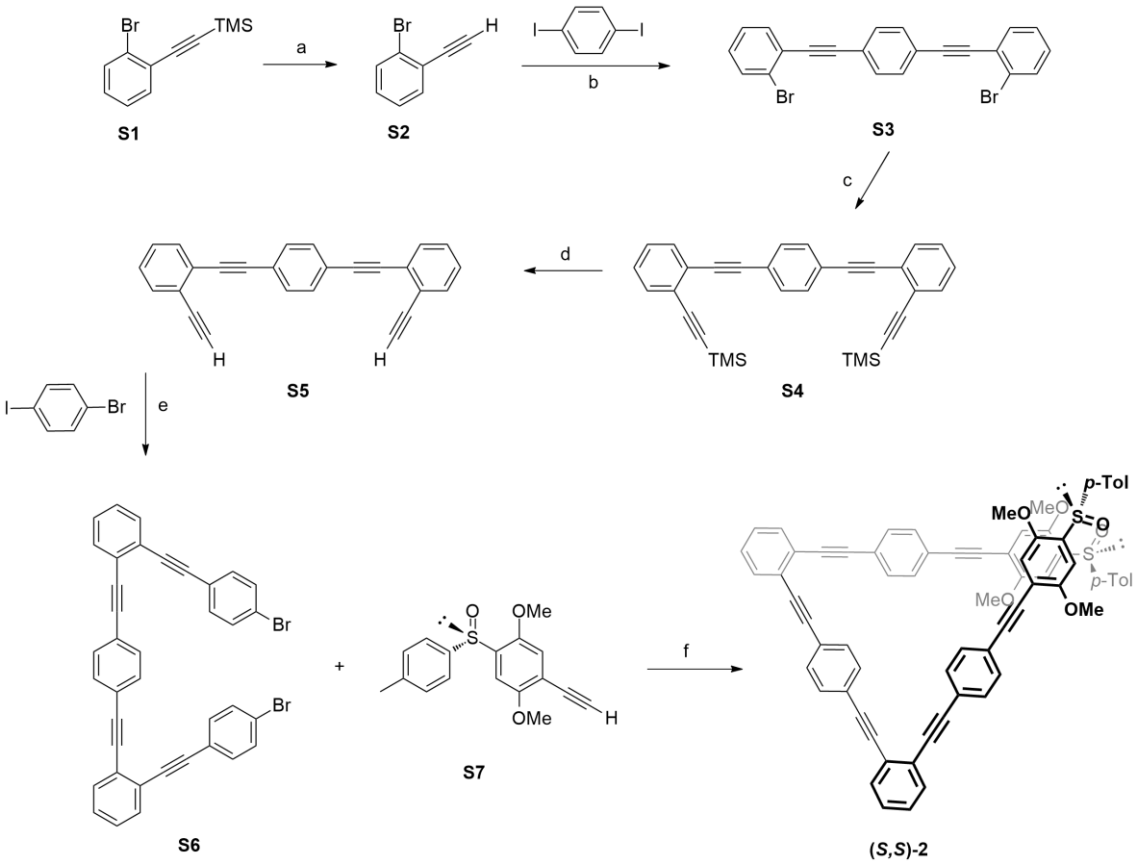
General Details

The following palladium catalysts, trans-dichlorobis(triphenylphosphine) palladium(II) ($Pd(PPh_3)_2Cl_2$) and trans-dichlorobis(acetonitrile)palladium(II) ($Pd(CH_3CN)_2Cl_2$), were prepared from palladium(II) chloride($PdCl_2$) according to previously described procedures.[1] All reagents and solvents (CH_2Cl_2, EtOAc, hexane, THF, iPr_2NH, Et_3N) were purchased from standard chemical suppliers and used without further purification. Dry THF was freshly distilled over Na/benzophenone. Thin-layer chromatography analysis was performed on aluminium-backed plates coated with silica gel 60 (230-240 mesh) with F254 indicator. The spots were visualized with UV light (254 nm and 360 nm) and/or stained with phosphomolybdic acid (10% ethanol solution) and subsequent heating. Chromatography purifications were performed with silica gel 60 (40-63 μm). ^1H and ^{13}C NMR spectra were recorded on Varian 400 or 500 MHz spectrometers, at a constant temperature of 298 K. Chemical shifts are reported in ppm using residual solvent peak as reference ($CDCl_3$: δ = 7.26 ppm, CD_2Cl_2: δ = 5.32 ppm, $(CD_3)_2CO$: δ = 2.05 ppm). Data are reported as follows: chemical shift, multiplicity (s: singlet, d: doublet, t: triplet, q: quartet, quint: quintuplet, hept: heptuplet, m: multiplet, dd: doublet of doublets, dt: doublet of triplets, td: triplet of doublets, bs: broad singlet), coupling constant (*J* in Hz) and integration; ^{13}C NMR spectra were recorded at 101 or 126 MHz using broadband proton decoupling and chemical shifts are reported in ppm using residual solvent peaks as reference ($CDCl_3$: δ = 77.16 ppm, CD_2Cl_2: δ = 54.00 ppm, $(CD_3)_2CO$: δ = 29.84 ppm). Carbon multiplicities were accomplished by DEPT techniques. High-resolution mass spectra (HRMS) were recorded using EI on a Micromass GCT Agilent Technologies 6890N (Waters), by APCI mass spectra carried out on a Bruker MAXIS II mass spectrometer or by ESI mass spectrometry carried out on a Waters Xevo G2-XS QTof mass spectrometer. The following known compounds were isolated as pure samples and showed NMR spectra identical to reported data: **S1**,[2] **S2**,[3] **S7**,[4] (*S*,*S*)-**1.**[4]

Table of used salts for complexation reactions

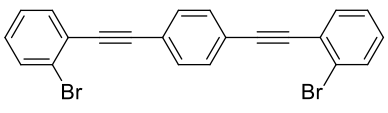
MONOVALENT CATIONIC SALTS		BIVALENT CATIONIC SALTS			TRIVALENT CATIONIC SALTS		TETRAVALENT CATIONIC SALTS	
LiOTf	TlOTf	$Ca(OTf)_2$	$Co(BF_4)_2$	$Ni(OTf)_2$	$Sc(OTf)_3$	$Ga(OTf)_3$	$Hf(OTf)_4$	$TiCp_2(OTf)_2$
$AgBF_4$	CuOTf	$Cu(OTf)_2$	$Zn(OTf)_2$	$Hg(OTf)_2$	$Fe(OTf)_3$	$Eu(OTf)_3$		
		$Fe(OTf)_2$	$Mg(OTf)_2$	$Sn(OTf)_2$	$Bi(OTf)_3$	$Al(OTf)_3$		
		$Mn(OTf)_2$	$Ba(OTf)_2$		$In(OTf)_3$	$La(OTf)_3$		

Synthesis and characterization of new compound ***(S,S)-2***



Scheme S1. Synthesis of compound (*S,S*)-**2.** Compound **S7**[4] was prepared according to literature procedures a) Bu_4NF, THF, rt b) $Pd(PPh_3)_2Cl_2$, CuI, 1,4-diiodobenzene, Et_3N/THF, rt c) $Pd(CH_3CN)_2Cl_2$, *t*$Bu_3P{\cdot}HBF_4$, CuI, trimethylsilyl acetylene, *i*Pr_2NH/THF, 60 ºC. d) Bu_4NF, THF, rt e) $Pd(PPh_3)_2Cl_2$, CuI, 1-bromo-4-iodobenzene, Et_3N/THF, rt f) $Pd(CH_3CN)_2Cl_2$, *t*$Bu_3P{\cdot}HBF_4$, CuI, **S7**, *i*Pr_2NH/THF, 70 ºC.

Compound S3.

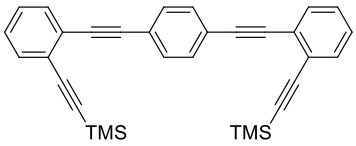


S3

A solution of compound **S2** (1.32 g, 8.02 mmol) dissolved in the minimum volume of THF and with 2 mL of Et_3N was added dropwise during 2 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (225 mg, 0.32 mmol), CuI (122 mg, 0.64 mmol) and the 1,4-diiodobenzene (1.06 g, 3.21 mmol) in 12 mL of Et_3N. The reaction was stirred during 5 h at room temperature under argon atmosphere. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane) to give **S3** (1.13 g, 81%) as a white solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.63 (dd, *J* = 8.1,

1.2 Hz, 2H), 7.57 (s, 4H), 7.56 (dd, *J* = 7.7, 1.7 Hz, 2H), 7.30 (td, *J* = 7.6, 1.2 Hz, 2H), 7.20 (td, *J* = 7.9, 1.7 Hz, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 133.4 (CH), 132.7 (CH), 131.8 (CH), 129.8 (CH), 127.2 (CH), 125.8 (C), 125.3 (C), 123.3 (C), 93.7 (C), 90.1 (C). **HRMS (APCI+):** *m*/*z* $[M+H]^+$ calcd for $C_{22}H_{13}Br_2$: 434.9379; found: 434.9380.

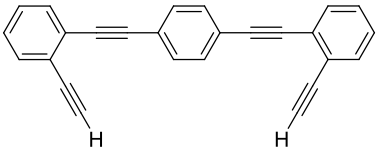
Compound S4.



S4

A solution of trimethylsilylacetylene (1.04 mL, 7.53 mmol) dissolved in 5 mL of THF was added dropwise at 60°C during 2 h to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (65 mg, 0.25 mmol), P*t*Bu_3·HBF_4 (145 mg, 0.50 mmol), CuI (48 mg, 0.25 mmol) and **S3** (1.10 g, 2.51 mmol) in 10 mL of *i*Pr_2NH. Afterwards, the reaction was stirred at room temperature under argon atmosphere during 16 h. The mixture was then diluted with EtOAc, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane) to give **S4** (748 mg, 63%) as a orange solid. **^{1}H NMR (500 MHz, CD_3Cl_3)** δ 7.55 (s, 4H), 7.54 – 7.49 (m, 4H), 7.32 – 7.27 (m, 4H), 0.28 (s, 18H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 132.5 (CH), 131.8 (CH), 131.7 (CH), 128.4 (CH), 128.2 (CH), 126.0 (C), 125.9 (C), 123.4 (C), 103.5 (C), 98.9 (C), 93.3 (C), 90.3 (C), 0.2 (CH_3). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{32}H_{30}Si_2$: 470.1886; found: 470.1871.

Compound S5.

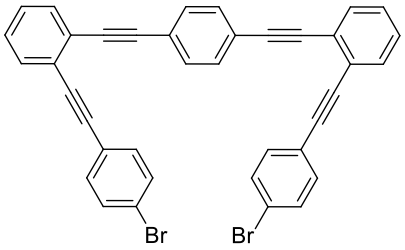


S5

To a solution of **S4** (748 mg, 1.59 mmol) in THF (10 ml) with a 4-5 drops of water, Bu_4NF (1.25 g, 3.97 mmol) was added, and the mixture was stirred at room temperature until complete consumption of the starting material (TLC, 1 h). The solution was then diluted with EtOAc, washed with brine, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane) to give **S5** (441 mg, 85%) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.55 (s, 4H), 7.56 – 7.53 (m, 4H), 7.34 (td, *J* = 7.6, 1.6 Hz, 2H), 7.30 (td, *J* = 7.6, 1.5 Hz, 2H), 3.38 (s, 2H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 132.79 (CH), 131.96 (CH), 131.82 (CH), 128.73

(CH), 128.29 (CH), 126.19 (C), 124.84 (C), 123.37 (C), 93.36 (C), 89.95 (C) , 82.27 (C), 81.41 (CH). **HRMS (EI):** *m*/*z* $[M]^+$ calcd for $C_{26}H_{14}$: 326.1096; found: 326.1080.

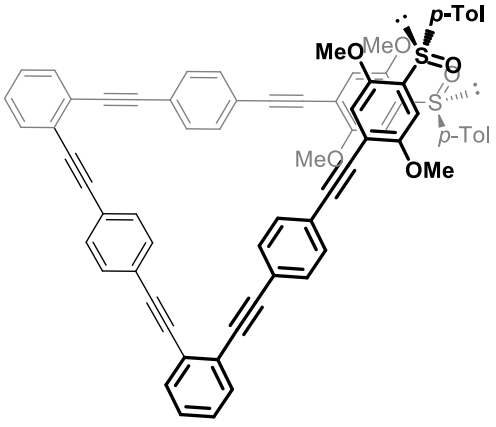
Compound S6.



S6

A solution of compound **S5** (441 mg, 1.35 mmol) dissolved in the minimum volume of THF and with 6 mL of Et_3N was added dropwise during 2 h to a carefully degassed solution of $Pd(PPh_3)_2Cl_2$ (29 mg, 0.04 mmol), CuI (26 mg, 0.14 mmol) and the 1-bromo-4-iodobenzene (956 mg, 3.38 mmol) in a mixture of Et_3N/THF (4:1, 12 mL). The reaction was stirred during 16 h at room temperature under argon atmosphere. The mixture was then diluted with CH_2Cl_2, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, Hexane/ CH_2Cl_2 8:2) to give **S6** (869 mg, 99%) as a brownish solid. **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.59 – 7.55 (m, 4H), 7.52 (s, 4H), 7.52 – 7.46 (m, 4H), 7.45 – 7.39 (m, 4H), 7.36 – 7.31 (m, 4H). **^{13}C NMR (126 MHz, $CDCl_3$)** δ 133.2 (CH), 132.02 (CH), 131.97 (CH), 131.9 (CH), 131.8 (CH), 128.5 (CH), 125.74 (C), 125.71 (C), 123.5 (C), 123.0 (C), 122.3 (C), 93.4 (C), 92.8 (C), 90.4 (C), 89.5 (C), (one CH signal was not observed). **HRMS (APCI+):** *m*/*z* $[M+H]^+$ calcd for $C_{38}H_{21}Br_2$: 635.0005; found: 635.0011.

Compound (*S*,*S*)-2.

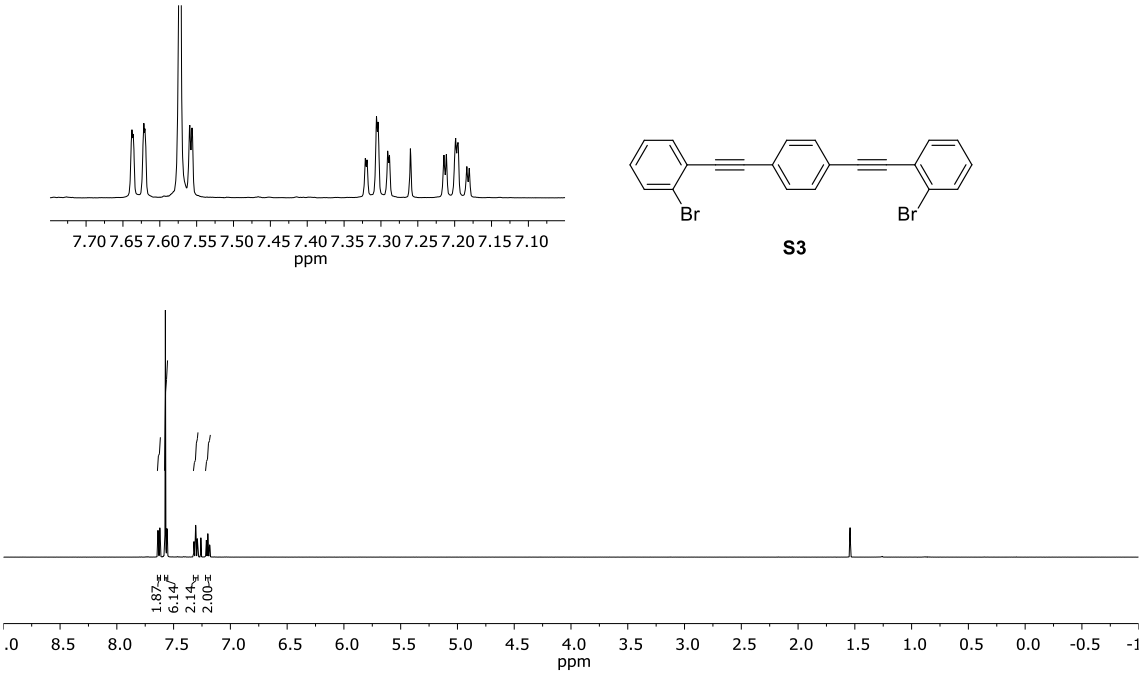


(*S*,*S*)-2

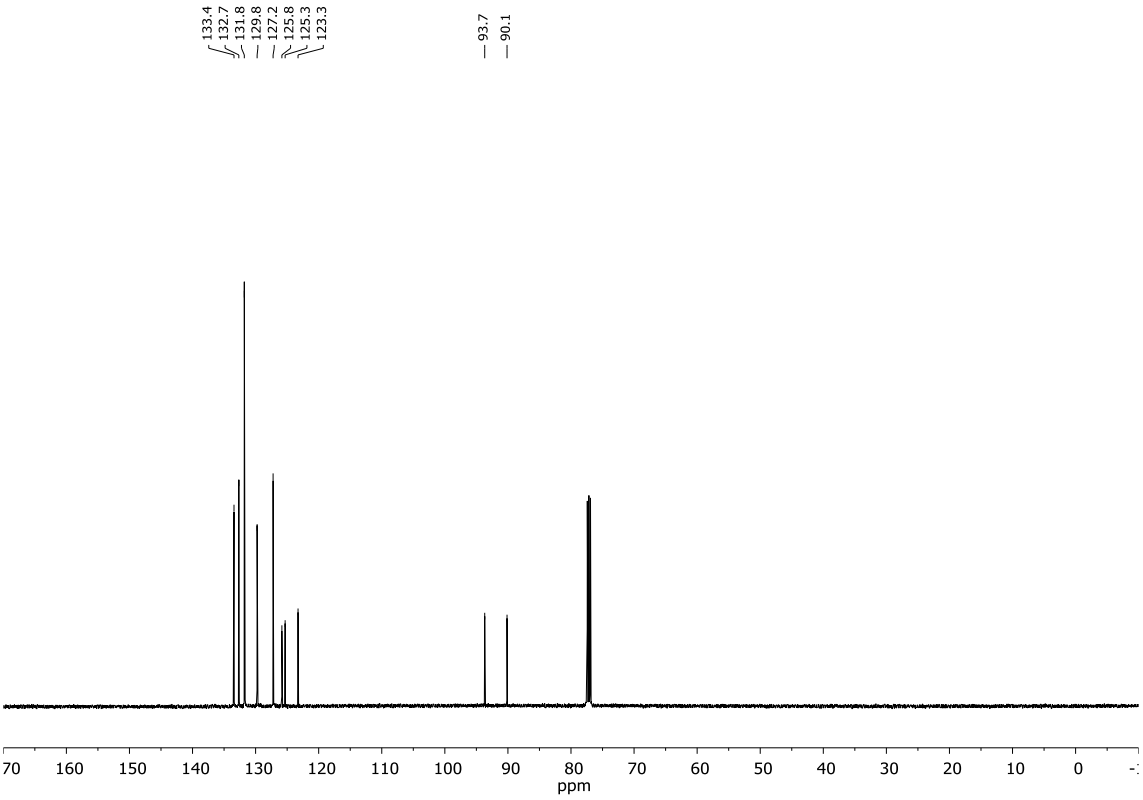
A solution of **S7** (282 mg, 0.94 mmol) dissolved in the minimum volume of THF and with 2 mL of *i*Pr_2NH was added dropwise at 70 °C during 2 h to a carefully degassed solution of $Pd(CH_3CN)_2Cl_2$ (26 mg, 0.10 mmol), P*t*Bu_3·HBF_4 (59 mg, 0.20 mmol), CuI (19 mg, 0.10 mmol) and **S6** (200 mg, 0.31 mmol) in a mixture of *i*Pr_2NH/THF (3:1, 20 mL). Afterwards, the reaction was stirred at room temperature under argon atmosphere during 16 h. The mixture was then diluted with CH_2Cl_2, washed with saturated aq NH_4Cl solution, dried over anhydrous Na_2SO_4 and the solvent was removed under reduced pressure. The residue was purified by flash chromatography (SiO_2, CH_2Cl_2/EtOAc 9:1) and subsequent preparative (TLC CH_2Cl_2/EtOAc 9:1) to give **(*S*,*S*)-2** (91 mg, 37%) as a white solid. **^{1}H NMR (400 MHz, $CDCl_3$)** δ 7.59 – 7.55 (m, 8H), 7.53 (d, *J* = 7.6 Hz, 8H), 7.52 (s, 4H), 7.50 (s, 2H), 7.34 (dd, *J* = 5.8, 3.3 Hz, 4H), 7.23 (d, *J* = 7.7 Hz, 4H), 6.94 (s, 2H), 3.93 (s, 6H), 3.71 (s, 6H), 2.36 (s, 6H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 155.5 (C), 149.0 (C), 142.2 (C), 141.8 (C), 134.9 (C), 132.0 (CH), 131.93 (CH), 131.85 (CH), 131.8 (CH), 131.7 (CH), 129.9 (CH), 128.5 (CH), 125.8 (C), 125.6 (CH), 123.5 (C), 123.4 (C), 123.3 (C), 116.2 (CH), 115.1 (C), 106.8 (CH), 94.9 (C), 93.6 (C), 93.5 (C), 90.5 (C), 87.3 (C), 56.8 (CH_3), 56.4 (CH_3), 21.6 (CH_3), (some carbon signals were not observed probably due to overlapping problems). **HRMS (ESI):** *m*/*z* $[M+Na]^+$ calcd for $C_{72}H_{50}O_6S_2Na$: 1097.2947; found: 1097.2958.

[1]H and [13]C NMR spectra of new compounds

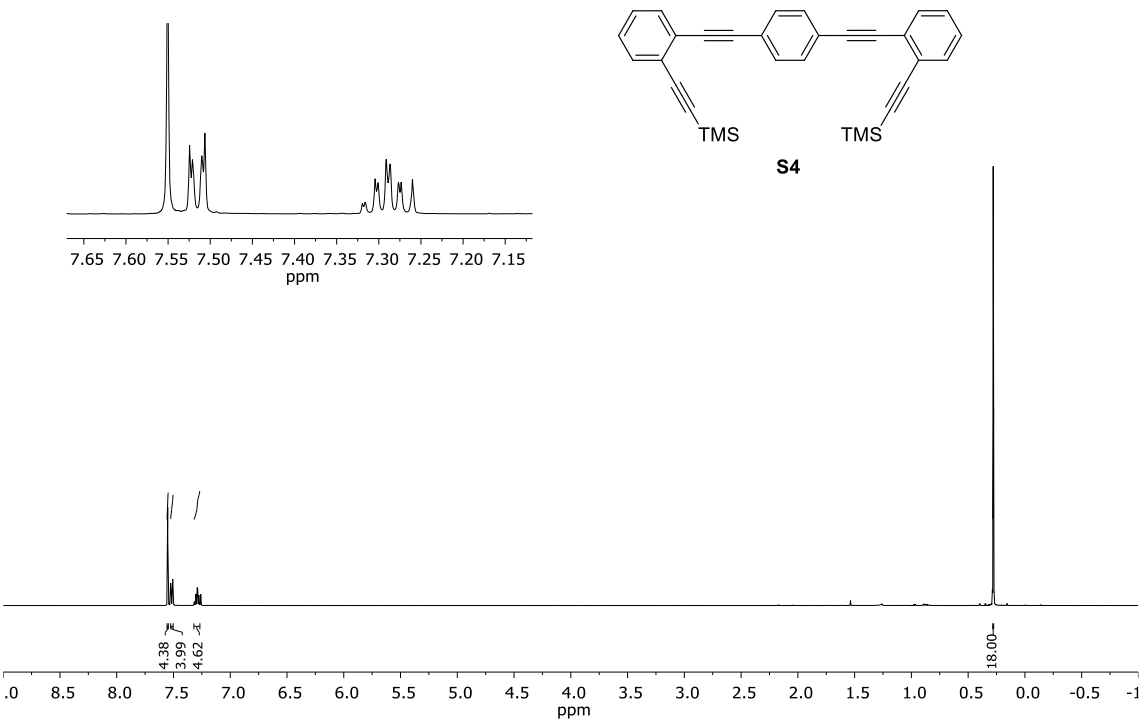
. [1]H NMR (500 MHz, $CDCl_3$) spectrum of compound **S3**



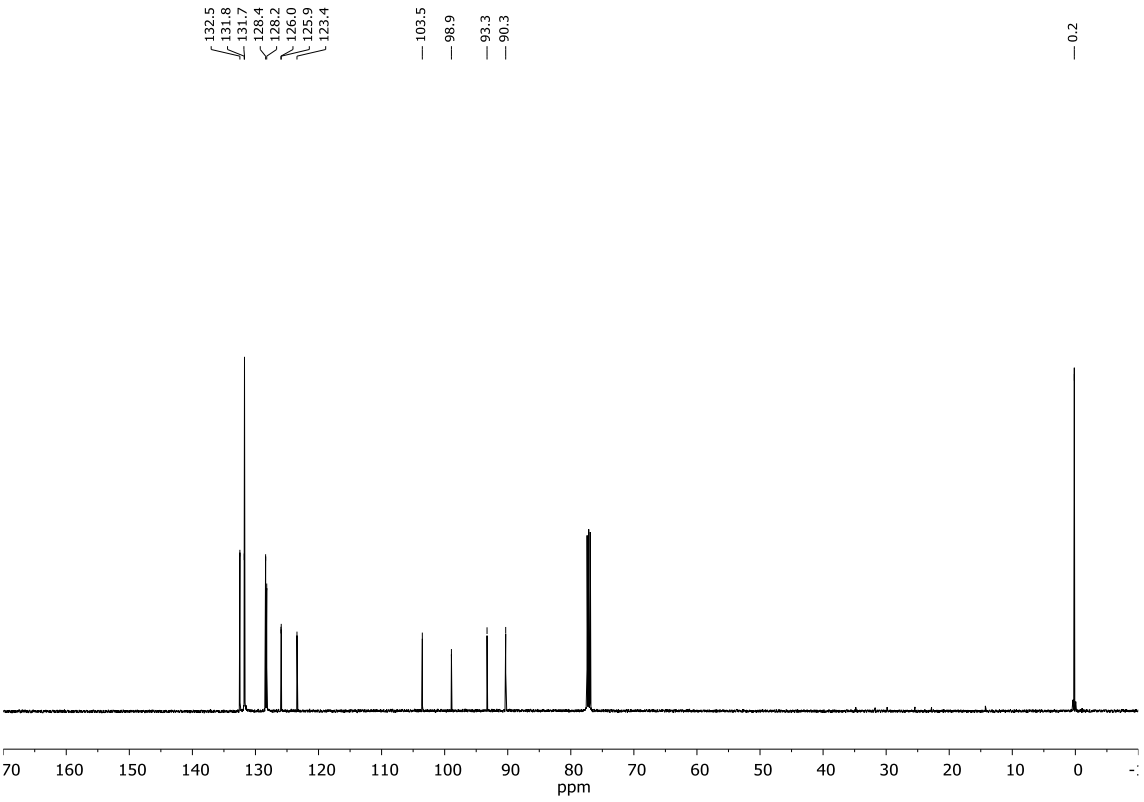
. [13]C NMR (126 MHz, $CDCl_3$) spectrum of compound **S3**



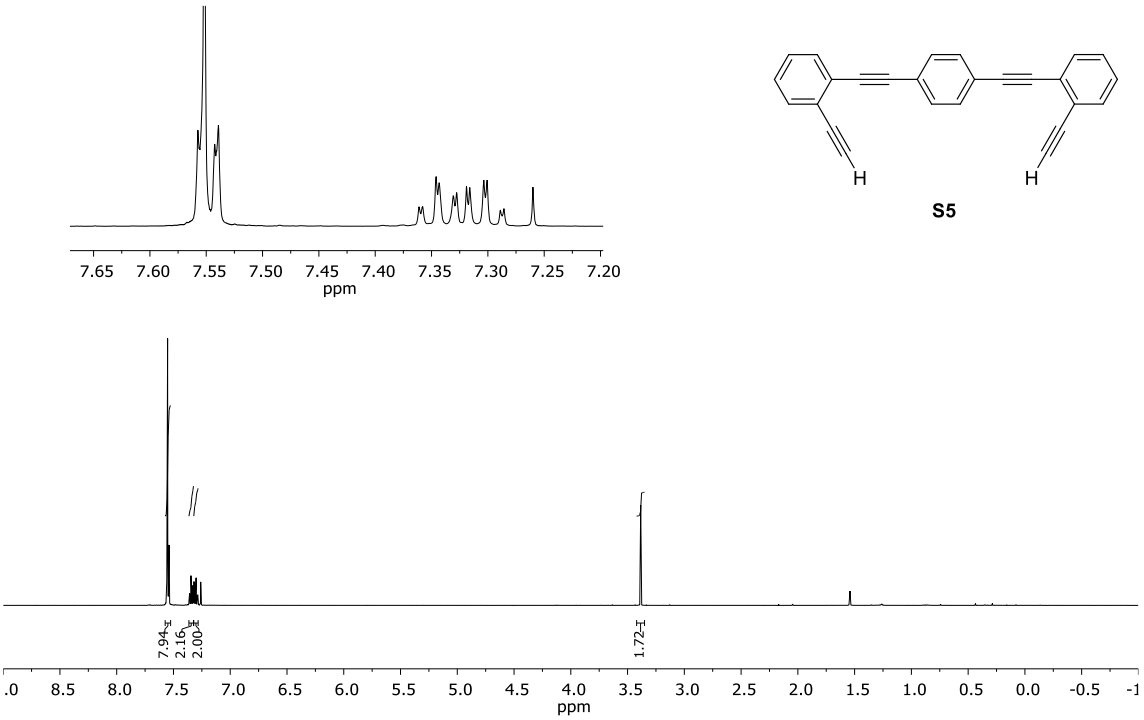
. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S4**



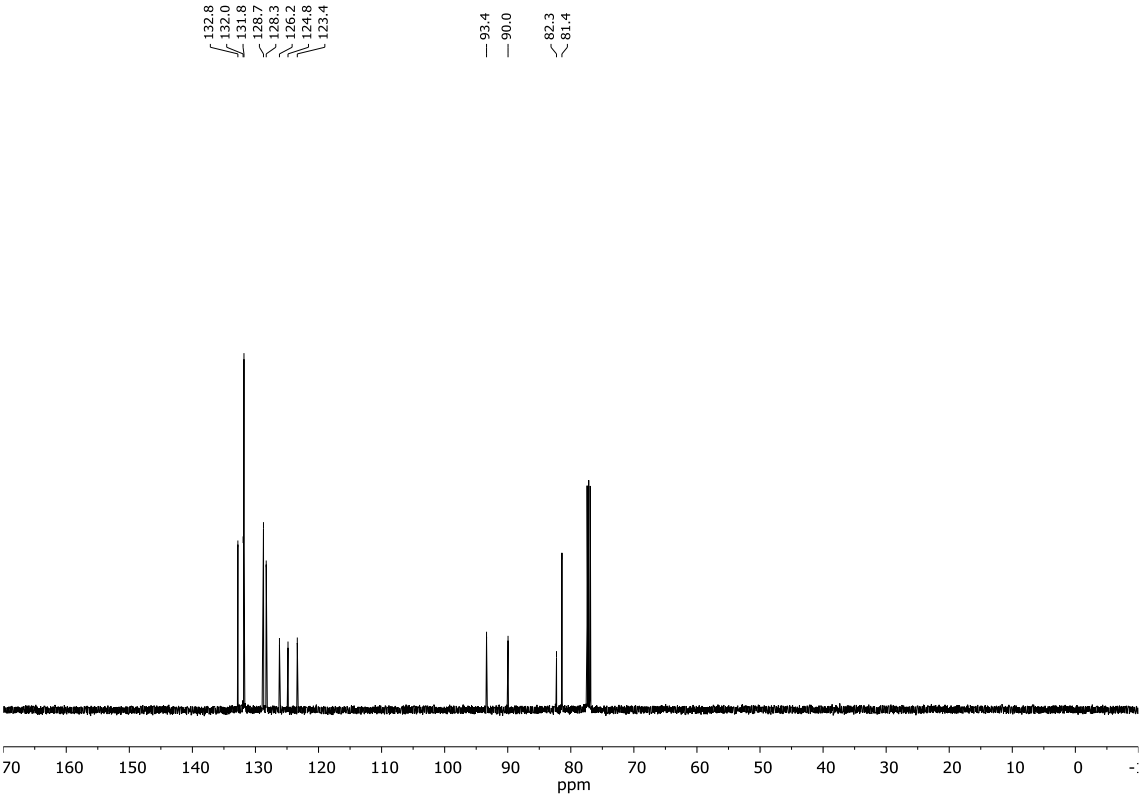
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S4**



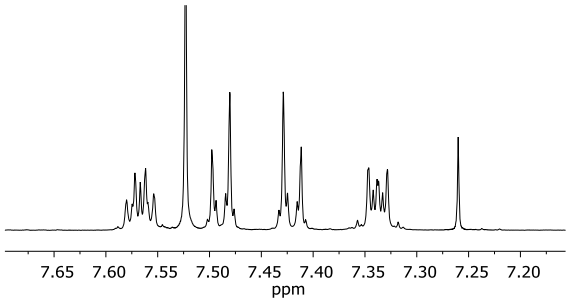
. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **S5**

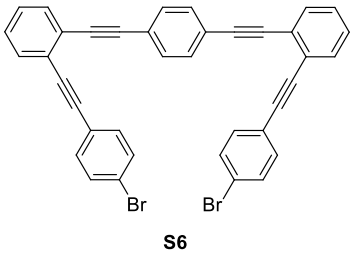


. ^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **S5**

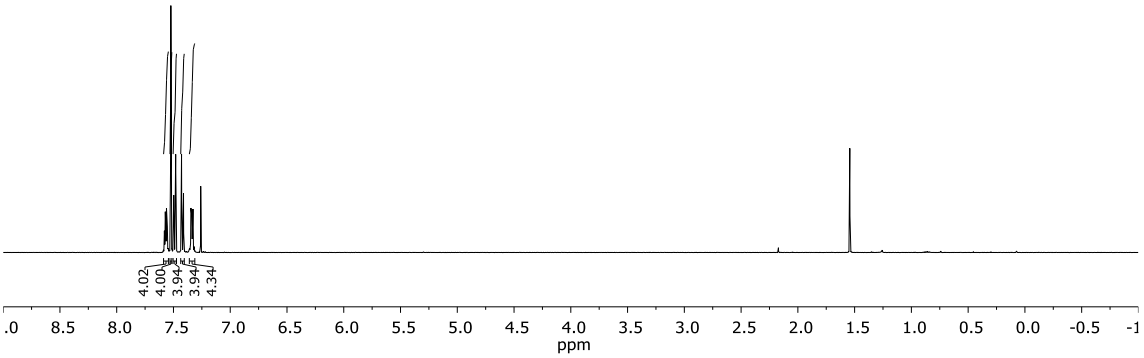


. **^{1}H NMR (500 MHz, $CDCl_3$)** spectrum of compound **S6**

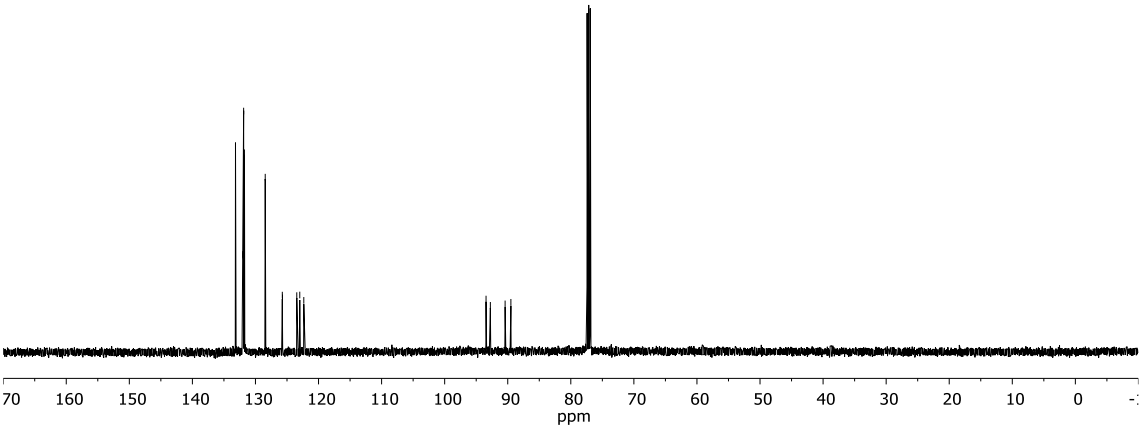




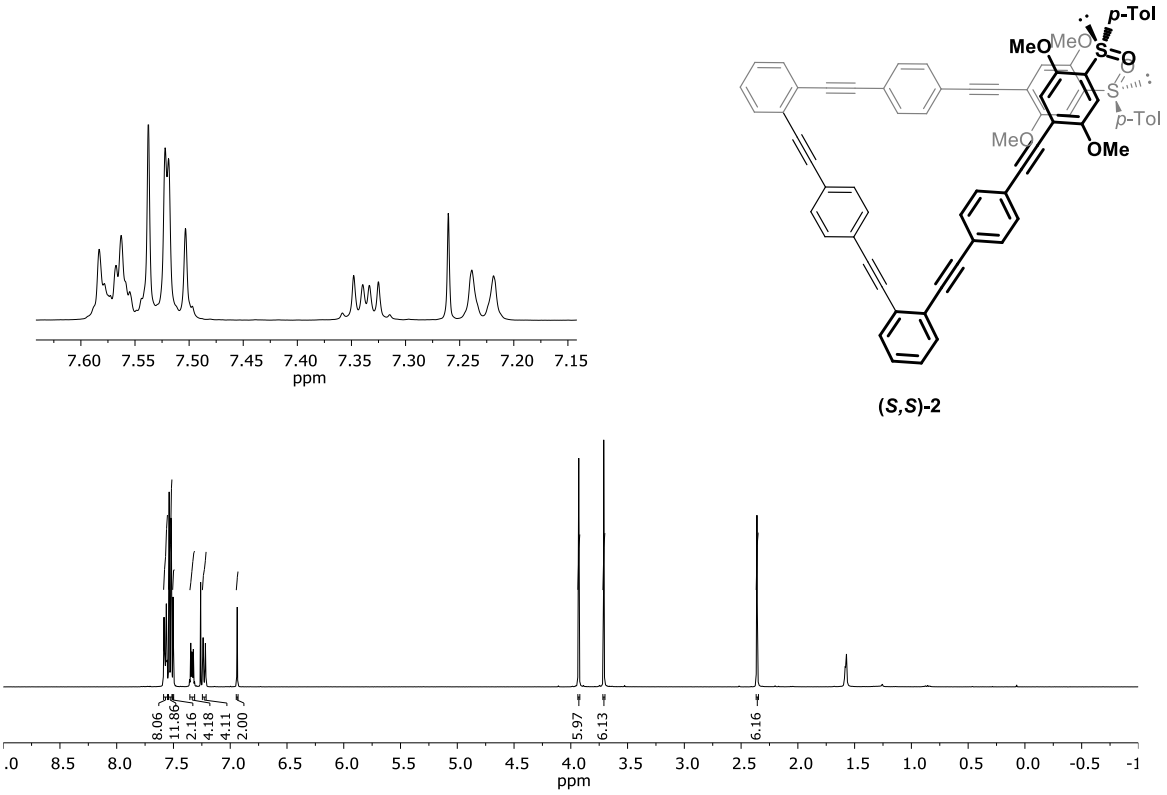
S6



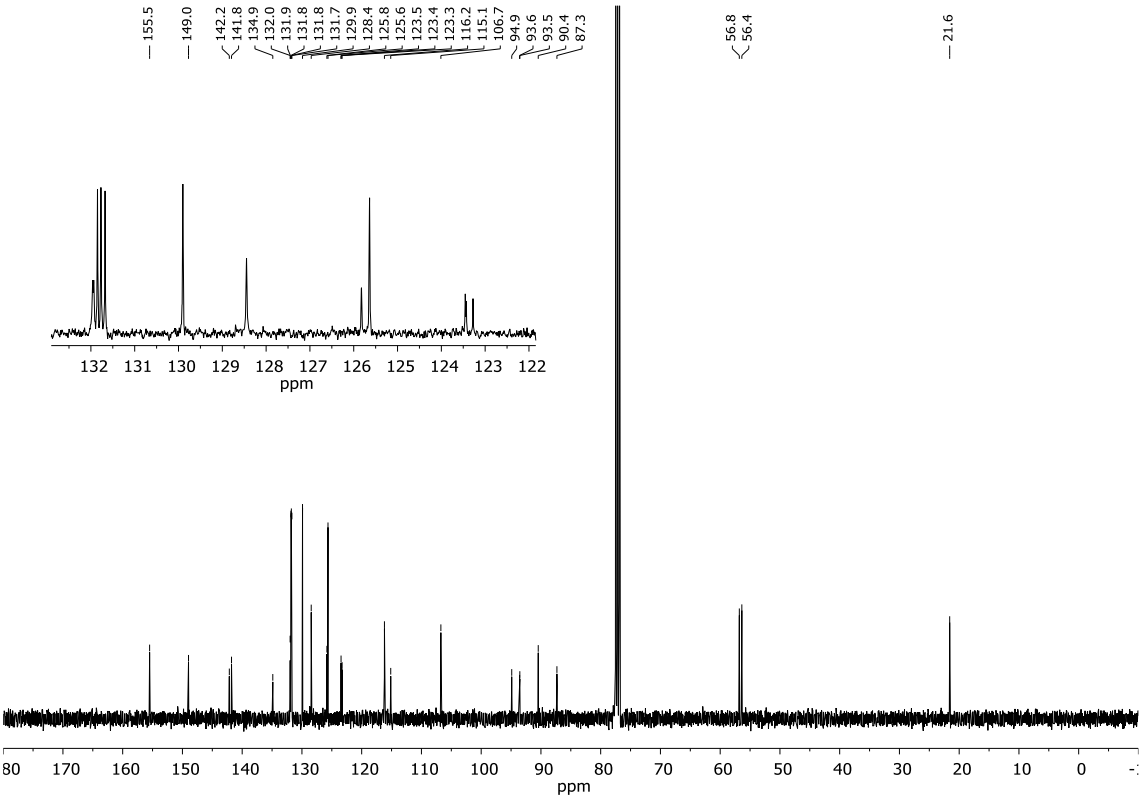
. **^{13}C NMR (126 MHz, $CDCl_3$)** spectrum of compound **S6**



^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **(*S*, *S*)-2**



^{13}C NMR (126 MHz, $CDCl_3$) spectrum of compound **(*S*, *S*)-2**



Synthesis and Spectroscopic Characterization of (S,S)-1 and (S,S)-2 complexes

The corresponding compounds (*S*,*S*)-**1** and (*S*,*S*)-**2** (0.024 mmol, 1 eq.) were dissolved in 0.5 mL of a 9:1 mixture of CD_2Cl_2: Acetone-d_6. On the other hand, a solution of corresponding metal salt (0.120 mmol, 5 eq.) in 0.5 mL of 9:1 CD_2Cl_2: Acetone-d_6 was prepared. Stepwise additions of 1 eq. (0.1 mL) of metal was performed and the corresponding a ^{1}H-NMR spectra recorded. Changes in the aromatic signals confirmed the binding phenomena.

Complex (*S*,*S*)-1·Zn(II):

^{1}H NMR (400 MHz, 9:1 CD_2Cl_2:Acetone-d_6) δ 7.68 – 7.65 (m, 2H), 7.65 – 7.61 (m, 2H), 7.56 (d, *J* = 8.1 Hz, 4H), 7.42 (s, 2H), 7.40 – 7.36 (m, 4H), 7.24 (d, *J* = 8.1 Hz, 4H), 6.76 (s, 2H), 4.03 (s, 6H), 3.67 (s, 6H), 2.34 (s, 6H). **^{13}C NMR (101 MHz, 9:1 CD_2Cl_2:Acetone-d_6)** δ 155.7 (C), 148.7 (C), 144.1 (C), 137.5 (C), 133.5 (CH), 133.2 (CH), 130.7 (CH), 129.14 (CH), 129.10 (CH), 128.2 (C), 127.2 (CH), 125.9 (C), 125.3 (C), 116.9 (C), 116.1 (CH), 105.9 (CH), 95.3 (C), 92.7 (C), 89.9 (C), 56.9 (CH_3), 56.1 (CH_3), 21.7 (CH_3).

Complex (*S*,*S*)-1·Ca(II):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) δ 7.68 – 7.63 (m, 2H), 7.64 – 7.60 (m, 2H), 7.48 (d, *J* = 8.3 Hz, 4H), 7.39 – 7.35 (m, 4H), 7.26 (s, 2H), 7.01 (d, *J* = 8.1 Hz, 4H), 6.75 (s, 2H), 3.98 (s, 6H), 3.75 (s, 6H), 2.23 (s, 6H). **^{13}C NMR (126 MHz, CD_2Cl_2:Acetone-d_6)** δ 155.7 (C), 148.8 (C), 142.4 (C), 140.0 (C), 133.0 (CH), 132.8 (CH), 131.5 (C), 130.2 (CH), 129.1 (CH), 128.9 (CH), 125.88 (C), 125.86 (C), 125.4 (CH), 116.5 (C), 116.1 (CH), 105.6 (CH), 94.6 (C), 92.6 (C), 90.5 (C), 57.2 (CH_3), 56.2 (CH_3), 21.6 (CH_3).

Complex (*S*,*S*)-1·Sc(III):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) δ 7.69 – 7.63 (m, 8H), 7.43 – 7.36 (m, 4H), 7.33 – 7.31 (m, 6H), 6.83 (s, 2H), 4.06 (s, 6H), 3.76 (s, 6H), 2.36 (s, 6H). **^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6)** δ 156.0 (C), 149.3 (C), 145.5 (C), 135.0 (C), 133.4 (CH), 133.3 (CH), 131.2 (CH), 129.4 (CH), 129.2 (CH), 127.3 (CH), 125.9 (C), 125.2 (C), 125.1 (C), 118.8 (C), 116.5 (CH), 105.3 (CH), 96.2 (C), 92.6 (C), 89.3 (C), 57.4 (CH_3), 56.6 (CH_3), 21.8 (CH_3).

Complex (*S*,*S*)-1·Ga(III):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) δ 7.71 – 7.62 (m, 8H), 7.56 (s, 2H), 7.43 – 7.36 (m, 4H), 7.31 (d, *J* = 8.1 Hz, 4H), 6.81 (s, 2H), 4.10 (s, 6H), 3.70 (s, 6H), 2.36 (s, 6H). **^{13}C NMR (126 MHz, CD_2Cl_2:Acetone-d_6)** δ 156.0 (C), 148.9 (C), 145.8 (C), 133.9 (C), 133.8 (CH), 133.4 (CH), 131.1 (CH), 129.5

(CH), 129.2 (CH), 128.0 (CH), 126.0 (C), 124.9 (C), 116.5 (CH), 106.1 (CH), 96.3 (C), 92.7 (C), 89.2 (C), 57.3 (CH_3), 56.5 (CH_3), 21.9 (CH_3).

Complex (*S,S*)-2·Zn(II):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$) δ 7.65 – 7.60 (m, 8H), 7.60 – 7.56 (m, 12H), 7.51 (s, 2H), 7.36 (dd, *J* = 5.8, 3.3 Hz, 4H), 7.26 (d, *J* = 8.1 Hz, 4H), 6.71 (s, 2H), 4.07 (s, 6H), 3.70 (s, 6H), 2.34 (s, 6H). **^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$)** δ 155.8 (C), 148.7 (C), 144.2 (C), 137.6 (C), 132.62 (CH), 132.56 (CH), 132.29 (CH), 132.25 (CH), 132.2 (CH), 130.7 (CH), 129.13 (CH), 129.10 (CH), 128.6 (C), 127.3 (CH), 125.91 (C), 125.89 (C), 124.1 (C), 123.9 (C), 123.7 (C), 116.3 (C), 115.8 (CH), 106.5 (CH), 95.9 (C), 93.7 (C), 93.60 (C), 90.9 (C), 90.8 (C), 87.9 (C), 57.1 (CH_3), 56.2 (CH_3), 21.7 (CH_3).

Complex (*S,S*)-2·Ca(II):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$) δ 7.61 (s, 4H), 7.60 – 7.54 (m, 12H), 7.53 (d, *J* = 8.3 Hz, 4H), 7.36 (dd, *J* = 5.8, 3.3 Hz, 4H), 7.32 (s, 2H), 7.12 (d, *J* = 8.1 Hz, 4H), 6.81 (s, 2H), 3.96 (s, 6H), 3.78 (s, 6H), 2.28 (s, 6H). **^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$)** δ 155.8 (C), 148.9 (C), 142.7 (C), 140.4 (C), 132.5 (CH), 132.4 (CH), 132.20 (CH), 132.17 (CH), 130.3 (CH), 129.1 (CH), 126.1 (C), 125.9 (C), 125.7 (CH), 123.93 (C), 123.89 (C), 123.8 (C), 116.0 (CH), 115.9 (C), 106.0 (CH), 95.2 (C), 93.72 (C), 93.69 (C), 90.82 (C), 90.78 (C), 88.3 (C), 57.1 (CH_3), 56.4 (CH_3), 21.6 (CH_3), (one C and two CH signals were not observed probably due to overlapping problems).

Complex (*S,S*)-2·Sc(III):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$) δ 7.68 – 7.62 (m, 12H), 7.61 – 7.57 (m, 10H), 7.37 (dd, *J* = 5.8, 3.3 Hz, 4H), 7.32 (d, *J* = 8.1 Hz, 4H), 6.84 (s, 2H), 4.06 (s, 6H), 3.81 (s, 6H), 2.36 (s, 6H). **^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$)** δ 156.1 (C), 149.3 (C), 145.5 (C), 135.0 (C), 132.6 (CH), 132.5 (CH), 132.4 (CH), 132.3 (CH), 132.2 (CH), 131.1 (CH), 129.2 (CH), 129.1 (CH), 127.4 (CH), 126.0 (C), 125.9 (C), 124.4 (C), 123.9 (C), 123.5 (C), 121.3 (C), 118.7 (C), 116.3 (CH), 105.8 (CH), 97.0 (C), 93.8 (C), 93.6 (C), 91.2 (C), 90.8 (C), 87.4 (C), 57.5 (CH_3), 56.7 (CH_3), 21.8 (CH_3).

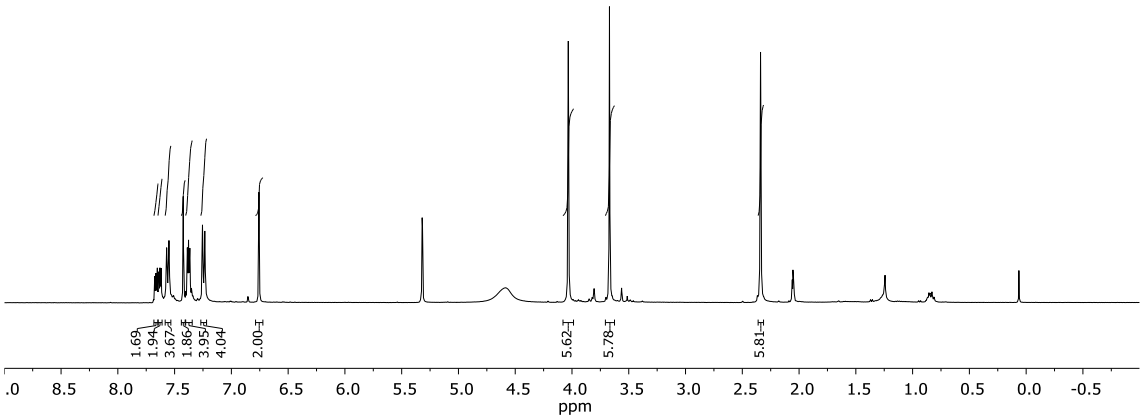
Complex (*S,S*)-2·Ga(III):

^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$) δ 7.67 – 7.54 (m, 22H), 7.36 (dd, *J* = 5.9, 3.3 Hz, 4H), 7.31 (d, *J* = 8.2 Hz, 4H), 6.74 (s, 2H), 4.12 (s, 6H), 3.75 – 3.66 (bs, 6H), 2.36 (s, 6H). **^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-*d*$_6$)** δ 156.0 (C), 148.9 (C), 132.7 (CH), 132.6 (CH), 132.4 (CH), 132.3 (CH), 132.2 (CH), 131.1 (CH), 129.2 (CH), 129.1 (CH), 125.9 (C), 125.8 (C), 124.4 (C), 123.9 (C), 123.4 (C), 116.1 (CH), 106.5

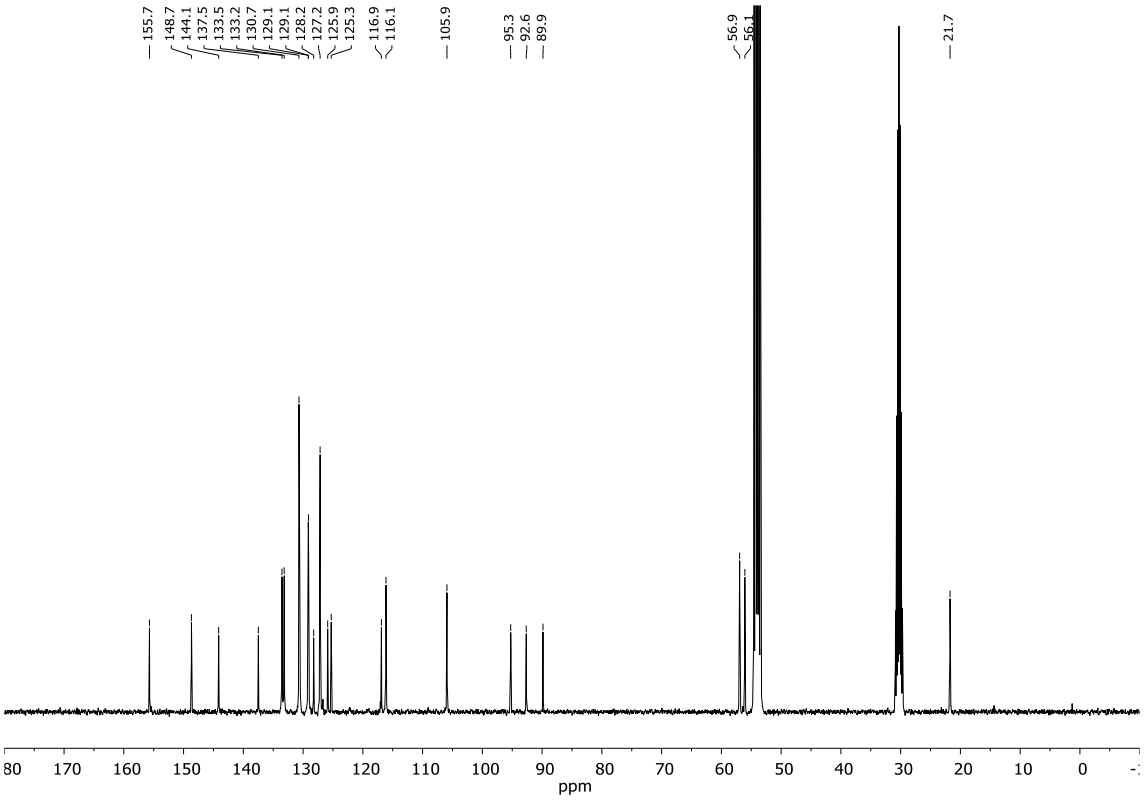
(C), 96.9 (C), 93.7 (C), 93.5 (C), 91.1 (C), 90.8 (C), 87.2 (C), 57.4 (CH_3), 56.6 (CH_3), 21.9 (CH_3), (some signals were not observed owing to they appear as broad signals).

[1]H and [13]C NMR spectra of the metal complexes

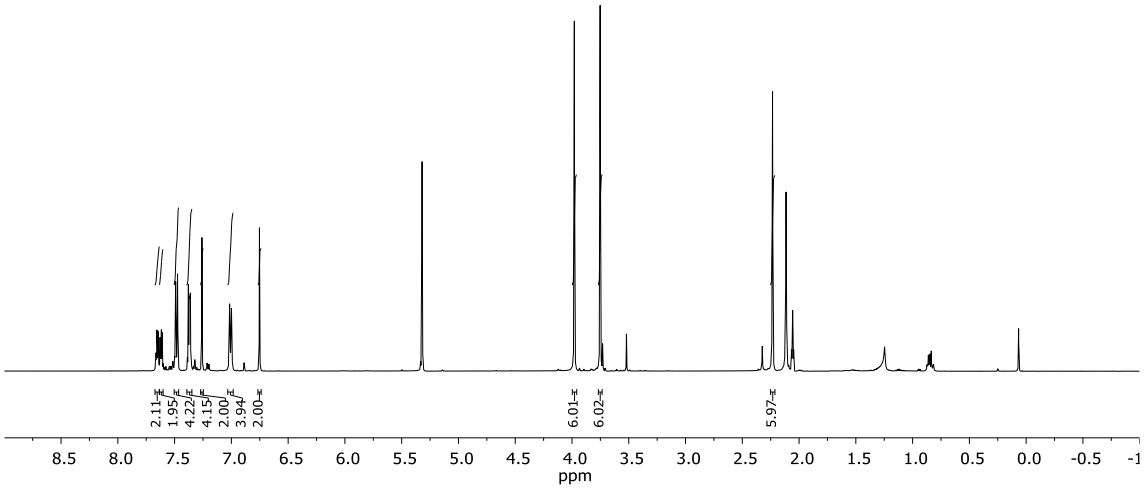
^{1}H NMR (400 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Zn(II) complex of compound (*S,S*)**-1.**



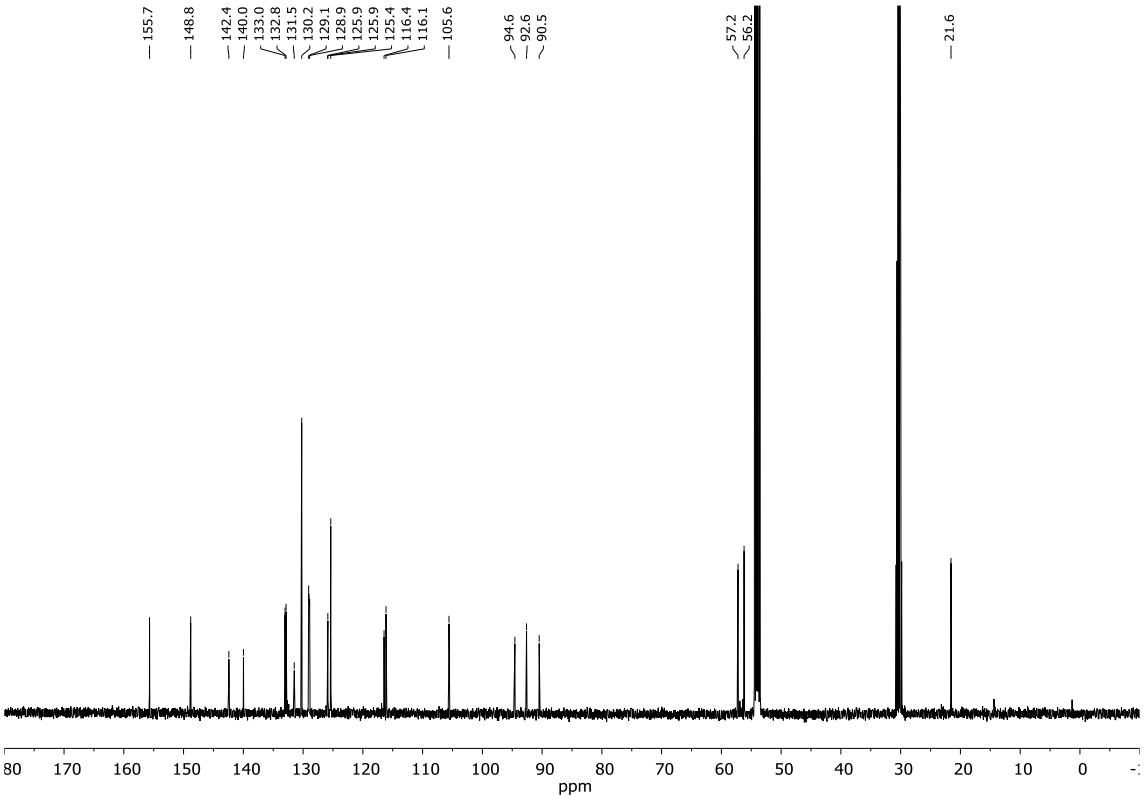
^{13}C NMR (101 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Zn(II) complex of compound (*S,S*)**-1.**



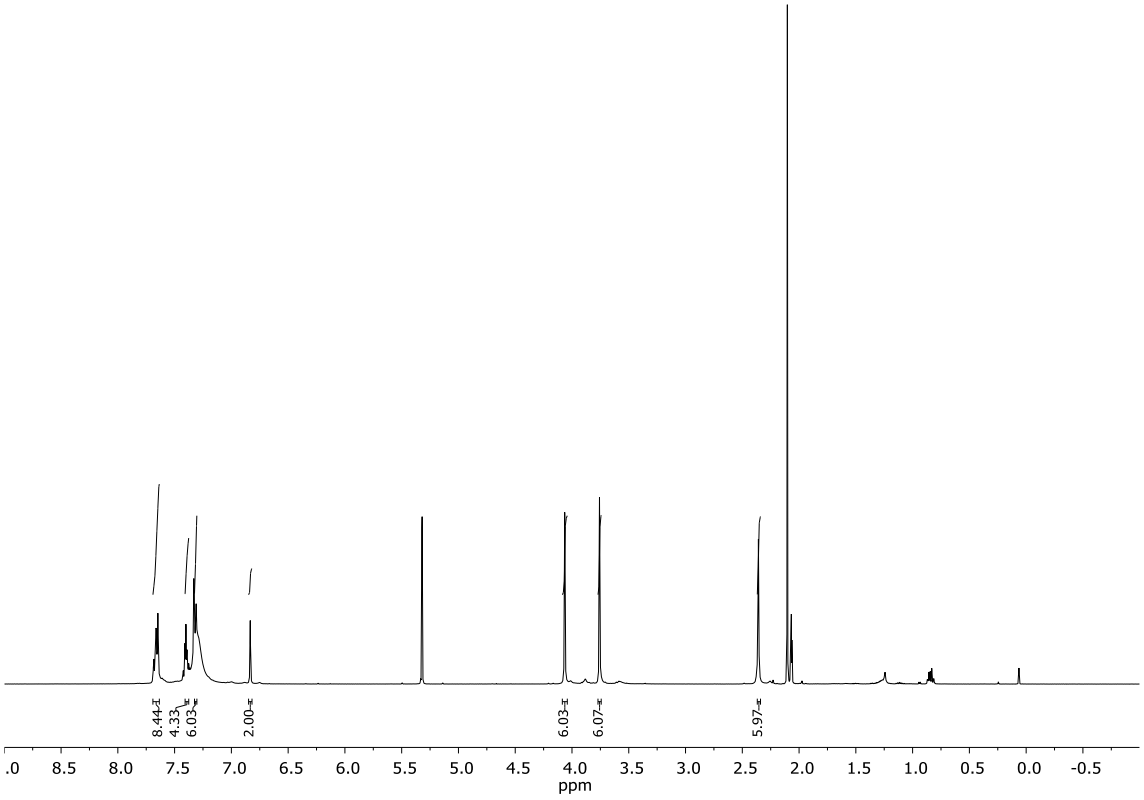
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ca(II) complex of compound (*S,S*)**-1.**



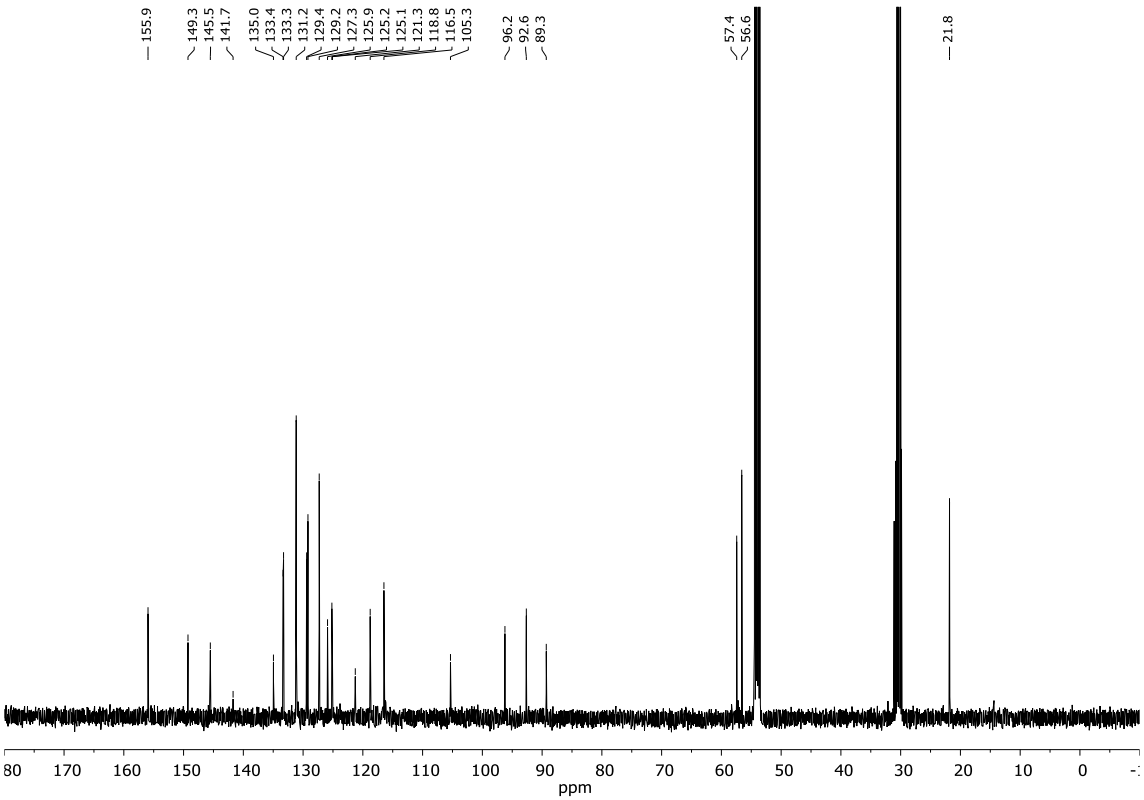
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ca(II) complex of compound (*S,S*)**-1.**



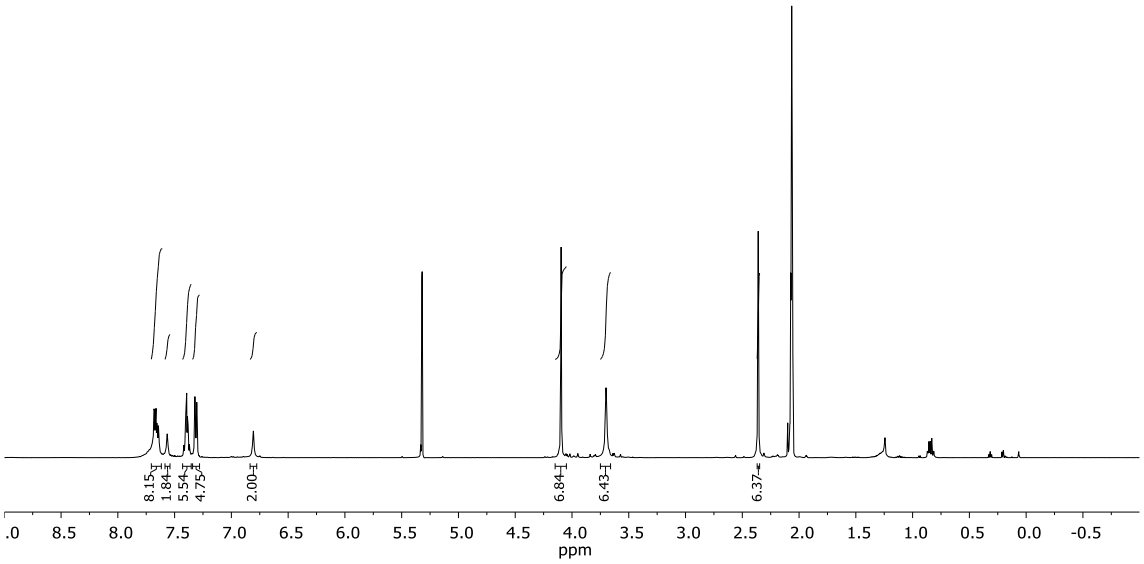
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Sc(III) complex of compound (*S*,*S*)**-1.**



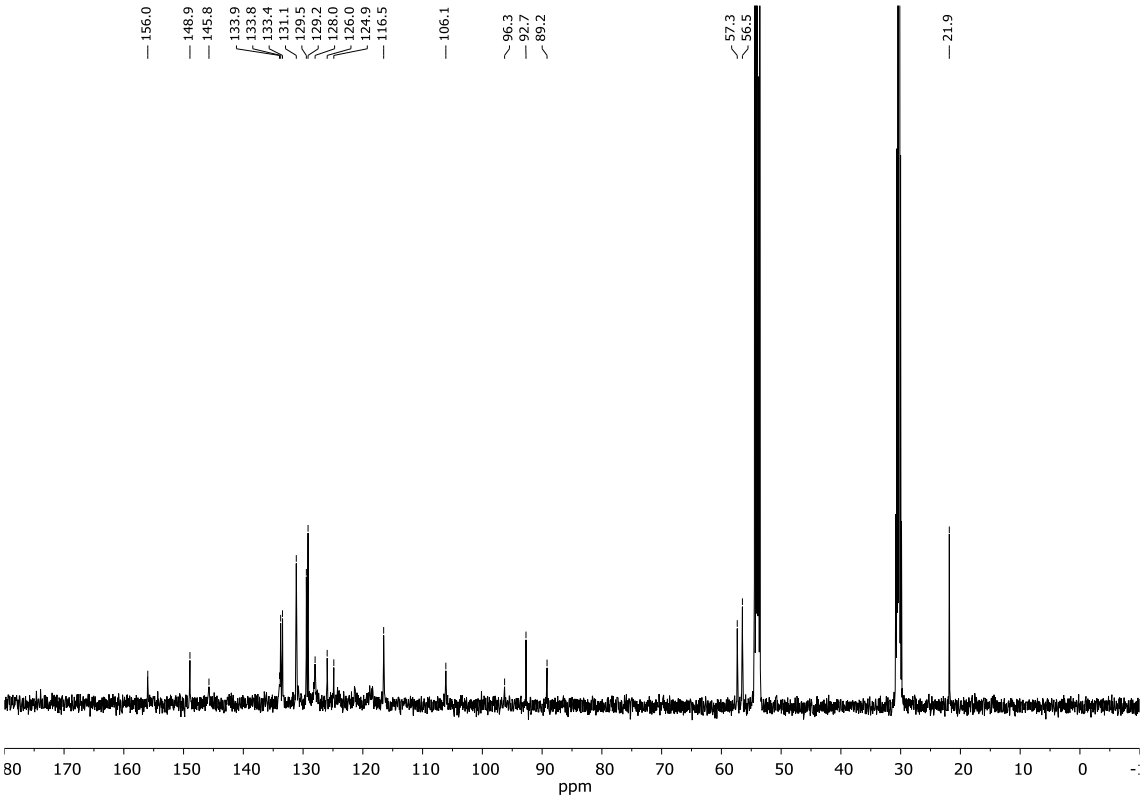
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Sc(III) complex of compound (*S*,*S*)**-1.**



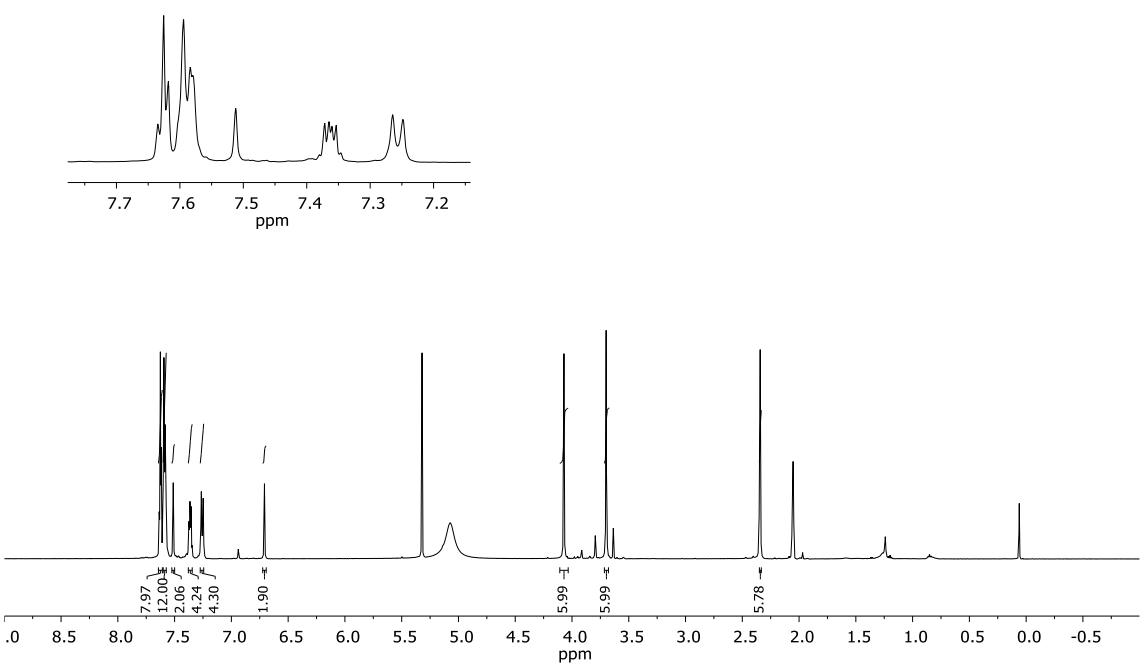
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ga(III) complex of compound (*S,S*)**-1.**



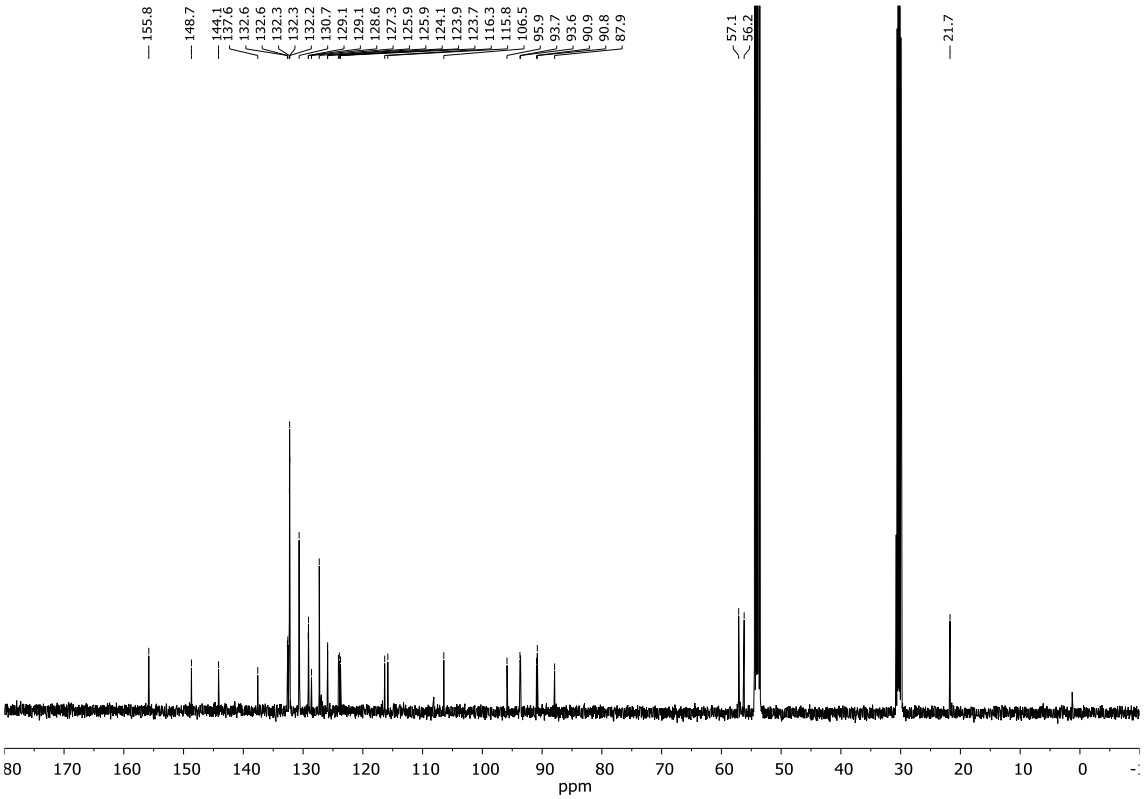
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ga(III) complex of compound (*S,S*)**-1.**



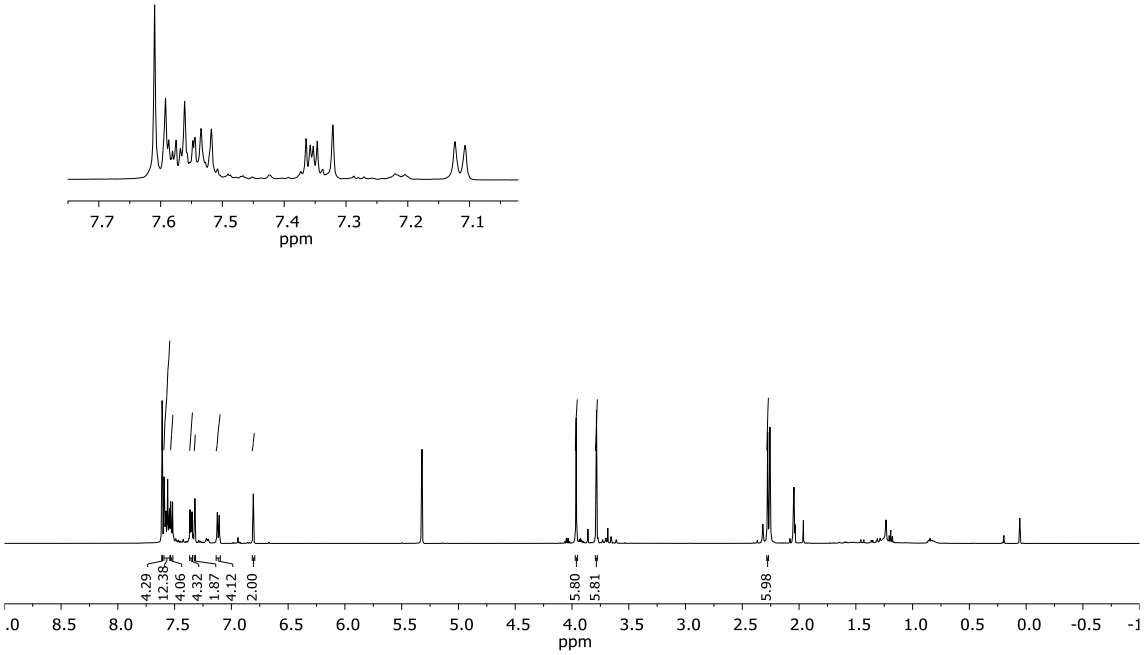
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Zn(II) complex of compound (*S,S*)**-2.**



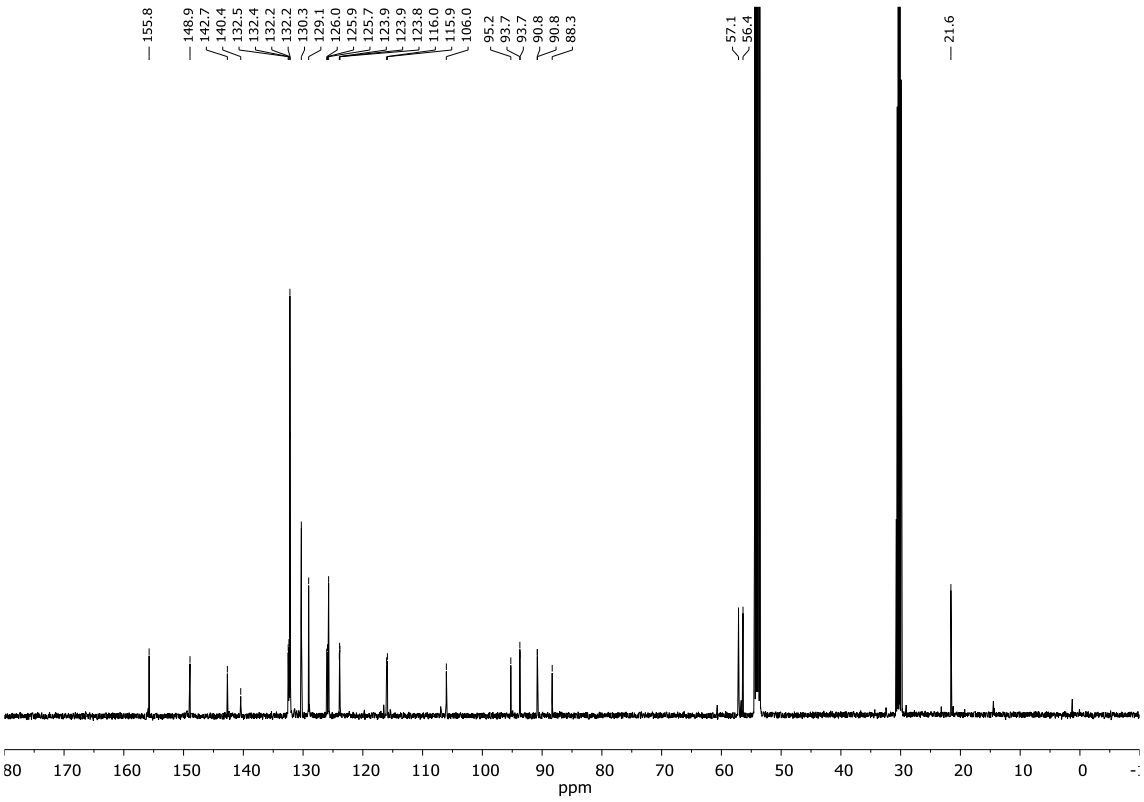
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Zn(II) complex of compound (*S,S*)**-2.**



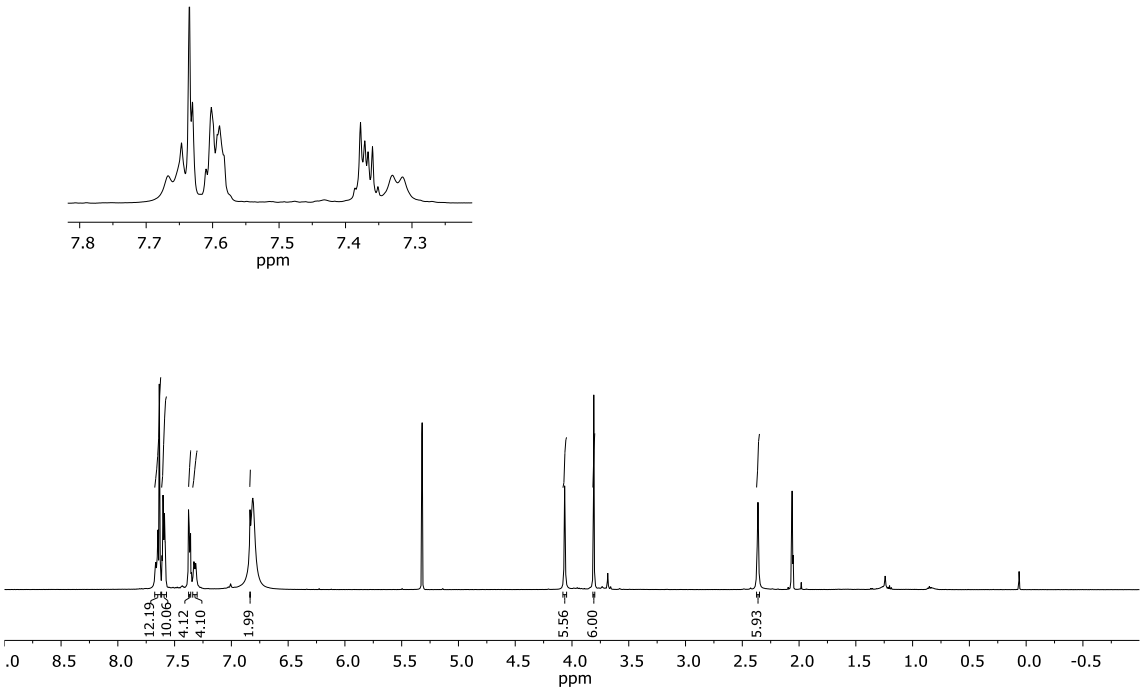
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ca(II) complex of compound (*S,S*)**-2.**



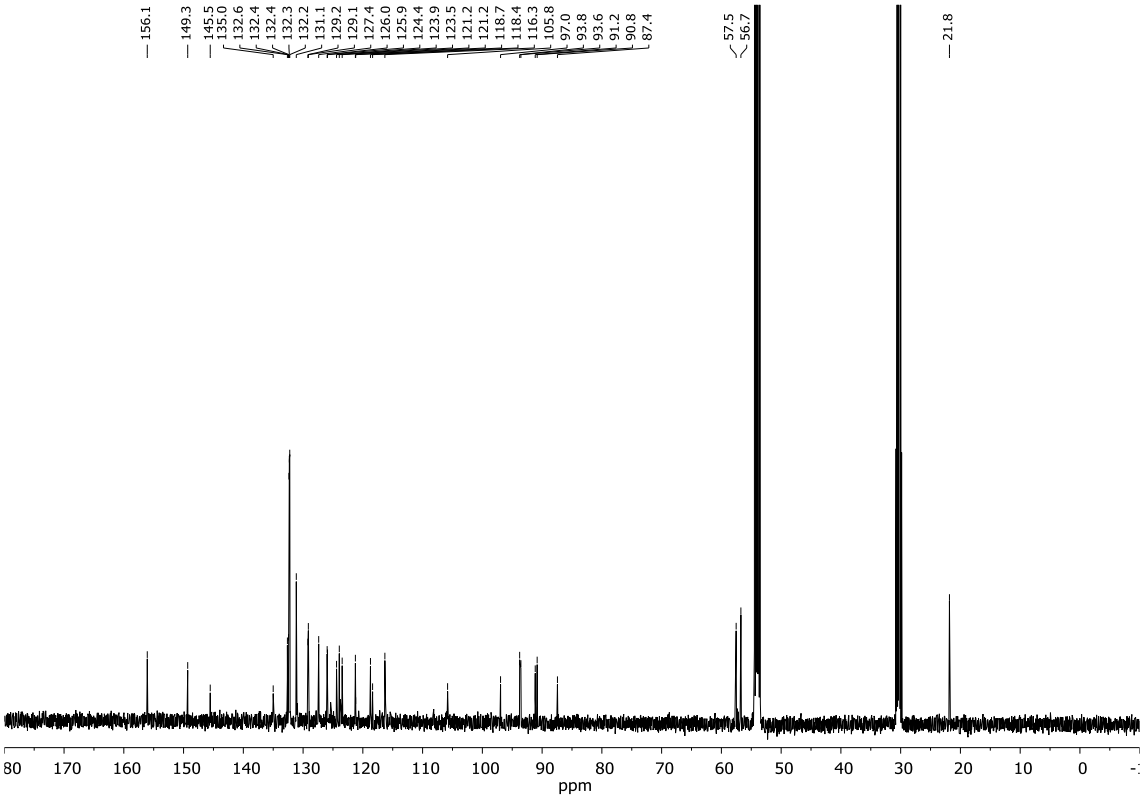
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ca(II) complex of compound (*S,S*)**-2.**



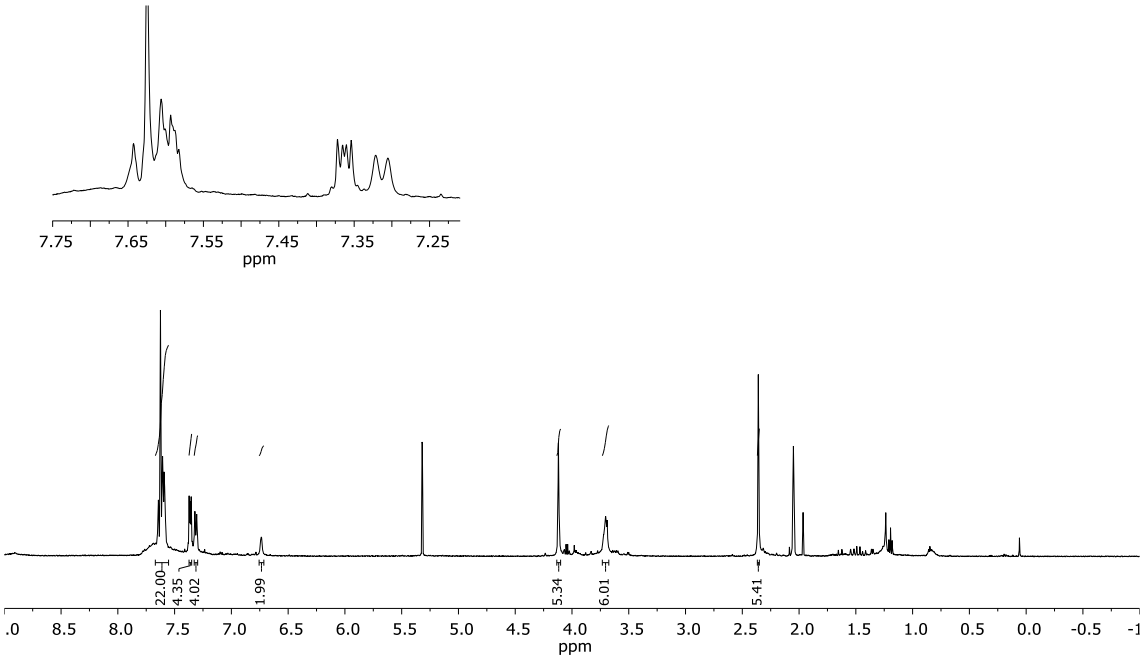
^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Sc(III) complex of compound (*S*,*S*)**-2.**



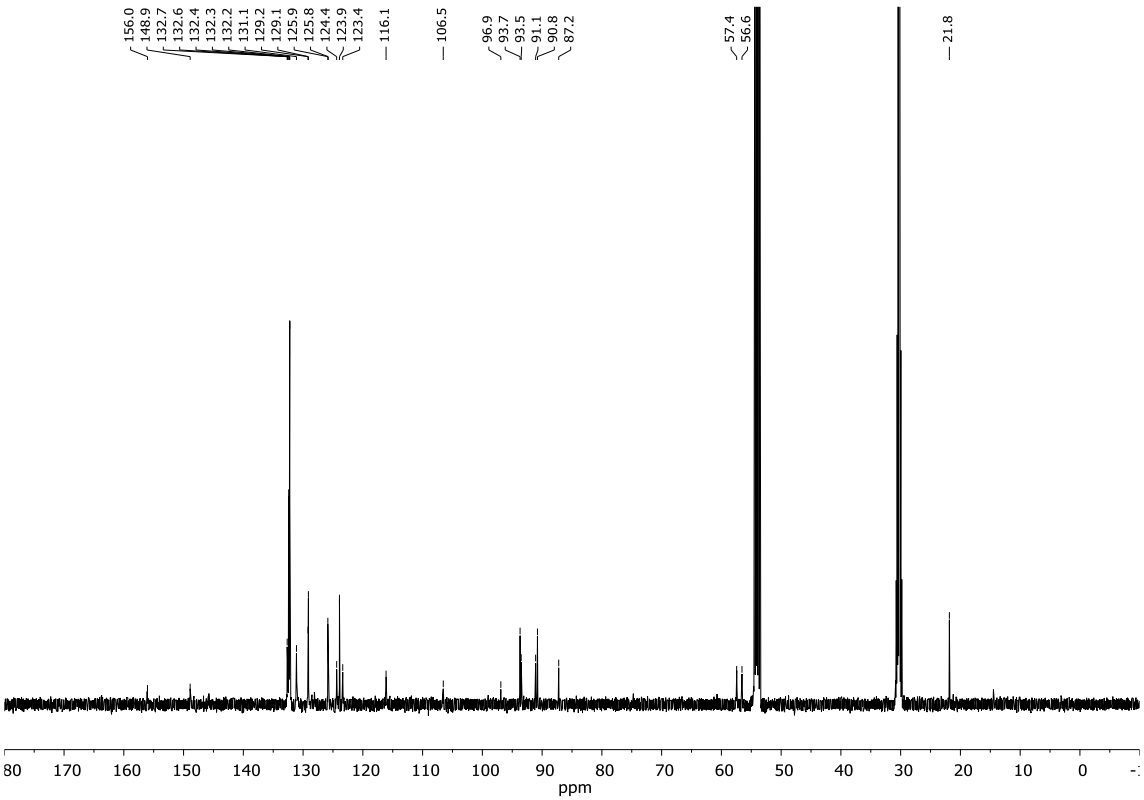
^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Sc(III) complex of compound (*S*,*S*)**-2.**



^{1}H NMR (500 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ga(III) complex of compound (*S,S*)**-2.**



^{13}C NMR (126 MHz, 9:1 CD_2Cl_2:Acetone-d_6) spectrum of Ga(III) complex of compound (*S,S*)**-2.**



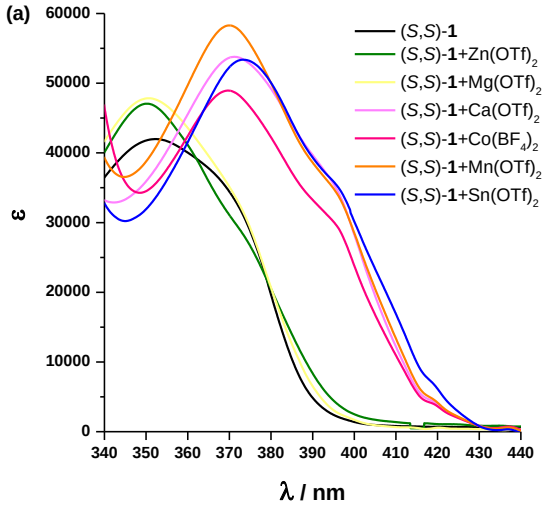
ABSORPTION AND STEADY-STATE FLUORESCENCE SPECTRA

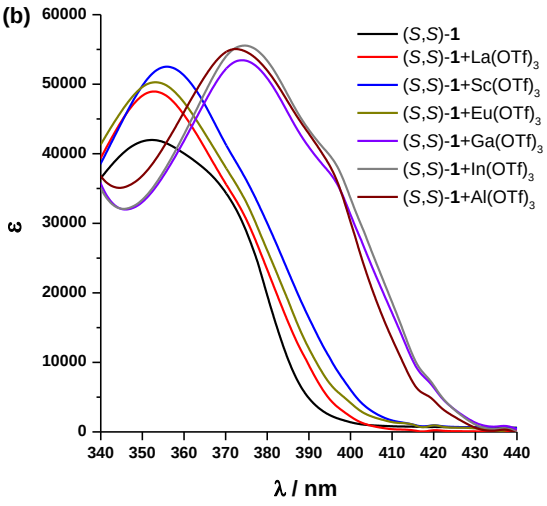
Experimental Conditions

Absorption measurements were conducted using a Jasco 815SE apparatus in a 2.0 mm path-length quartz cell on $4x10^{-5}$M solutions in presence of 30 equivalents of salt.

Steady-state fluorescence spectra were recorded using a JASCO FP-8300 spectrofluorometer in 10 × 10 mm cuvettes on $2.5x10^{-5}$M solutions in presence of 30 equivalents of salt.

Figure S1. Absorption spectra of compound (*S,S*)-**1** in 9:1 mixtures of CH_2Cl_2:Acetone in absence and presence of 10equivalents of different (a) bivalent, (b) trivalent and (c) tetravalent metal salts.





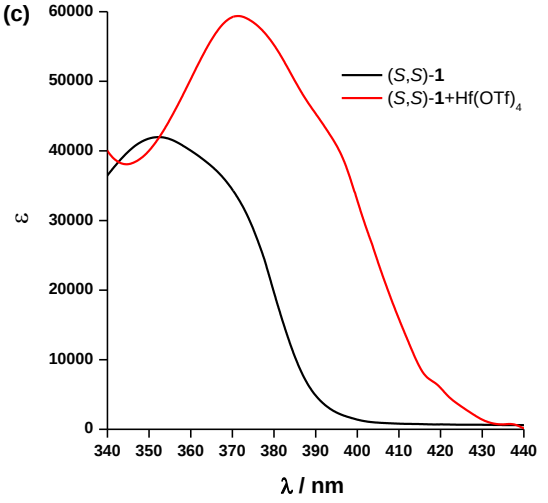


Figure S2. Absorption spectra of compound (*S,S*)-**2** in 9:1 mixtures of CH_2Cl_2:Acetone in absence and presence of 10equivalents of different (a) bivalent, (b) trivalent and (c) tetravalent metal salts.

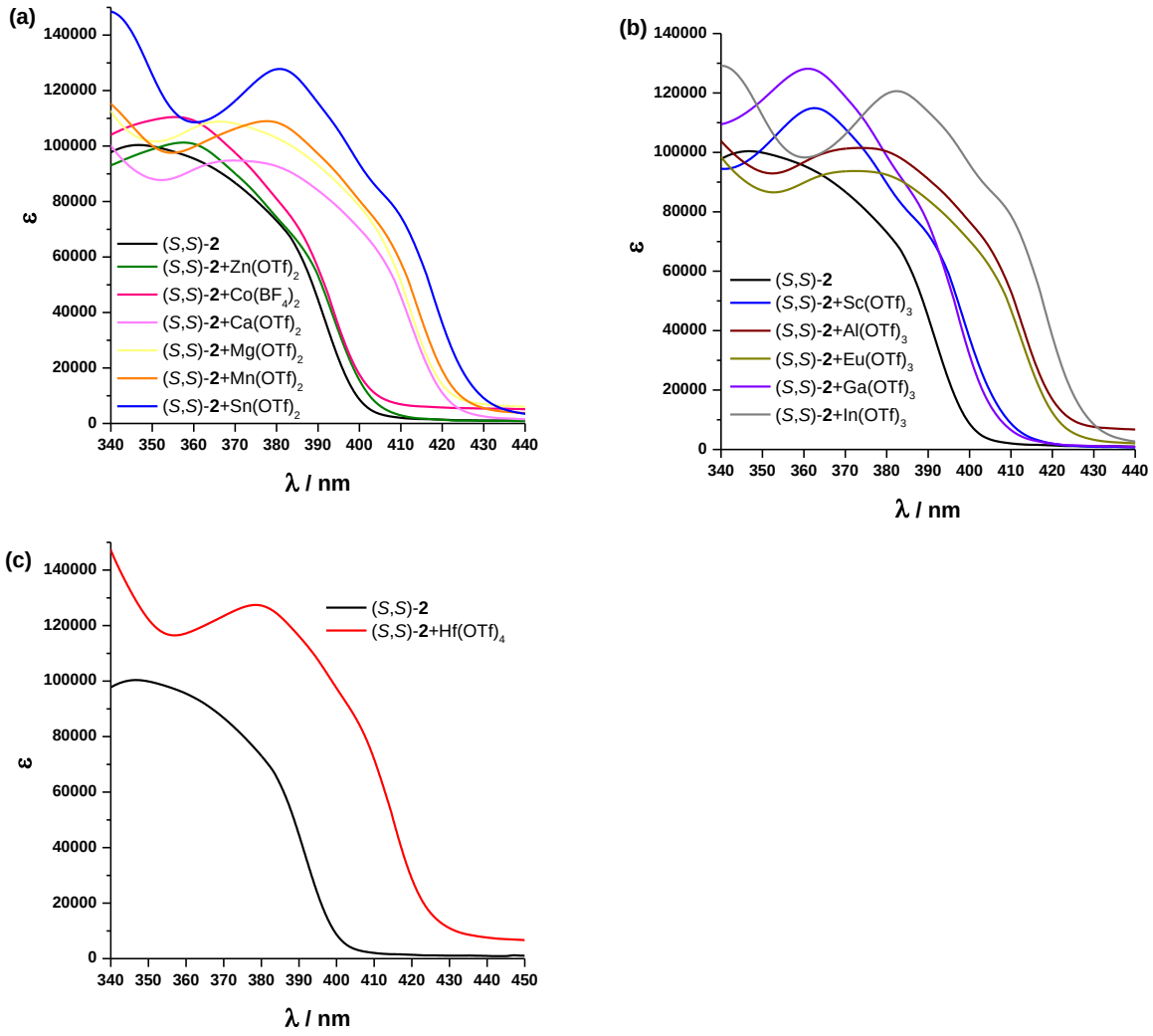
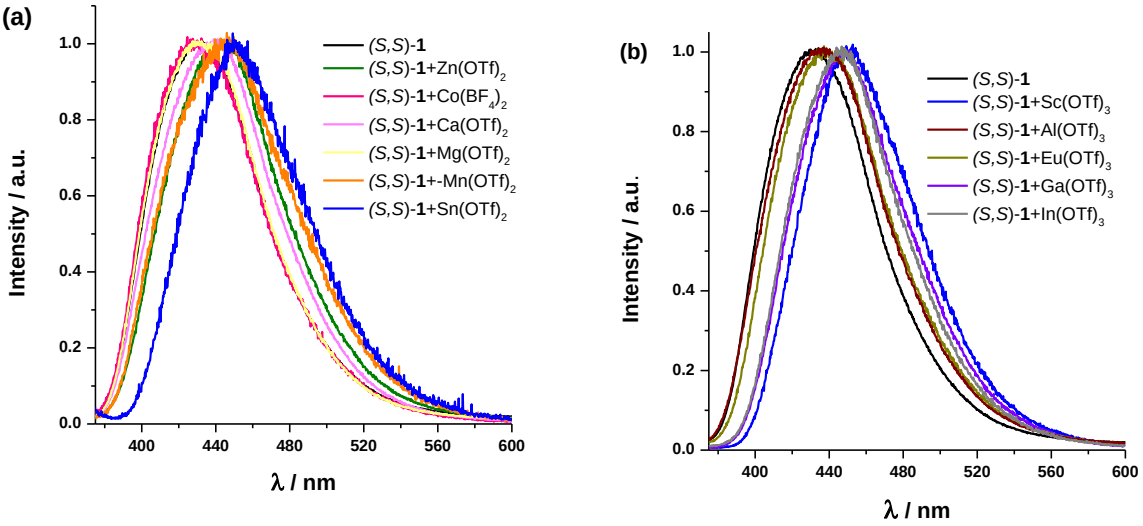


Figure S3. Normalized emission spectra of compound (*S,S*)-**1** in 9:1 mixtures of CH_2Cl_2:Acetone in absence and presence of 10equivalents of different (a) bivalent, (b) trivalent and (c) tetravalent metal salts (λ_{exc}= 365 nm).



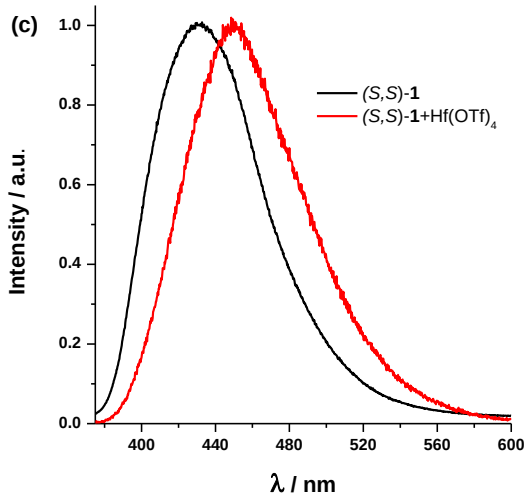
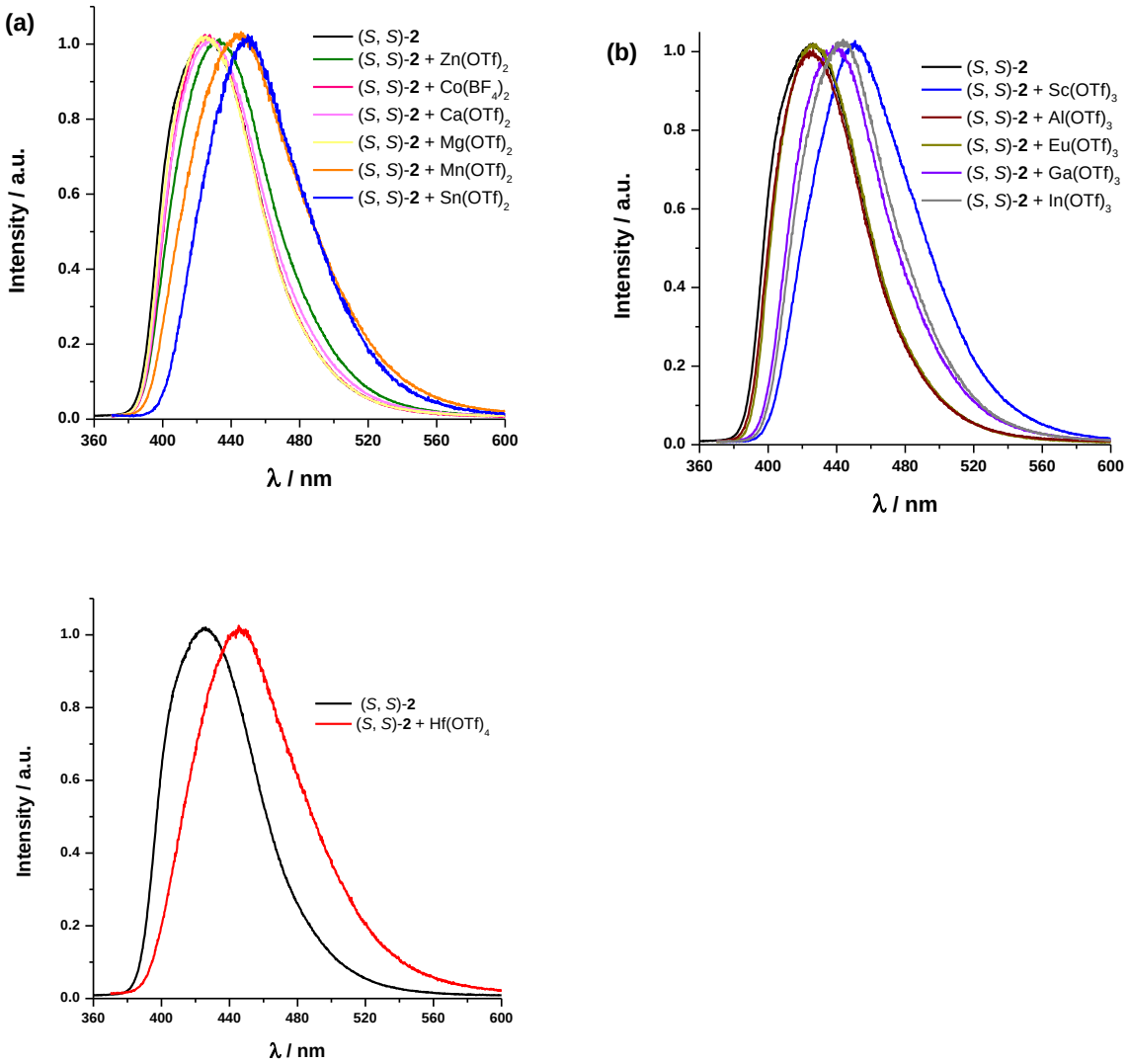


Figure S4. Normalized emission spectra of compound (*S,S*)-**2** in 9:1 mixtures of CH_2Cl_2:Acetone in absence and presence of 10equivalents of different (a) bivalent, (b) trivalent and (c) tetravalent metal salts (λ_{exc}= 365 nm).



LIFETIMES, QUANTUM YIELDS and TRES DECONVOLUTION OF COMPOUNDS (S, S)-1-2 with DIFFERENT METALS

Quantum yields were determined by measuring both absorbance and fluorescence of compounds (*P*,*S*,*S*)-**2**-**3** and quinine in 0.1 M H_2SO_4 quinine sulphate as standard (Φr = 0.54).[5] For the relative determination of the fluorescence quantum yield Φ in a series of solvents, the following formula was used:[6,7]

$$\Phi_x = \Phi_r \, \mathrm{x} \, \frac{F_x}{F_r} \, \mathrm{x} \, \frac{1-10^{-A_r(\lambda_{ex})}}{1-10^{-A_x(\lambda_{ex})}} \, \mathrm{x} \, \frac{n_x^2}{n_r^2} \qquad \text{(eq. S1)}$$

The subscripts ***x*** and ***r*** refer respectively to sample and reference (standard) fluorophore with known quantum yield Φ_r in a specific solvent; *F* stands for the spectrally corrected, integrated fluorescence spectra; $A(\lambda_{ex})$ denotes the absorbance at the used excitation wavelength λ_{ex}; and *n* represents the refractive index of the solvent (in principle at the average emission wavelength). To minimize inner filter effects, the absorbance at the excitation wavelength λ_{ex} was kept under 0.1. The measurements were performed using 10×10 mm cuvettes on non-degassed samples.

Time-resolved fluorescence decay traces were collected via the time-correlated single photon counting (TCSPC) method using a FluoTime 200 fluoromoter (PicoQuant, GmbH). The excitation source was a 375-nm pulsed diode laser (LDH-P-C-375B PicoQuant, GmbH) using a 20 MHz excitation frequency. The full width at half maximum (fwhm) of the laser pulses was around 40 ps. The fluorescence emission was collected at a 90° geometry, focused at the detector after crossing through a polarizer (set at the magic angle), 2-mm slits, and a 2-nm bandwidth monochromator. TCSPC was achieved by a TimeHarp200 board, set at 36 ps/channel. Fluorescence decay traces were collected for the necessary time to reach 20,000 counts at the peak channel. For both compounds (*S*,*S*)-**1** and (*S*,*S*)-**2** decay traces were collected at 400, 405 and 410 nm, where the maximum of emission was observed (corresponding to *OPE* structure).

Time-resolved emission spectroscopy (TRES) of compounds (*S*,*S*)-**1**-**2** in absence and presence of metals dissolved in CH_2Cl_2: Acetone (9:1 mixture) was performed by collecting 52 fluorescence decay traces in the 390-598 nm emission range ($\Delta\lambda_{em}$ = 4 nm) at 20 MHz excitation frequency during a fixed amount of time (500 s), to maintain the overall intensity information.

The fluorescence decay traces were fitted to a three -exponential function, by using a Levenberg-Marquard algorithm-based nonlinear least-squares error minimization deconvolution method iterative reconvolution methods (FluoFit 4.4 package, Picoquant GmbH). For each sample, the decay traces were fitted globally with the decay times linked as shared parameters, whereas the pre-exponential factors were local adjustable parameters. The quality of fittings was assessed by the value of the reduced chi-squared, χ^2, parameter and random distributions of the weighted residuals and the autocorrelation functions.

For the TRES (Time Resolved Emission Spectroscopy) analysis and the estimation of the species-associated emission spectra (SAEMS), the fitting procedure described above was performed, by fitting globally the 66 decay traces. The SAEMS of each species *i* at any given emission wavelength ($SAEMS_i(\lambda_{em})$) is given by the fluorescence intensity emitted by the species *i* ($A_{i,\lambda em} \times \tau_i$), normalized by the total intensity and corrected for the different detection sensitivity using the total intensity of the steady-state spectrum ($I_{ss,\lambda em}$):

$$SAEMS_i(\lambda_{em}) = \frac{A_{i,\lambda em} \times \tau_i}{\sum_i A_{i,\lambda em} \times \tau_i} \cdot I_{ss,\lambda em} \qquad \text{(eq. S2)}$$

The approximate contribution of each species can be assessed as the area under the SAEMS. This estimation assumes equal excitation rate for all the species, as the initial amount of each form in the excited state (after the pulse excitation) is unknown. Figures S5-S6 show the SAEMS of compounds (*S*,*S*)-**1**-**2** dissolved in 9:1 mixtures of dichloromethane:acetone.

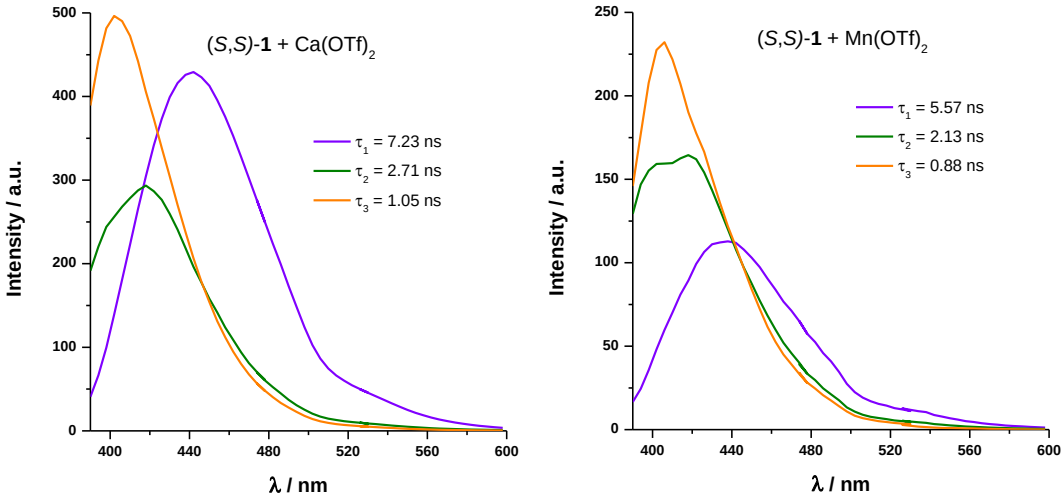
Table S1. Quantum yields and lifetimes (average of signals at 410, 415 and 420 nm) of compound (*S*,*S*)-**1** in absence and presence of 10 equivalents of different metal salts.

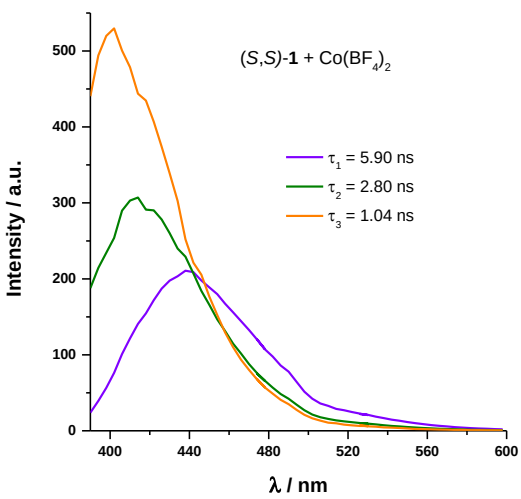
METAL	Φ	τ_1	τ_2	τ_3
(*S*,*S*)-1	0.404±0.004	4.919±0.045	1.970±0.023	1.042±0.012
+LiOTf	0.344±0.009	5.016±0.045	1.88±0.020	0.996±0.013
+CuOTf	0.053±0.003	4.748±0.046	1.567±0.014	0.730±0.013
+TlOTf	0.360±0.002	4.987±0.049	2.125±0.024	1.059±0.011
+Mg(OTf)$_2$	0.343±0.003	6.008±0.047	2.042±0.024	0.999±0.0012
+Ca(OTf)$_2$	0.249±0.002	6.857±0.048	1.987±0.022	0.906±0.013
+Ba(OTf)$_2$	0.331±0.002	5.568±0.053	2.05±0.022	1.008±0.012
+Mn(OTf)$_2$	0.082±0.004	4.605±0.043	1.376±0.011	0.558±0.018
+Fe(OTf)$_2$	0.02081±0.0004	5.83±0.02	1.778±0.019	0.6846±0.0072
+ Co(BF$_4$)$_2$	0.1512±0.0002	4.922±0.044	1.769±0.019	0.902±0.012
+Ni(OTf)$_2$	0.263±0.005	4.779±0.043	1.831±0.019	0.974±0.013
+Cu(OTf)$_2$	0.1804±0.0009	4.816±0.042	1.678±0.016	0.883±0.014
+Zn(OTf)$_2$	0.28±0.01	5.998±0.043	1.934±0.024	0.928±0.014
+Hg(OTf)$_2$	0.15±0.02	4.779±0.049	1.623±0.014	0.740±0.013
+Sn(OTf)$_2$	0.053±0.003	4.922±0.044	1.768±0.019	0.902±0.013
+Bi(OTf)$_3$	0.186±0.004	4.945±0.041	1.684±0.015	0.862±0.015
+Al(OTf)$_3$	0.25±0.01	5.612±0.037	1.824±0.020	0.890±0.015
+Ga(OTf)$_3$	0.161±0.011	4.683±0.037	1.839±0.019	0.834±0.014
+Sc(OTf)$_3$	0.0910±0.0005	6.632±0.038	2.085±0.055	0.659±0.008
+In(OTf)$_3$	0.075±0.002	4.613±0.046	1.799±0.017	0.7005±0.0098
+La(OTf)$_3$	0.162±0.002	6.482±0.035	1.760±0.029	0.729±0.011
+Fe(OTf)$_3$	0.0078±0.0003	5.003±0.180	1.479±0.020	0.645±0.006
+Eu(OTf)$_3$	0.110±0.002	5.006±0.046	1.611±0.015	0.774±0.014
+TiCp$_2$(OTf)$_2$	0.345±0.009	5.014±0.046	1.967±0.023	1.025±0.012
+Hf(OTf)$_4$	0.124±0.003	6.707±0.037	1.773±0.033	0.701±0.010

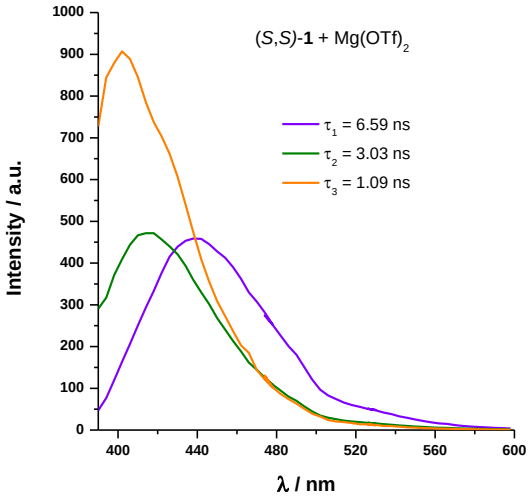
Table S2. Quantum yields and lifetimes (average of signals at 410, 415 and 420 nm) of compound (*S*,*S*)-**2** in absence and presence of 10 equivalents of different metal salts.

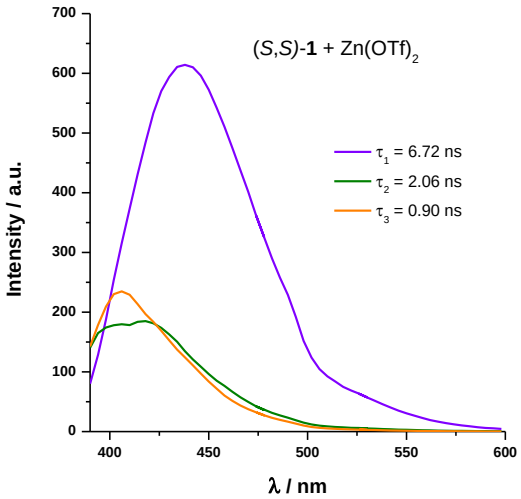
METAL	Φ	τ_1	τ_2	τ_3
(*S*,*S*)-2	0.862±0.007	3.367±0.046	1.961±0.008	1.011±0.011
+Ca(OTf)$_2$	0.843±0.007	4.320±0.069	2.011±0.008	1.024±0.012
+Mn(OTf)$_2$	0.341±0.023	4.701±0.047	2.132±0.009	1.024±0.009
+ Co(BF$_4$)$_2$	0.524±0.015	3.456±0.040	1.935±0.008	1.029±0.011
+Zn(OTf)$_2$	0.654±0.010	5.246±0.014	1.931±0.018	0.955±0.020
+Ga(OTf)$_3$	0.757±0.157	4.688±0.045	2.002±0.008	1.029±0.011
+Sc(OTf)$_3$	0.385±0.005	6.262±0.013	2.206±0.047	0.531±0.027
+In(OTf)$_3$	0.335±0.004	4.419±0.012	1.955±0.017	0.938±0.018

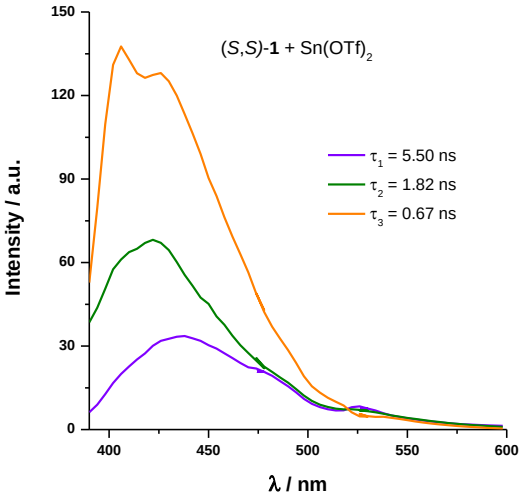
Figure S5. SAEMS spectra of compound (*S*,*S*)-**1** in presence of 30 equivalents of Ca(OTf)$_2$, Mn(OTf)$_2$, Co(BF$_4$)$_2$, Mg(OTf)$_2$, Zn(OTf)$_2$, Sn(OTf)$_2$, Al(OTf)$_3$, Sc(OTf)$_3$, In(OTf)$_3$, Ga(OTf)$_3$, and Hf(OTf)$_4$.

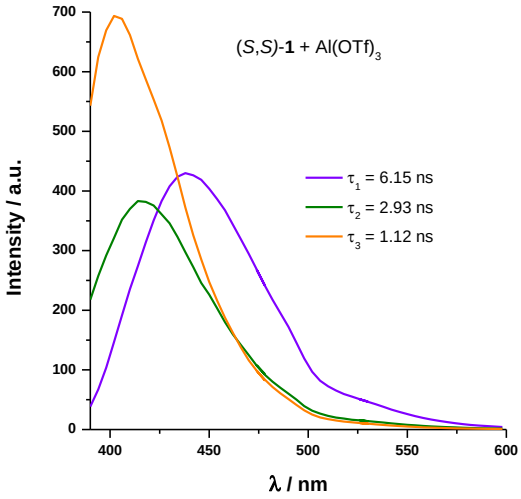


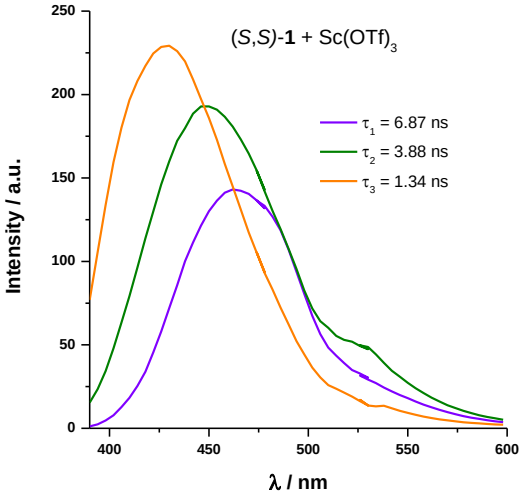

(S,S)-1 + Co(BF4)2
τ1 = 5.90 ns
τ2 = 2.80 ns
τ3 = 1.04 ns
Intensity / a.u.
λ / nm


(S,S)-1 + Mg(OTf)2
τ1 = 6.59 ns
τ2 = 3.03 ns
τ3 = 1.09 ns
Intensity / a.u.
λ / nm


(S,S)-1 + Zn(OTf)2
τ1 = 6.72 ns
τ2 = 2.06 ns
τ3 = 0.90 ns
Intensity / a.u.
λ / nm


(S,S)-1 + Sn(OTf)2
τ1 = 5.50 ns
τ2 = 1.82 ns
τ3 = 0.67 ns
Intensity / a.u.
λ / nm


(S,S)-1 + Al(OTf)3
τ1 = 6.15 ns
τ2 = 2.93 ns
τ3 = 1.12 ns
Intensity / a.u.
λ / nm


(S,S)-1 + Sc(OTf)3
τ1 = 6.87 ns
τ2 = 3.88 ns
τ3 = 1.34 ns
Intensity / a.u.
λ / nm

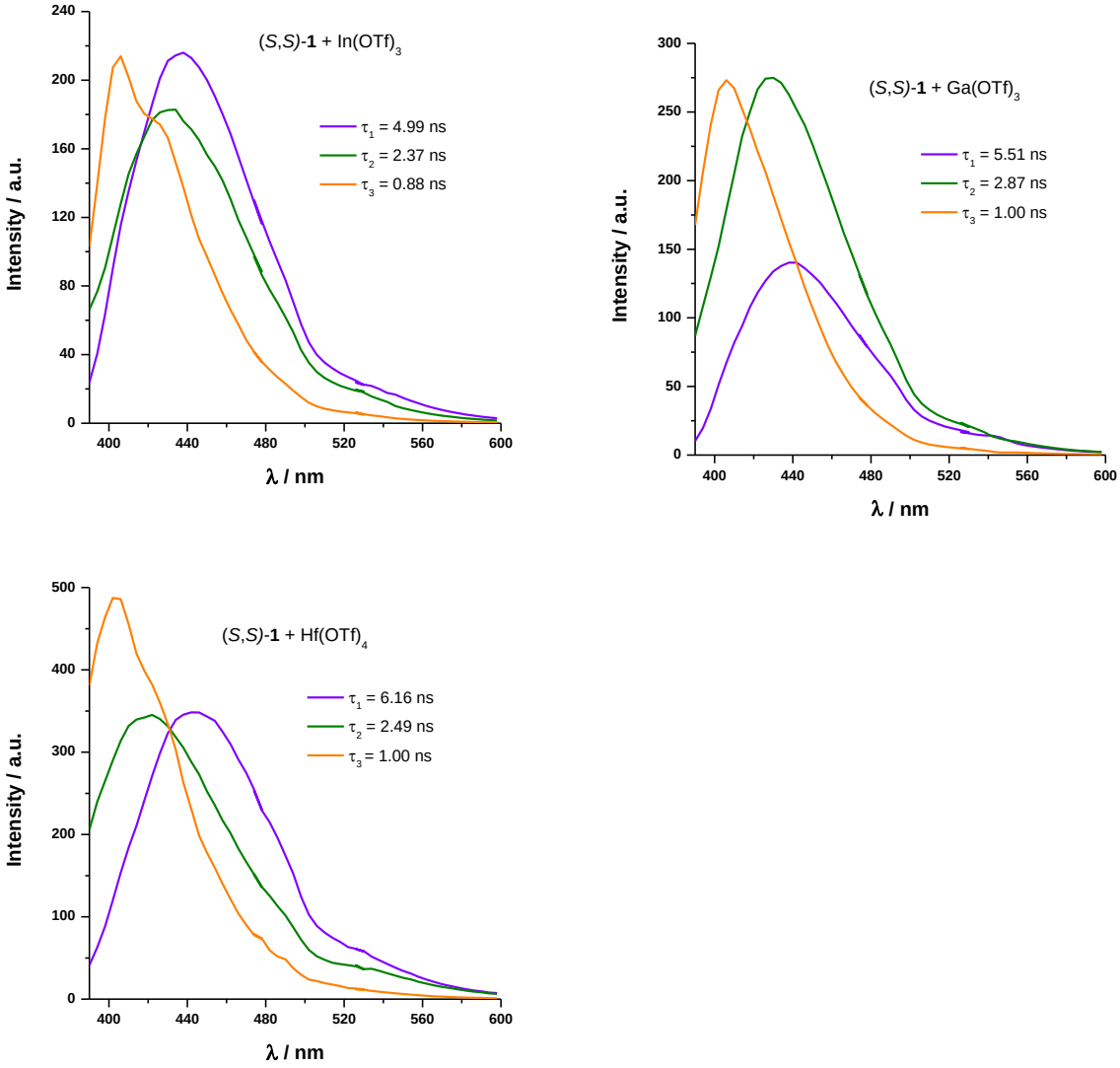
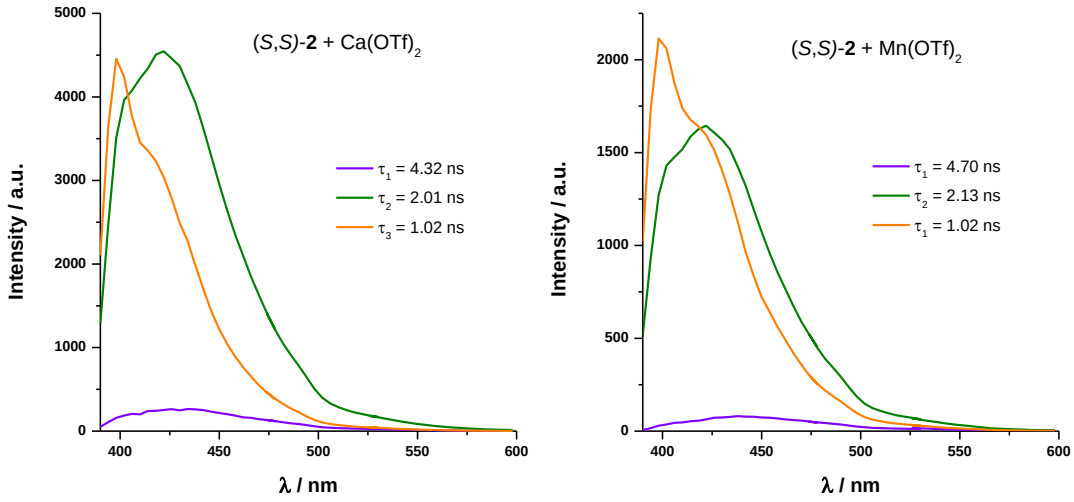
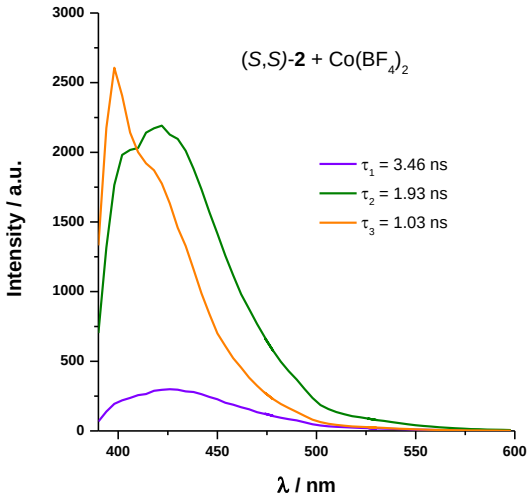
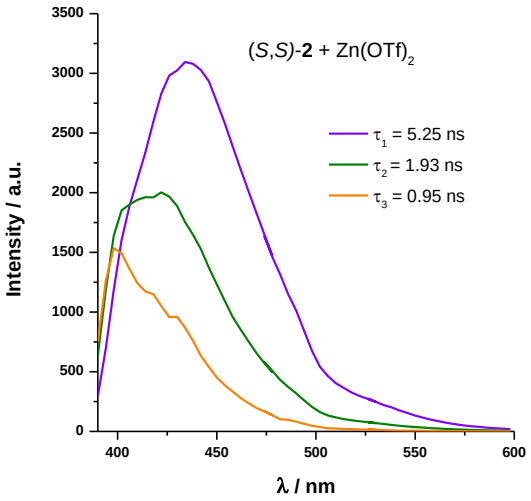
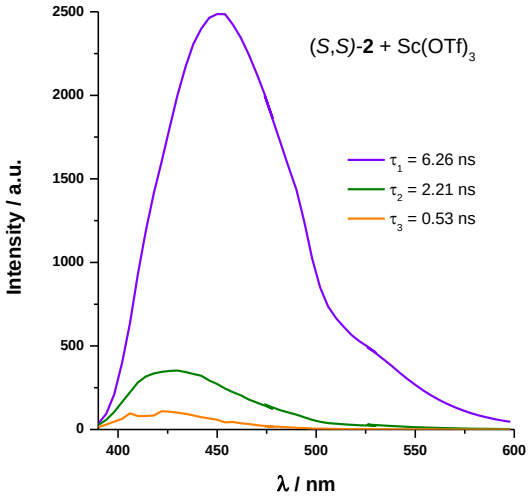


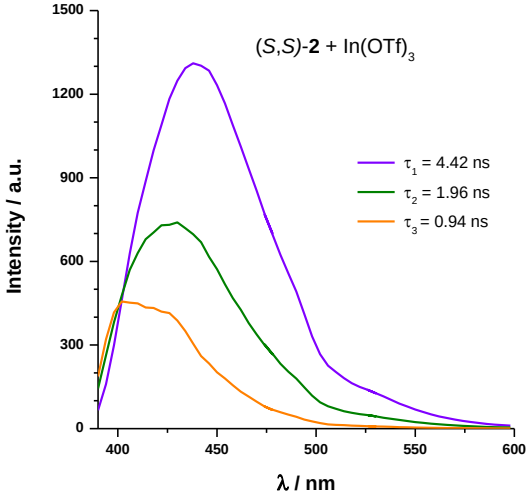
Figure S6. SAEMS spectra of compound (*S,S*)-**2** in presence of 30 equivalents of $Ca(OTf)_2$, $Mn(OTf)_2$, $Co(BF_4)_2$, $Zn(OTf)_2$, $Sc(OTf)_3$, $In(OTf)_3$, $Ga(OTf)_3$.

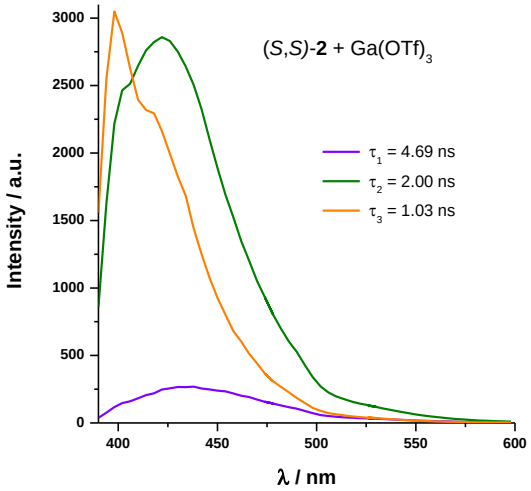



(S,S)-2 + Co(BF4)2
τ1 = 3.46 ns
τ2 = 1.93 ns
τ3 = 1.03 ns
Intensity / a.u.
λ / nm


(S,S)-2 + Zn(OTf)2
τ1 = 5.25 ns
τ2 = 1.93 ns
τ3 = 0.95 ns
Intensity / a.u.
λ / nm

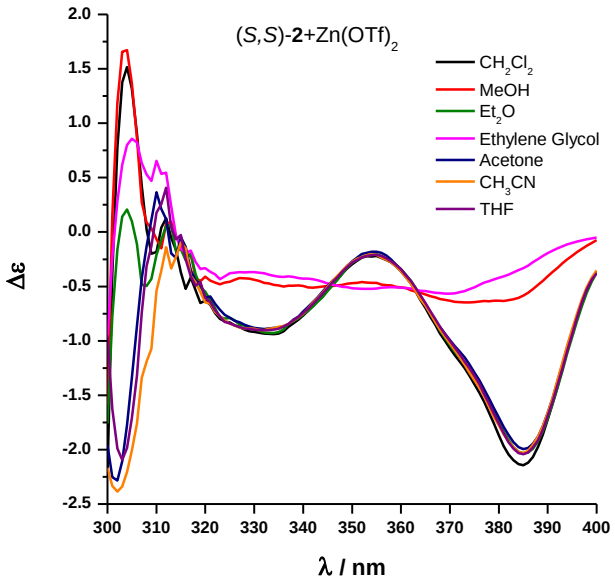

(S,S)-2 + Sc(OTf)3
τ1 = 6.26 ns
τ2 = 2.21 ns
τ3 = 0.53 ns
Intensity / a.u.
λ / nm


(S,S)-2 + In(OTf)3
τ1 = 4.42 ns
τ2 = 1.96 ns
τ3 = 0.94 ns
Intensity / a.u.
λ / nm


(S,S)-2 + Ga(OTf)3
τ1 = 4.69 ns
τ2 = 2.00 ns
τ3 = 1.03 ns
Intensity / a.u.
λ / nm

CD SPECTRA OF COMPOUND (S,S)-2 IN DIFFERENT SOLVENTS

Figure S7. CD spectra of $Zn(OTf)_2$ complex of compound (*S,S*)-**2** in different solvents



In this experiment, 10 equivalents of ethylendiaminetetraacetic acid (EDTA) were also added to try to trap the metal, thus releasing the ligand. However, no differences were observed in CD spectra after EDTA addition.

CD TITRATION OF COMPOUNDS (S,S)-1 and (S,S)-2 WITH DIFFERENT METALS

Experimental

CD titrations were performed in an Olis DSM172 spectrophotometer with a xenon lamp of 150 W with a1.0 cm path-length quartz cell. In all the cases a fixed slit-width of 1 mm and 0.2s of integration time were selected, the ECD spectra showed in Figures S7-S14 are an average spectra calculated after 30 scans (each one).

*General procedure for the CD-titration of compounds (S,S)-**1-2***

Titrations of compounds (*S*,*S*)-**1**-**2** were carried out by addition of progressive quantities of a $2.5x10^{-4}$M solution of the corresponding metal salt, which was commercially available, to a $2.5x10^{-5}$M solution of the corresponding compound in 90:10 mixture of CH_2Cl_2:acetone (some drops of methanol were added in the cases that salts were not soluble at all). To make the fitting of the kinetic constant easier, concentration of ligands (*S*,*S*)-**1**-**2** was kept constant during the titration. To ensure this, $2.5x10^{-5}$M solution of these compounds was used as solvent to prepare the metal solution. The fitting was carried out with DynaFit program (v. 4.06019), which has been previously used to study guest-host complexation equilibria.[8]

Fig. S8. CD titration of compound (*S*,*S*)-**1** with monovalent metals

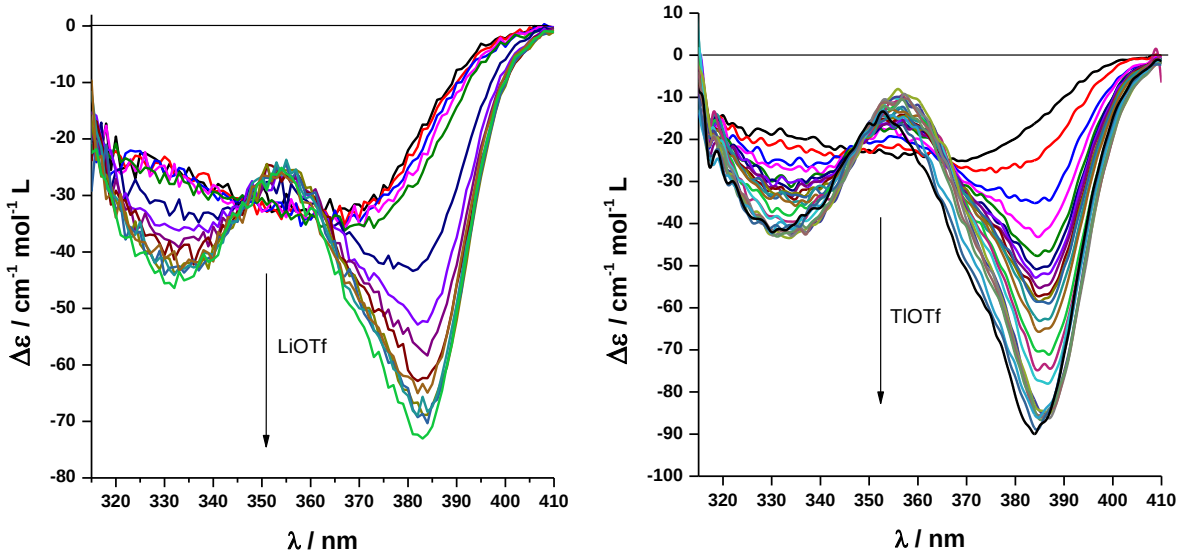
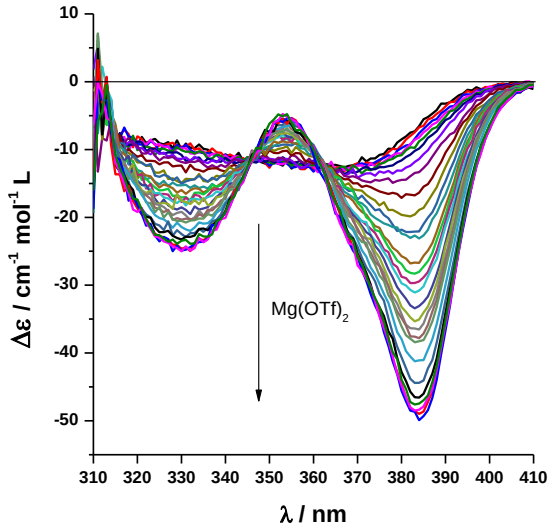
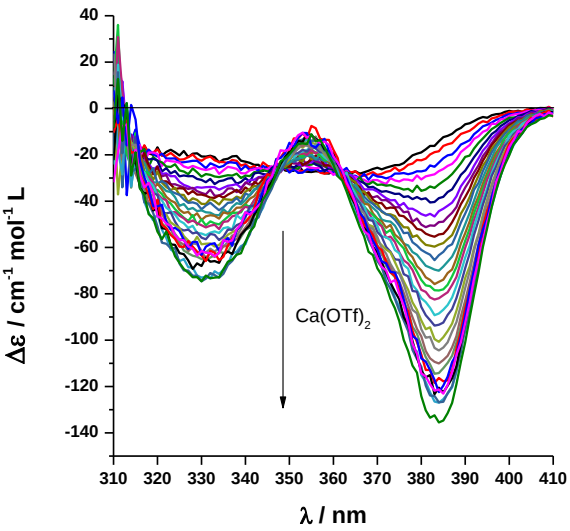
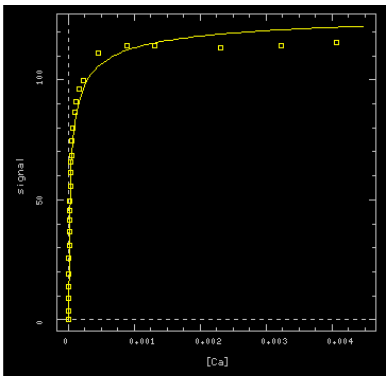
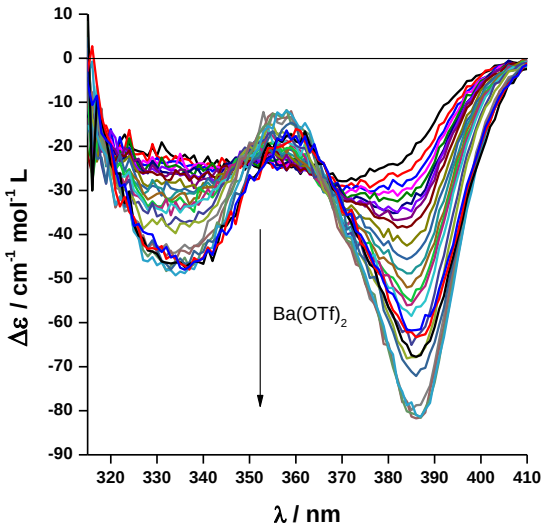


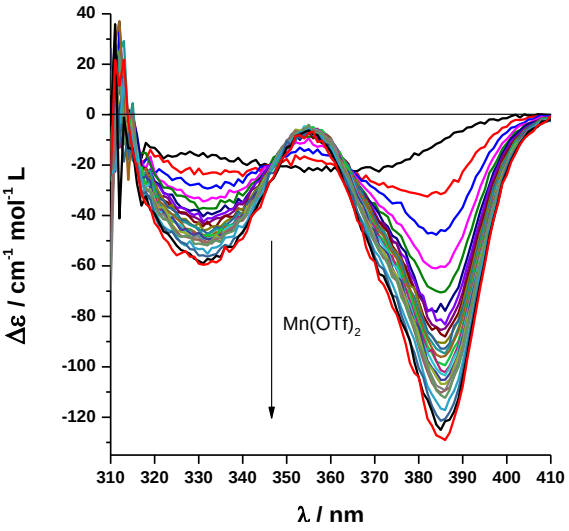
Fig. S9. CD titration of compound (*S,S*)-**1** with bivalent metals

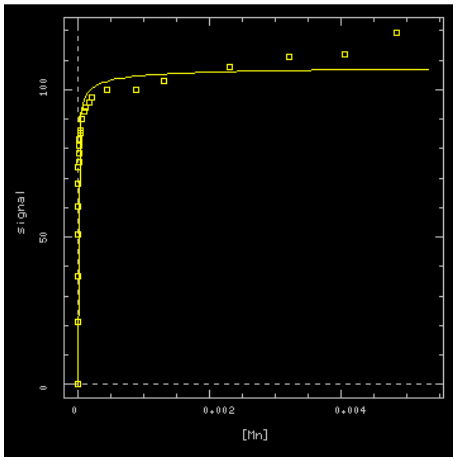


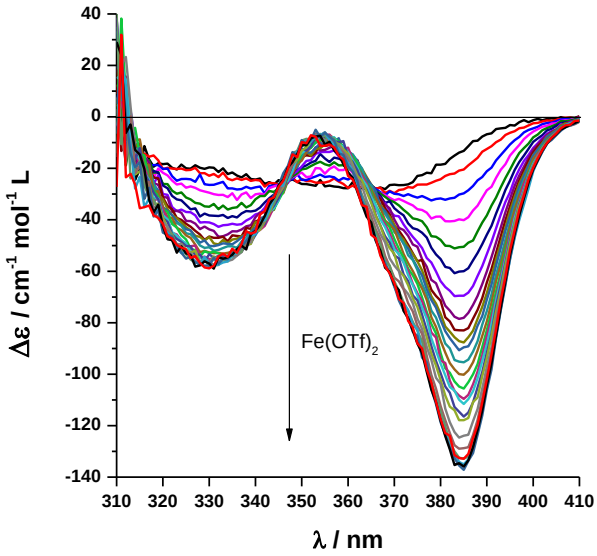


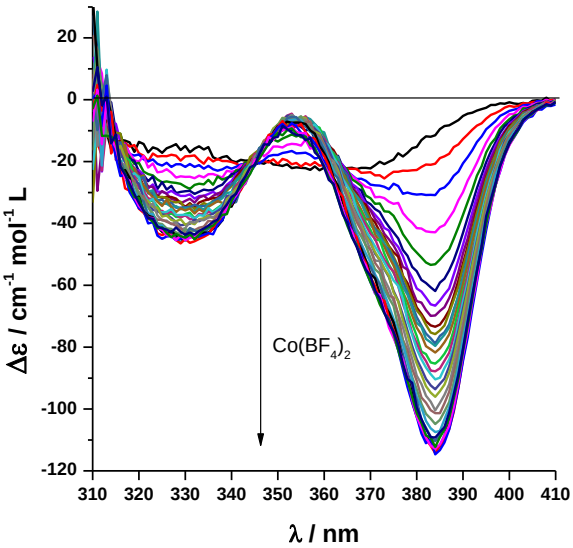


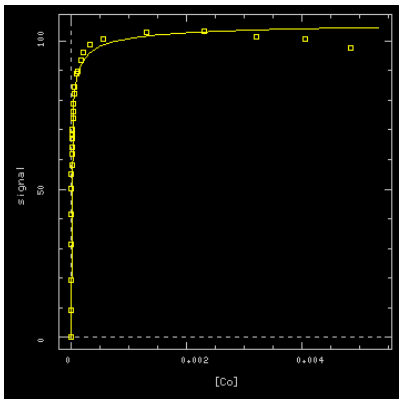


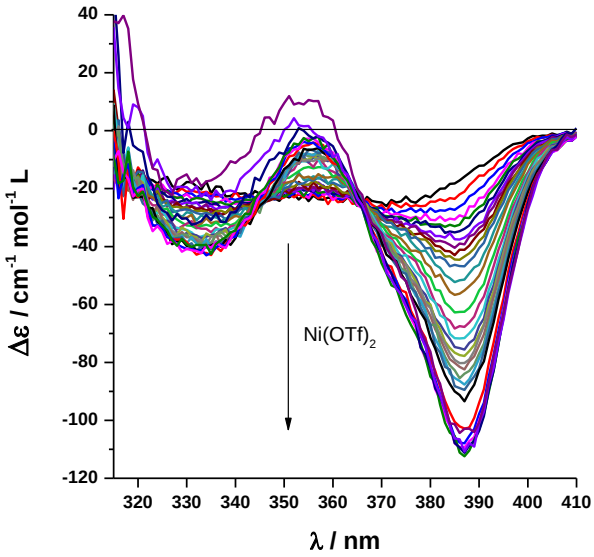

Δε / cm-1 mol-1 L
λ / nm
Mn(OTf)2

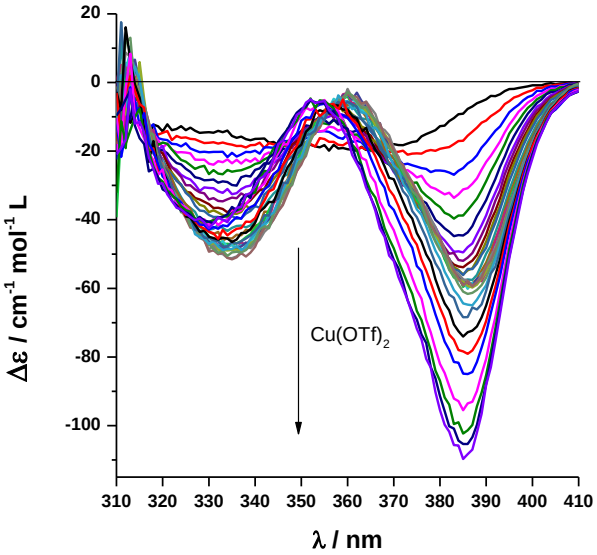

signal
[Mn]

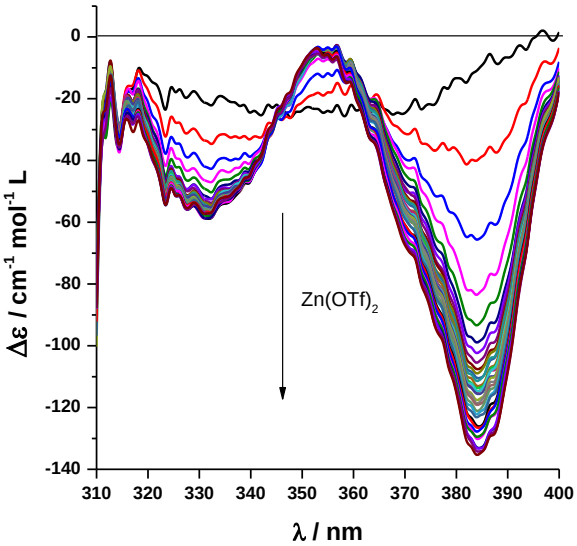

Δε / cm-1 mol-1 L
λ / nm
Fe(OTf)2

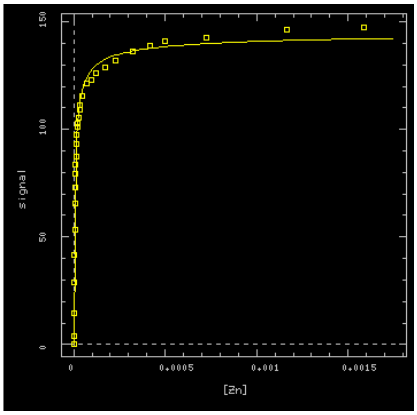

Δε / cm-1 mol-1 L
λ / nm
Co(BF4)2


signal
[Co]


Δε / cm-1 mol-1 L
λ / nm
Ni(OTf)2


Δε / cm-1 mol-1 L
λ / nm
Cu(OTf)2


Δε / cm-1 mol-1 L
λ / nm
Zn(OTf)2


signal
[Zn]

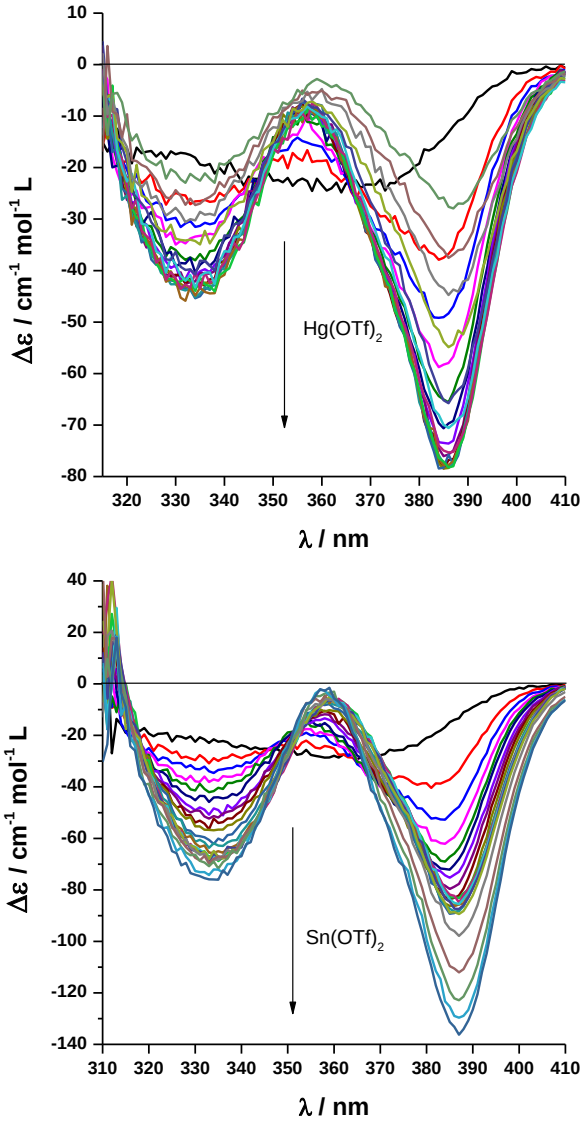
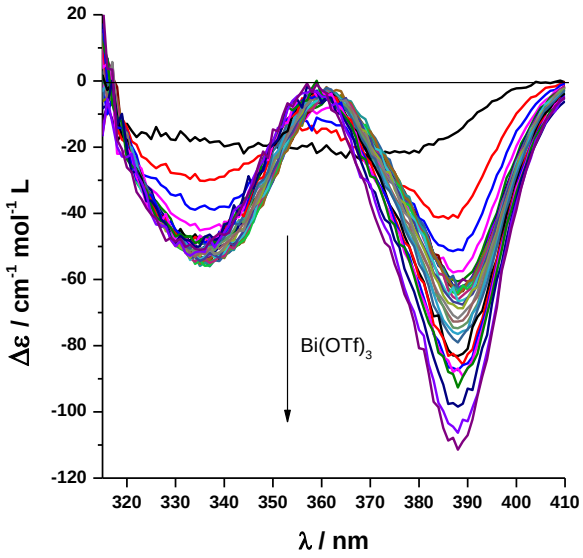
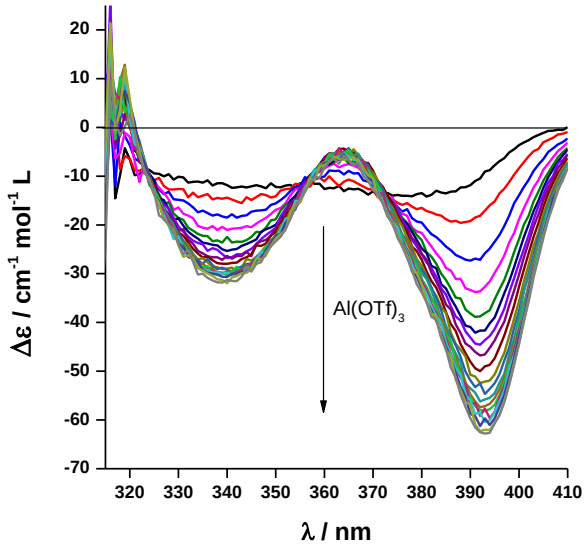
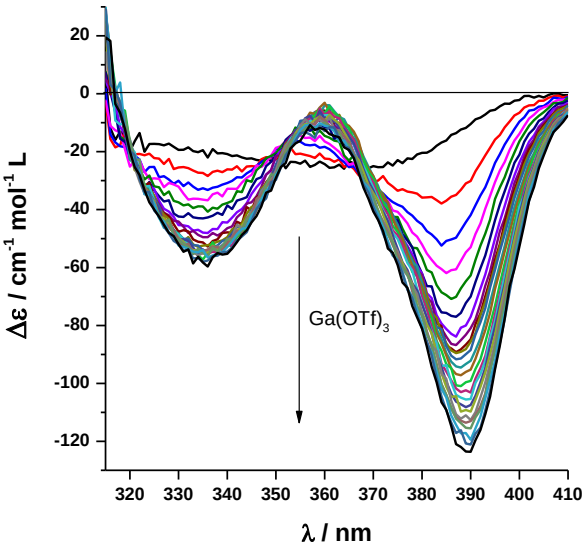
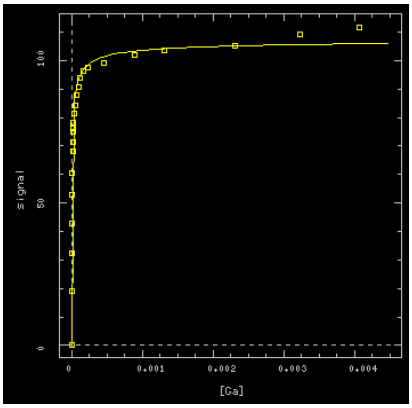


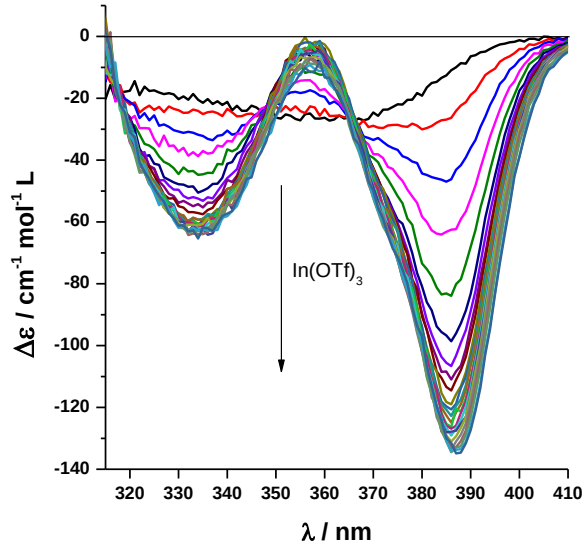
Fig. S10. CD titration of compound (*S,S*)-**1** with trivalent metals

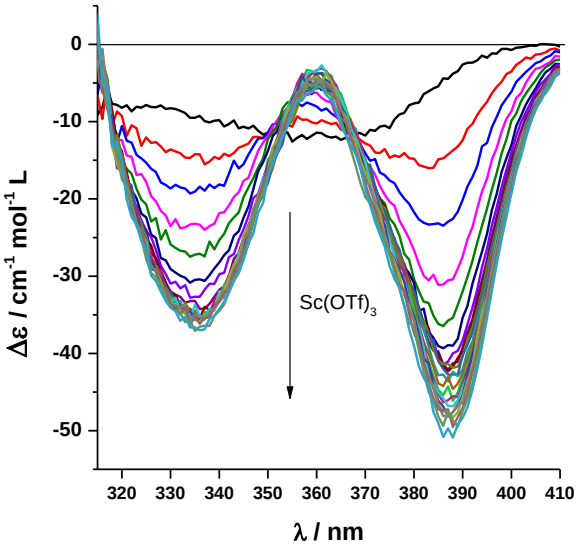


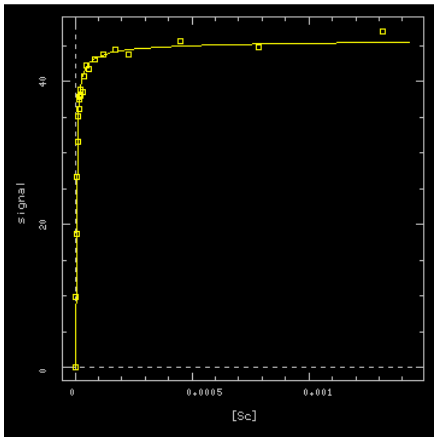

Δε / cm-1 mol-1 L
λ / nm
Al(OTf)3

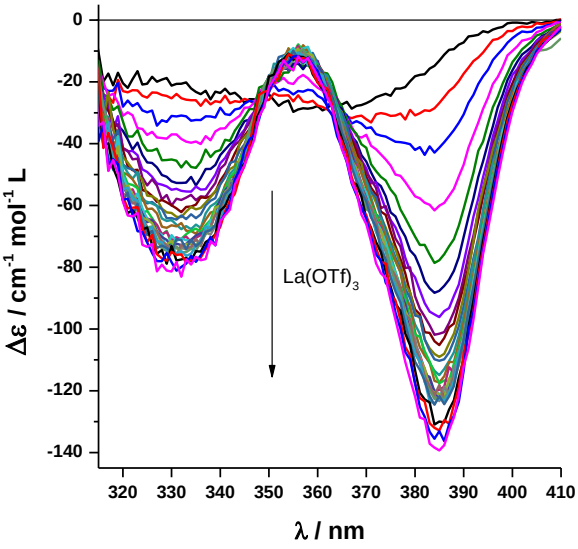

Δε / cm-1 mol-1 L
λ / nm
Ga(OTf)3

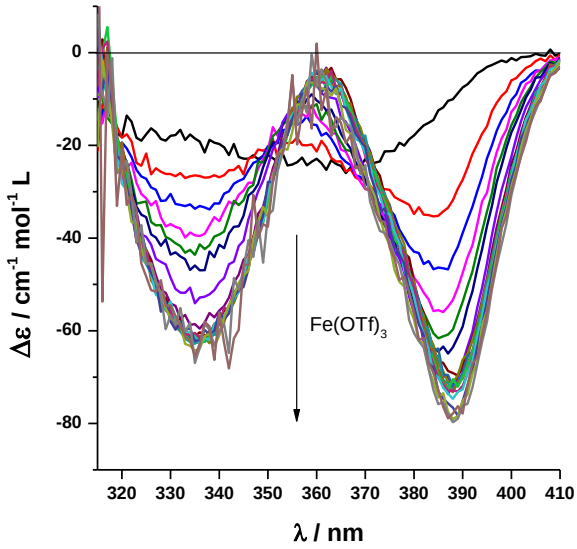

signal
[Ga]


Δε / cm-1 mol-1 L
λ / nm
In(OTf)3


Δε / cm-1 mol-1 L
λ / nm
Sc(OTf)3


signal
[Sc]


Δε / cm-1 mol-1 L
λ / nm
La(OTf)3


Δε / cm-1 mol-1 L
λ / nm
Fe(OTf)3

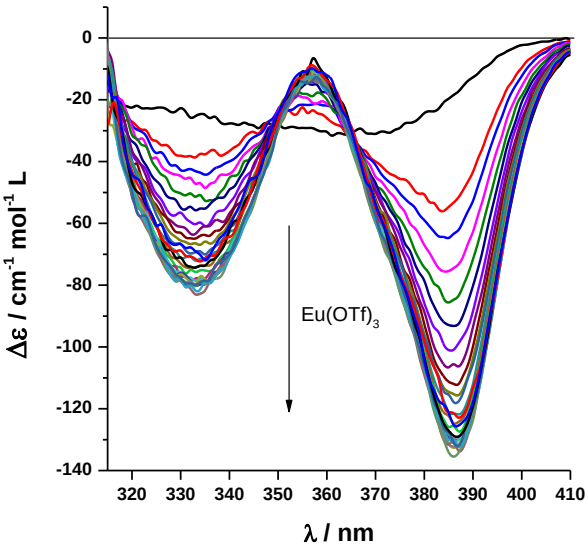
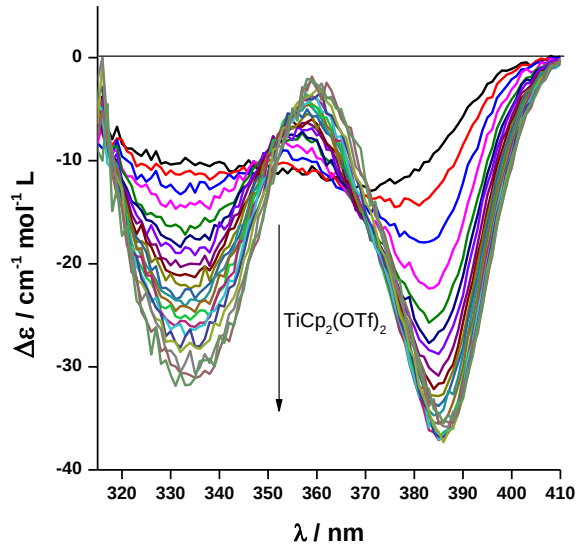


Fig. S11. CD titration of compound (*S*,*S*)-**1** with tetravalent metals



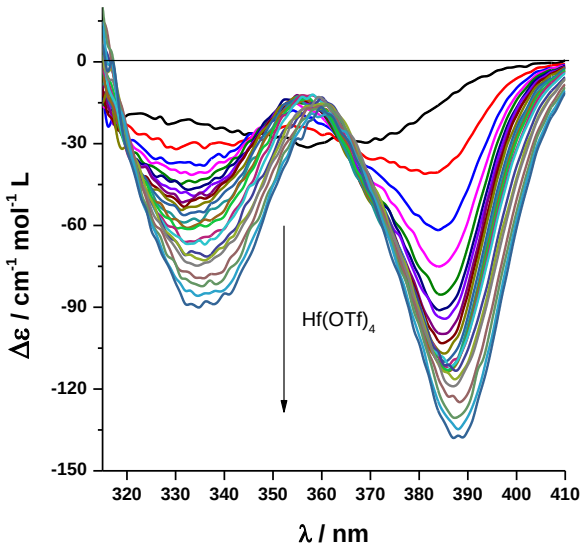


Fig. S12. CD titration of compound (*S,S*)-**2** with monovalent metals

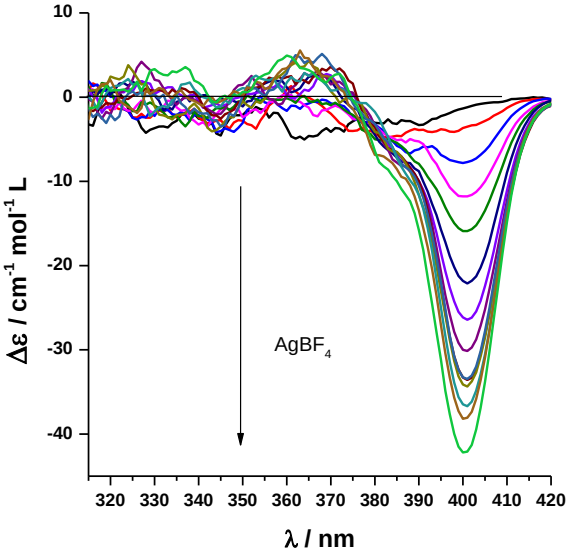
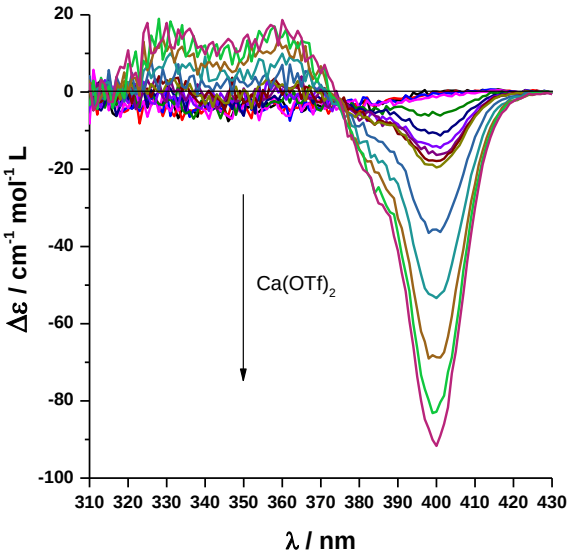
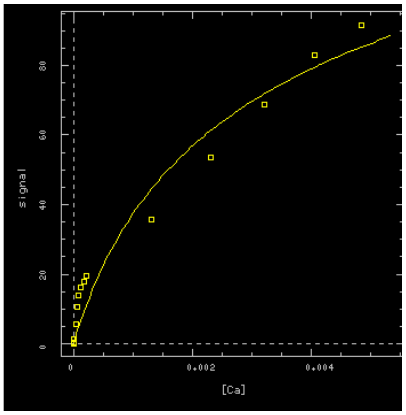
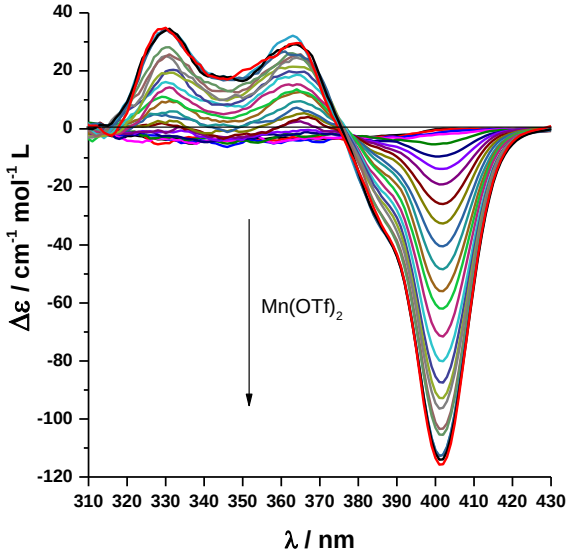
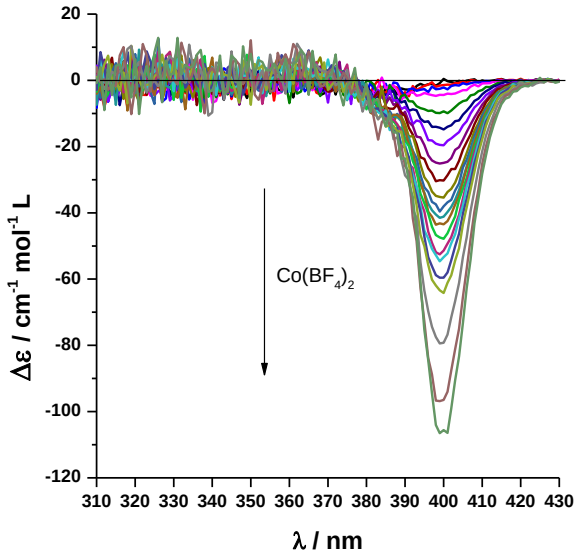


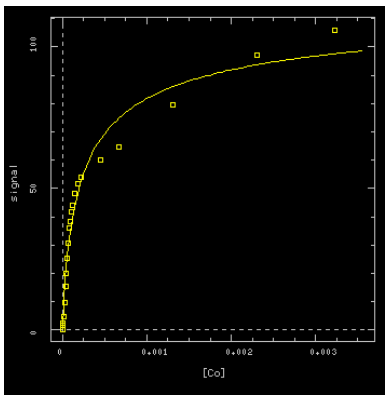
Fig. S13. CD titration of compound (*S,S*)-**2** with bivalent metals

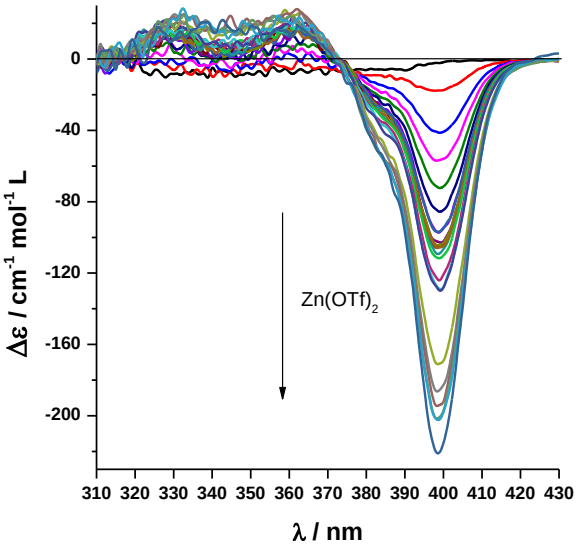







20
0
-20
-40
-60
-80
-100
-120
Δε / cm-1 mol-1 L
Co(BF4)2
310 320 330 340 350 360 370 380 390 400 410 420 430
λ / nm


signal
100
50
0
0
0.001
0.002
0.003
[Co]


0
-40
-80
-120
-160
-200
Δε / cm-1 mol-1 L
Zn(OTf)2
310 320 330 340 350 360 370 380 390 400 410 420 430
λ / nm

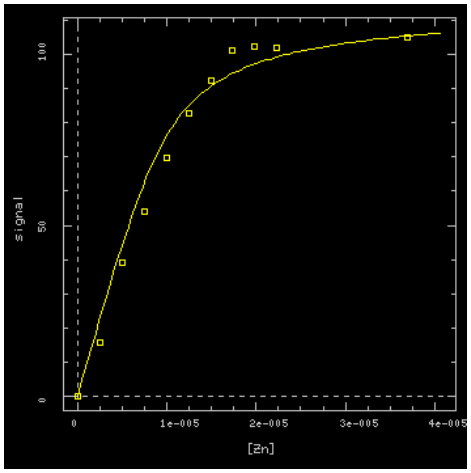
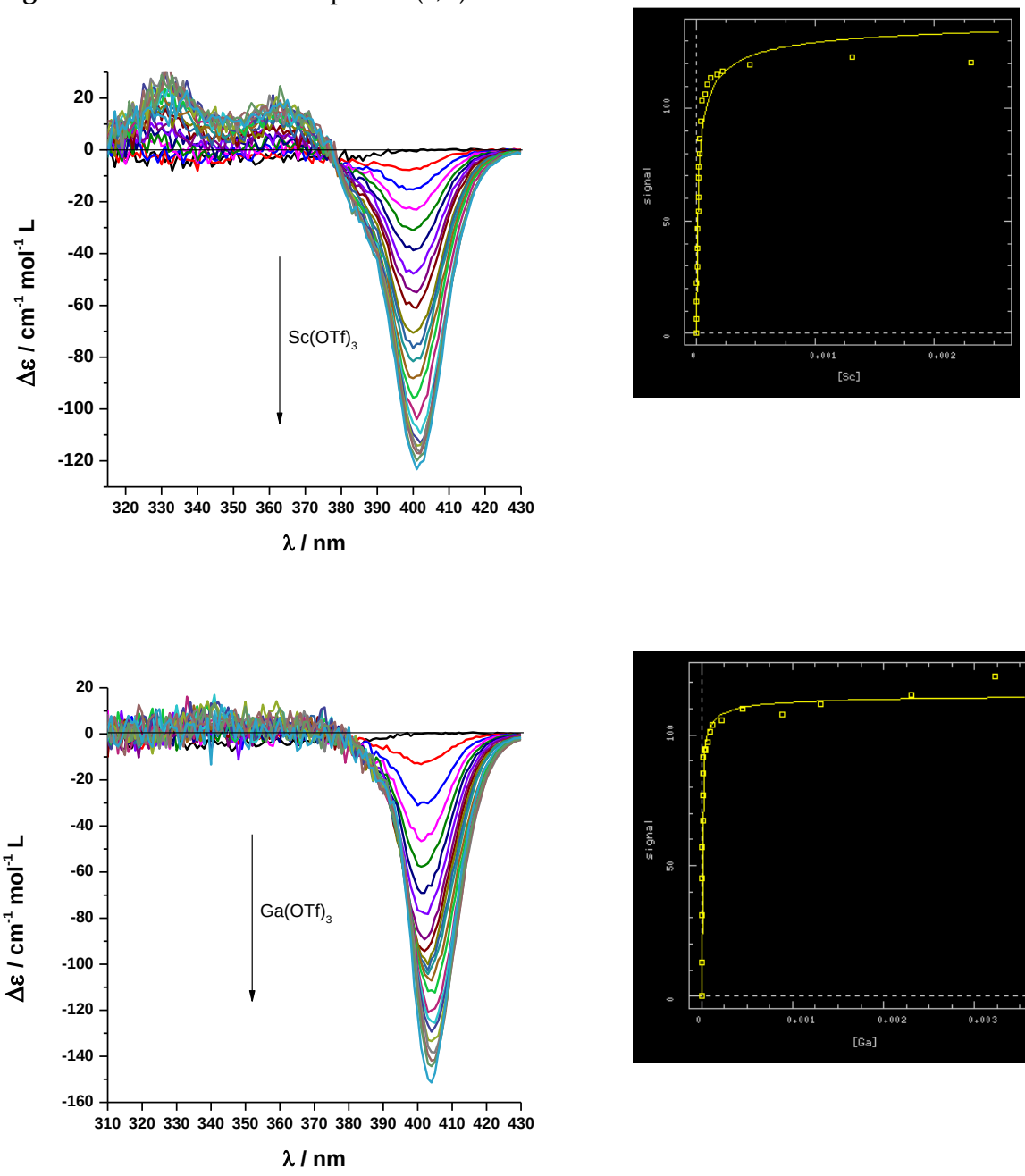

signal
100
50
0
0
1e-005
2e-005
3e-005
4e-005
[Zn]

Fig. S14. CD titration of compound (*S,S*)-**2** with trivalent metals



CPL MEASUREMENTS

Experimental

Circularly polarized luminiscence (CPL) measurements were recorded in anOlis DSM172 spectrophotometer.The spectra were recorded at 1×10^{-5} M concentrations in HPLC grade solvents. A fixed wavelength LED (372 nm) as the excitation source was used. CPL spectra in Figure S14 were collected by accumulating 150 scans and with 0.5 s of integration time. Some of the measurements were also carried out in a home –made apparatus,[9] with the excitation radiation brought to the sample from a Jasco FP8200 fluorimeter through an optical fiber. . In this case a 2.0 mm path-length quartz cell has been used with $4x10^{-5}$M solutions in presence of 30 equivalents of salt

Fig. S15. ΔI values obtained for compound (*S,S*)-**1** in a 9:1 CH_2Cl_2:Acetone mixture as solvent in the absence and presence of 30equivalents of different salts.

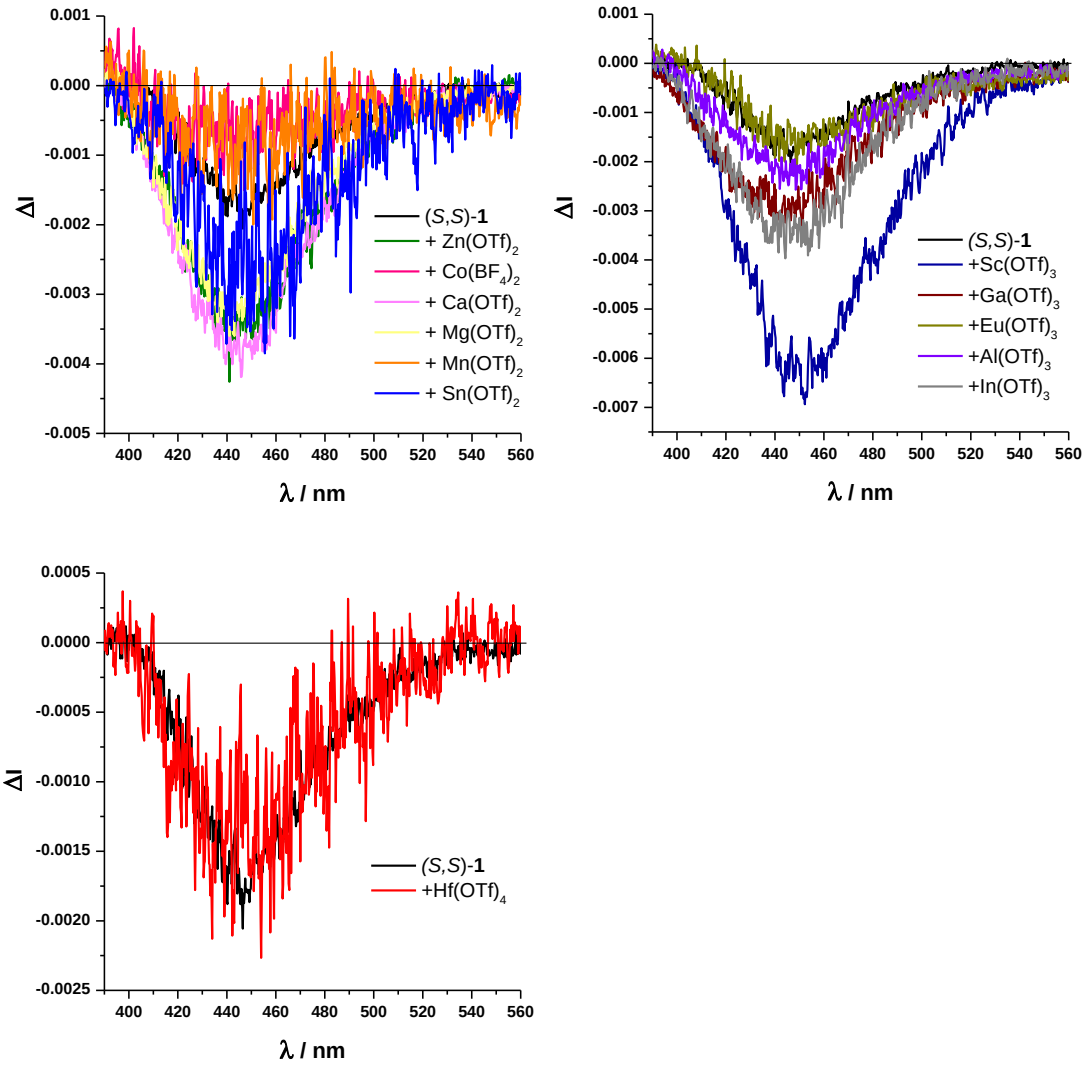
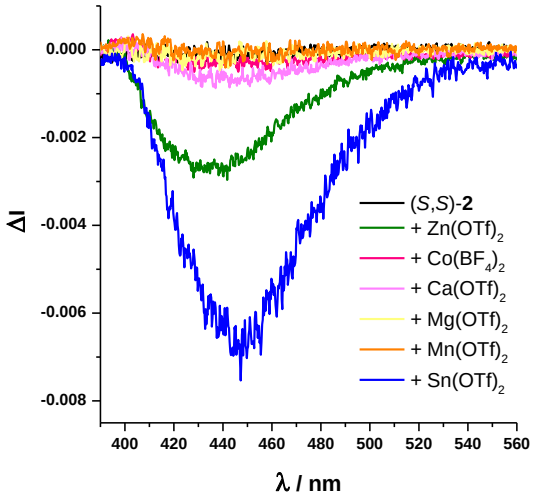
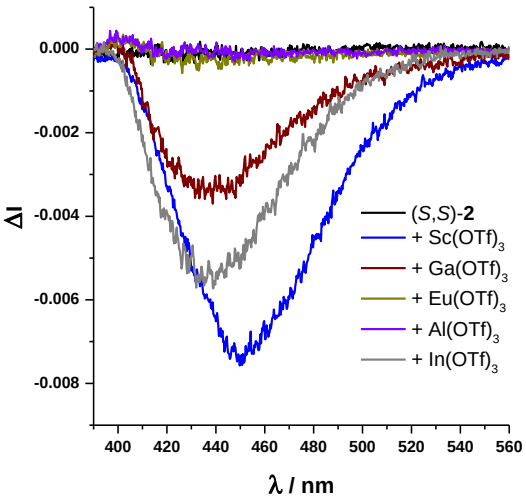
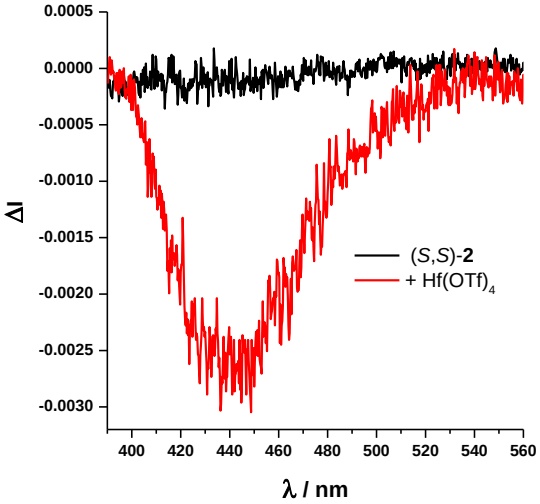


Fig. S16. ΔI values obtained for compound (*S,S*)-**2** in a 9:1 CH_2Cl_2:Acetone mixture as solvent in the absence and presence of 30equivalents of different salts.







X-RAY DIFFRACTION

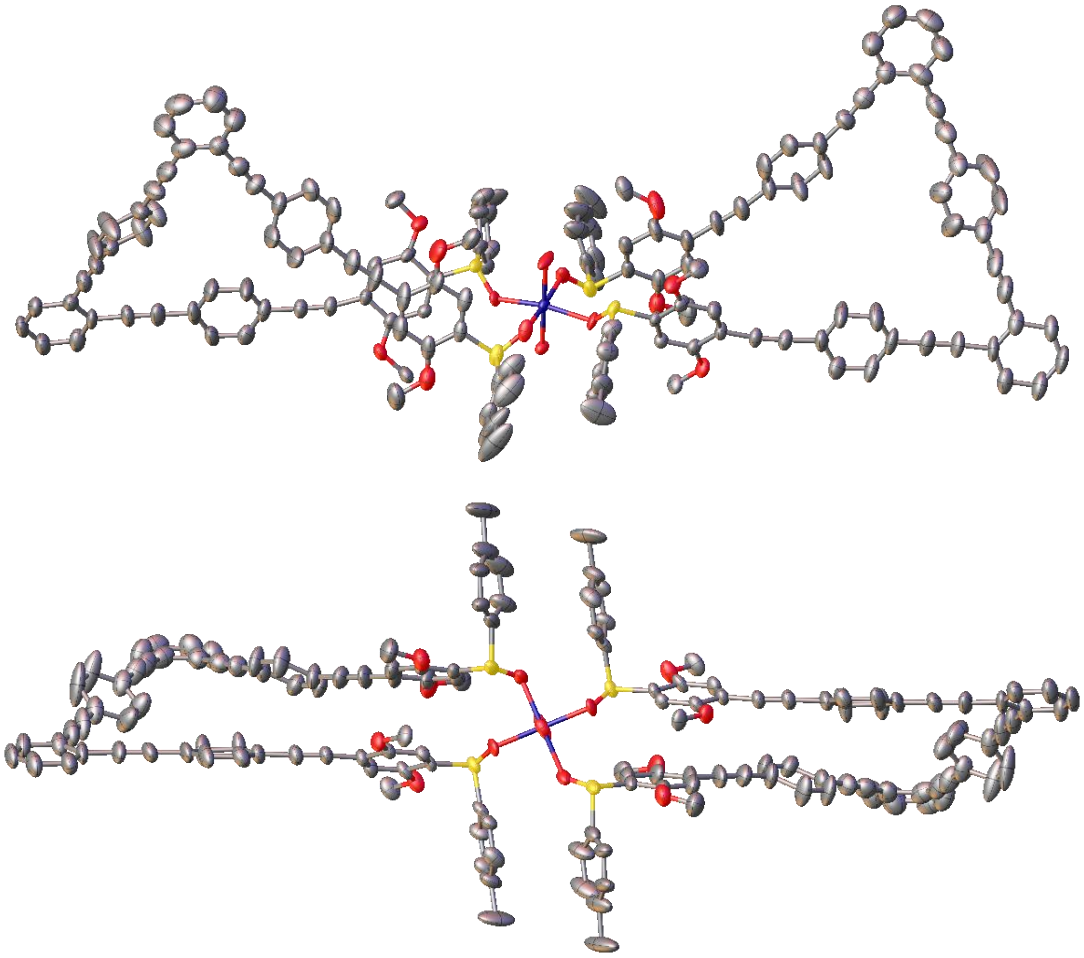
X-ray diffraction quality crystals of [((*S*,*S*)-**2**)$_2$(H_2O)$_2$:Zn](OTf)$_2$ were grown in a NMR tube by slow diffusion of hexane into a CH_2Cl_2 solution of the complex. The X-ray diffraction data were collected on a Bruker D8 Venture diffractometer equipped with a Photon 100 detector using Cu radiation source. The structure was solved with SHELXT[10] and refined using the full-matrix least-squares against F^2 procedure with SHELX 2018[11] using the WinGX32[12] software. C–H hydrogen atoms were placed in idealized positions (U_{eq}(H) = 1.2U_{eq}(C) or U_{eq}(H) = 1.5U_{eq}(C)) and were allowed to ride on their parent atoms. The H atoms of the two water molecules coordinated to the Zn ion could not be located but were included in the formula. During refinement the structure of the complex was obtained unambiguously. However, there was some density corresponding to what it seemed hexane solvent molecules which could not be modeled and was removed using the SQUEEZE[13]routine in PLATON[14], which showed an electron density removed of 343 electrons/cell, which could correspond to 6 molecules of hexane per unit cell. These solvent molecules removed with SQUEEZE were added to the cell unit contents and a last cycle of refinement was performed.

Summary of the X-ray diffraction measurement and refinement data: Chemical formula, $C_{82}H_{75}F_3O_{10}S_3Zn_{0.50}$; *Mr*, 1406.28; crystal size [mm^3], 0.776 x 0.265 x 0.184; temperature, 100(2) K; wavelength [Å], 1.54178 (Cu Kα), crystal system, monoclinic; space group, *C*2; *a* [Å], 28.5163(15); *b* [Å], 9.9416(5); *c* [Å], 26.6193(13); α [°], 90; β [°], 110.609(3); γ [°], 90; *V* [Å^3], 7063.6(6); *Z*, 4; ρ_{calcd} [Mg m^{-3}], 1.322; μ [mm^{-1}], 1.699; F(000), 2948; θ range [°], 3.158 to 75.479; *hkl* ranges, -35/35, -11/12, -33/33; reflections collected, 114741; independent reflections, 14299; R_{int}, 0.0642; completeness to θ = 67.679°, 100.0%); absorption correction, numerical; refinement method; full-matrix least-squares on F^2; Final *R* indices [$I>2\sigma(I)$], R_1 = 0.0963, wR_2 = 0.2528; *R* indices (all data), R_1 = 0.1010, wR_2 = 0.2584; goodness-of-fit on F^2, 1.046; absolute structure parameter, 0.14(4).

The structure shows a slightly distorted octahedral coordination geometry around the metal centre with the four sulfoxide O atoms located in a slightly distorted equatorial plane. Two water molecules are located on the axial positions to complete the coordination sphere. The Zn−O distances are 2.06 and 2.12 Å for the sulfoxide O atoms and 2.03 and 2.14 Å for the water O atoms. The O−Zn−O equatorial angles are 89.3º and 91.3º while the O−Zn−O angles between the O atoms of the sulfoxides and the water molecules range between 84.0º and 96º. Both units of (*S*,*S*)-**2** adopt a folded conformation with *M* helicity. The dimethoxybenzene units on the each edge are partially overlapped. The π-π distance, measured between the centroid of one ring and the mean plan of the other, is 3.52 Å, suggesting the establishment of π-π interactions.

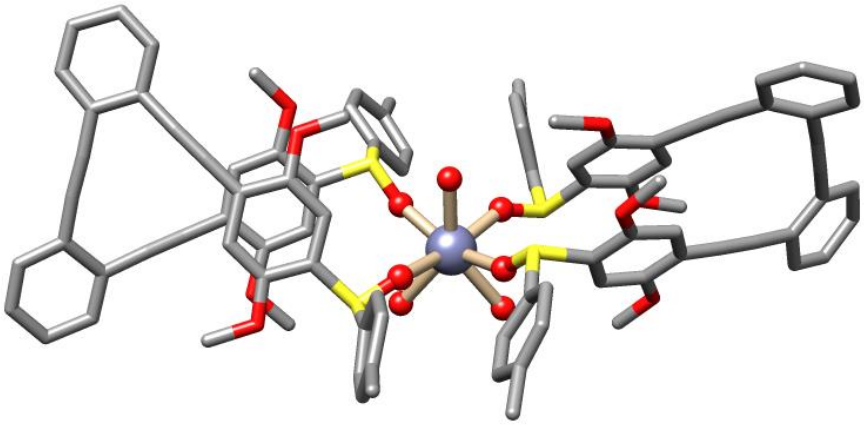
CCDC-1871394 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/?

Figure S17. Different views of the ORTEP-type[15] drawing of the crystal structure of [((*S*,*S*)-**2**)$_2$(H_2O)$_2$:Zn](OTf)$_2$ showing the ellipsoids at ellipsoids at 50% probability: a) Color code: C: gray, O: red, S: yellow, Zn: violet. Hydrogen atoms and counterions have been omitted for clarity.



Single crystals of [((*S*,*S*)-**1**)$_2$(H_2O)$_3$:Ca](OTf)$_2$ were also grown in a NMR tube by slow diffusion of hexane into a CH_2Cl_2 solution of the complex. The X-ray diffraction data were collected on a Bruker D8 Venture diffractometer equipped with a Photon 100 detector using a Mo radiation source. The structure was solved with SHELXT[S1] and refined using the full-matrix least-squares against F^2 procedure with SHELX 2016[S2] using the WinGX32[S3] software. However during refinement, due to the limited quality of the crystals obtained, the anisotropy of an important number of atoms had to be modeled using ISOR restraints. Therefore, we consider that the overall quality of the data is not sufficient for its publication. Nevertheless, as the position and connectivity of the different atoms in the complex were established unambiguously the chemical structure and the XYZ atomic coordinates are shown in Figure S18 and Table S3.

Figure S18. Single crystal X-ray diffraction structure of [((S,S)-1)$_2$(H_2O)$_3$:Ca](OTf)$_2$. Color code: C: gray, O: red, S: yellow, Ca: violet. Couterions and hydrogen atoms have been omitted for clarity.



The structure shows 7 O atoms coordinated to the metal centre with a capped octahedral geometry. The arrangement is quite similar to that observed for of [((*S,S*)-**2**)$_2$(H_2O)$_2$:Zn](OTf)$_2$ with the difference of the presence of 3 water molecules, one on one side of the plane formed by the four sulfoxide O atoms and two on the other. The Zn–O distances range between 2.31 and 2.38 Å for the sulfoxide O atoms and between 2.36 and 2.47 Å for the water O atoms. The O–Zn–O angles for the sulfoxide units are between 78.4º and 101.3º while the O–Zn–O angles between the O atoms of the sulfoxides and the water molecules range between 72.4º and 125.8º. Again, both units of (*S,S*)-**1** adopt the *M* folded conformation with the end dimethoxybenzene aromatic rings at a π-π distance of 3.39 and 3.46, optimal for the establishment of π-π interactions.

Table S3. Atomic coordinates for the X-ray diffraction structure of [((*S,S*)-**1**)$_2$(H_2O)$_3$:Ca](OTf)$_2$

Atom	X	Y	Z
C	2,445923	22,592957	17,951122
H	2,60924	22,029905	18,735998
H	1,509205	22,894196	17,958695
H	3,036683	23,371264	17,974992
C	2,697512	21,817013	16,726808
C	1,594642	21,501909	15,807888
H	0,728852	21,867706	15,947206
C	1,844778	20,666884	14,732848
H	1,136907	20,428626	14,145328
C	3,134373	20,166656	14,505515
C	4,173826	20,493576	15,301181
H	5,047129	20,170122	15,111454
C	3,947103	21,30103	16,398134
H	4,684379	21,515537	16,957264
C	2,220255	17,799437	13,503056
C	1,174943	17,744294	12,62796
H	1,082122	18,387185	11,934538
C	0,187749	16,649308	12,795036
C	0,43462	15,711873	13,734498
C	1,497004	15,782772	14,610964
H	1,596408	15,128537	15,293677
C	2,461276	16,858064	14,486342
C	3,890989	15,95214	16,087262
H	3,154723	15,774382	16,709649
H	4,698179	16,18059	16,592285
H	4,060243	15,149964	15,547263
C	-1,139555	17,452823	10,939393
H	-1,201882	18,330742	11,369724
H	-1,991589	17,242018	10,502392
H	-0,424324	17,466845	10,269677
C	-0,369186	14,518417	13,824884
C	-1,012524	13,549472	13,875555
C	-1,769512	12,283542	13,872816
C	-2,902614	12,115749	13,085366
H	-3,201128	12,825914	12,526783
C	-3,599606	10,914415	13,114125
H	-4,373988	10,801686	12,576193

C	-3,16301	9,87851	13,931703	H	3,861748	15,143268	2,945433
H	-3,639082	9,056955	13,951588	C	2,388121	17,653702	1,320177
C	-2,029909	10,044728	14,719153	H	2,706784	18,152905	0,539725
H	-1,731316	9,336492	15,277599	H	1,426471	17,48646	1,230819
C	-1,332916	11,245274	14,690394	H	2,863574	16,797446	1,375942
C	-0,098372	11,335866	15,360069	C	2,639402	18,433584	2,537643
C	1,024946	11,367377	15,764065	C	3,890989	18,925934	2,819756
C	2,363377	11,501296	16,374853	H	4,590085	18,721589	2,209763
C	2,606861	11,115294	17,690921	C	4,220304	19,721572	3,957792
H	1,903117	10,778644	18,239918	H	5,105793	20,016115	4,136879
C	3,967721	11,249213	18,197628	C	3,128781	20,036676	4,798652
H	4,180202	11,031909	19,097814	C	1,845983	19,49706	4,582275
C	4,995831	11,721869	17,280078	H	1,139492	19,688564	5,188159
H	5,899331	11,753261	17,570928	C	1,617636	18,681728	3,489431
C	4,69187	12,115749	16,027005	H	0,762426	18,286194	3,37182
H	5,378814	12,437588	15,454755	C	2,331382	22,411772	5,780568
C	3,372472	12,048789	15,560013	C	1,182792	22,48267	6,609102
C	3,128989	12,615976	14,257639	H	1,043891	21,83076	7,28442
C	2,942592	13,175286	13,219574	C	0,242397	23,530391	6,43107
C	2,726919	13,907903	12,02265	C	0,461325	24,55054	5,462849
C	1,552851	13,746412	11,298196	C	1,64308	24,400866	4,598708
H	0,937577	13,06366	11,538307	H	1,787847	25,029538	3,899877
C	1,277681	14,585376	10,219047	C	2,520067	23,40435	4,771263
C	2,263889	15,617342	9,915023	C	4,040754	24,282702	3,171712
C	3,4721	15,759139	10,653172	H	4,245318	25,072471	3,71523
H	4,119256	16,421645	10,444696	H	3,315083	24,48815	2,551393
C	3,639475	14,865031	11,695345	H	4,843041	24,025498	2,662773
C	5,777803	15,908813	12,1281	C	-1,118782	22,801713	8,212762
H	6,137336	15,700293	11,241609	H	-1,171976	21,9067	7,813696
H	6,502375	15,88971	12,788271	H	-1,976353	23,021538	8,63289
H	5,374125	16,803197	12,114638	H	-0,410549	22,813727	8,89016
C	-0,847958	13,596738	9,887634	C	-0,357611	25,661282	5,401223
H	-0,59309	13,177767	10,738669	C	-1,02778	26,649921	5,401223
H	-0,972057	12,902642	9,208331	C	-1,785248	27,8355	5,501194
H	-1,68585	14,090781	10,008244	C	-3,019206	27,843377	6,183195
C	2,207108	16,113631	7,170589	H	-3,310956	27,044392	6,608746
C	3,313274	16,582348	6,469416	C	-3,787895	28,926547	6,24893
H	3,85797	17,271284	6,827863	H	-4,63189	28,893067	6,683534
C	3,612171	16,003344	5,202648	C	-3,301166	30,186963	5,629925
H	4,388522	16,265038	4,721756	H	-3,801586	30,990754	5,719448
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C	1,635817	14,731112	5,323162	H	-1,890036	30,98713	4,51061
H	1,04247	14,103464	4,932916	C	-1,295598	29,068344	4,816455
C	1,327651	15,298299	6,572127	C	-0,081635	29,028956	4,17417
H	0,495463	15,104077	6,990064	C	0,995767	29,111671	3,660616
C	3,236955	14,5066	3,347005	C	2,26583	29,127426	3,142953
H	2,467071	14,383749	2,747598	C	2,650584	29,93488	2,043262
H	3,68074	13,648493	3,487623	H	1,993438	30,489581	1,640306

C	3,894797	29,954574	1,540663
H	4,06799	30,49608	0,778494
C	4,938622	29,225896	2,082977
H	5,805945	29,256225	1,698687
C	4,673372	28,406626	3,257989
H	5,378506	27,894621	3,634719
C	3,434042	28,35936	3,834539
C	3,14782	27,646437	5,016399
C	2,981085	27,063495	6,051725
C	2,739735	26,311184	7,228107
C	3,626978	25,267402	7,569107
C	3,333916	24,428438	8,608541
H	3,922408	23,717012	8,82737
C	2,163371	24,625378	9,350798
C	1,257594	25,614016	9,007059
C	1,519437	26,445103	7,92928
H	0,883762	27,096896	7,663053
C	-0,974815	26,516002	9,312453
H	-0,962498	27,324086	9,861381
H	-1,8352	26,063237	9,403359
H	-0,83153	26,759616	8,369608
C	5,78427	24,274824	7,21989
H	5,827542	24,294203	8,199272
H	6,653043	24,532973	6,849254
H	5,55784	23,368388	6,922042
C	2,077239	24,215742	12,069213
C	3,243019	23,739148	12,849815
H	3,822056	23,062068	12,518196
C	3,445525	24,32209	14,075498
H	4,125973	23,973664	14,638559
C	2,685157	25,432832	14,539752
C	1,681799	25,885794	13,768735
H	1,131572	26,596708	14,084783
C	1,424663	25,334362	12,518402
H	0,780148	25,748054	11,956094
C	3,05302	26,043346	15,890057
H	3,570888	26,864073	15,746084
H	3,588061	25,405181	16,403694
H	2,235051	26,259664	16,387342
O	5,175785	18,772321	10,298477
O	2,957617	19,768837	11,922678
O	2,834486	17,984561	8,95091
O	3,002151	20,442372	7,313014
O	2,792649	22,32118	10,443642
O	-0,837074	16,409041	11,97198
O	3,547552	17,011677	15,249141
O	0,198723	14,510539	9,465834
O	4,802816	14,963501	12,474578
O	0,079731	25,63371	9,734252
O	-0,834984	23,727331	7,232215
O	5,19813	21,513726	9,052252
O	3,649155	23,179838	4,041331
O	4,774594	25,196504	6,765223
O	0,877196	20,174534	9,650714
S	3,44692	19,051188	13,145623
S	1,794099	16,894301	8,733163
S	3,491275	21,135601	6,098287
S	1,744045	23,383868	10,572236
Ca	3,23937	20,138297	9,657561
C	-2,172902	22,258159	13,594811
O	-0,831721	20,915028	11,81449
O	-2,720834	22,238465	11,029779
O	-3,060213	20,150901	12,319827
F	-1,323738	23,27043	13,478406
F	-1,707521	21,46646	14,520579
F	-3,264469	22,687488	13,830362
S	-2,1579	21,249038	11,982935
C	-2,065203	18,177562	5,690183
O	-3,062549	20,064247	7,080203
O	-0,845198	19,256793	7,625255
O	-2,807864	17,882152	8,173047
F	-1,582886	18,965322	4,765785
F	-3,250955	17,728539	5,258797
F	-1,244315	17,078637	5,751809
S	-2,220676	18,950748	7,310275

CHECKCIF of [((S,S)-2)$_2$(H_2O)$_2$:Zn](OTf)$_2$

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SS-2-Zn

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: SS-2-Zn

Bond precision: C-C = 0.0190 A Wavelength=1.54178

Cell: a=28.5163(15) b=9.9416(5) c=26.6193(13)
alpha=90 beta=110.609(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	7063.6(6)	7063.6(6)
Space group	C 2	C 2
Hall group	: C 2y	C 2y
Moiety formula	C144 H100 O14 S4 Zn, 2(C F3 O3 S) [+ solvent]	?
Sum formula	C146 H100 F6 O20 S6 Zn [+ solvent]	C82 H75 F3 O10 S3 Zn0.50
Mr	2546.02	1406.28
Dx,g cm-3	1.197	1.322
Z	2	4
Mu (mm-1)	1.653	1.699
F000	2632.0	2948.0
F000'	2640.75	
h,k,lmax	35,12,33	35,12,33
Nref	14637[7756]	14299
Tmin,Tmax	0.612,0.732	0.343,1.000
Tmin'	0.255	

Correction method= # Reported T Limits: Tmin=0.343 Tmax=1.000
AbsCorr = NUMERICAL

Data completeness= 1.84/0.98 Theta(max)= 75.479

R(reflections)= 0.0963(13421) wR2(reflections)= 0.2584(14299)

S = 1.046 Npar= 815

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

Alert level B

```
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01897 Ang.
PLAT430_ALERT_2_B Short Inter D...A Contact  O5       ..O10      .       2.76 Ang.
                                           x,1+y,z  =      1_565 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O5       ..O10      .       2.76 Ang.
                                        1-x,1+y,-z  =      2_665 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O6       ..O11      .       2.77 Ang.
                                         1-x,y,-z  =      2_655 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O6       ..O11      .       2.77 Ang.
                                           x,y,z  =      1_555 Check
```

Alert level C

```
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.26 Report
PLAT213_ALERT_2_C Atom C5              has ADP max/min Ratio .....        3.3 prolat
PLAT213_ALERT_2_C Atom C56             has ADP max/min Ratio .....        3.2 prolat
PLAT213_ALERT_2_C Atom C62             has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range        4.7 Ratio
PLAT222_ALERT_3_C Non-Solv.  Resd 1  H   Uiso(max)/Uiso(min) Range        5.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C1       --C2       .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C6       --C7       .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14      --C15      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C18      --C19      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C20      --C22      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23      --C24      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C28      --C62      .       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C52      --C53      .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C54      --C55      .       0.18 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C60 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C62 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C81 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C25 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C28 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of         S3 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       ZN1      0.079 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        S3      0.077 Check
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
            C144 H100 O14 S4 Zn
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .          1 Check
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
```

Alert level G

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FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C82 H75 F3 O10 S3 Zn0.5
           Atom count from the _atom_site data:  C73 H50 F3 O10 S3 Zn0.5
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
           symmetry error - see SYMMG tests
          From the CIF: _cell_formula_units_Z    4
          From the CIF: _chemical_formula_sum  C82 H75 F3 O10 S3 Zn0.50
```

```
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          C        328.00    292.00   36.00
          H        300.00    200.00  100.00
          F         12.00     12.00    0.00
          O         40.00     40.00    0.00
          S         12.00     12.00    0.00
          Zn         2.00      2.00    0.00
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.140 Note
PLAT041_ALERT_1_G Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT051_ALERT_1_G Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .       2.73 %
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size ....       0.78 mm
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      31.92 Why ?
PLAT244_ALERT_4_G Low    'Solvent' Ueq as Compared to Neighbors of        C80 Check
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C11      - C12      .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C13      - C14      .       1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C17      - C18      .       1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C22      - C23      .       1.46 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C24      - C25      .       1.42 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C28      - C29      .       1.41 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C30      - C31      .       1.44 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C32      - C37      .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C38      - C39      .       1.43 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C42      - C43      .       1.45 Ang.
PLAT371_ALERT_2_G Long   C(sp2)-C(sp1) Bond  C44      - C45      .       1.45 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F5       ..C68              2.80 Ang.
                                                 1-x,-1+y,-z  =      2_645 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure       ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .       2.12 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        43 Note

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

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

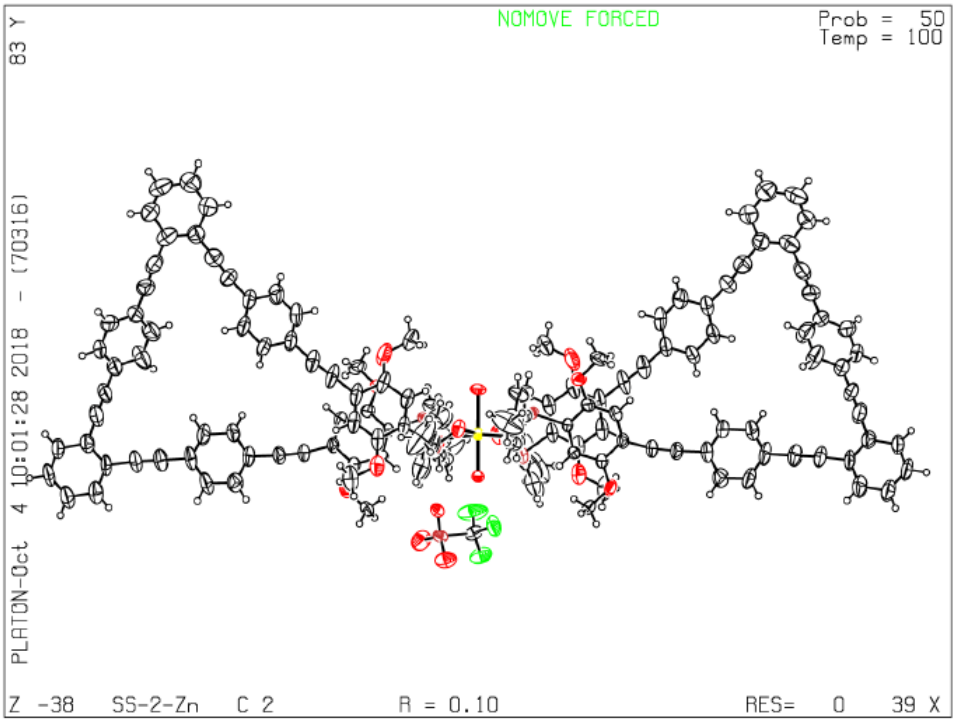
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 26/09/2018; check.def file version of 13/09/2018

Datablock SS-2-Zn - ellipsoid plot



IR, VCD and RAMAN EXPERIMENTS

General details

IR and VCD spectra were taken with a Jasco FVS6000 FTIR spectrometer equipped with a VCD module, comprised of a wire-grid linear polarizer, a ZnSe Photo Elastic Modulator (PEM) to produce 50 kHz modulated circularly polarized radiation and a liquid N_2-cooled MCT detector. The spectra were taken for 0.011-0.023 M CD_2Cl_2 solutions with maximum quantity of salt up to the solubility limit, in 200 μm BaF_2 cells. 5000 scans were taken for each spectra and subtraction of VA and VCD spectra of the solvent were performed.

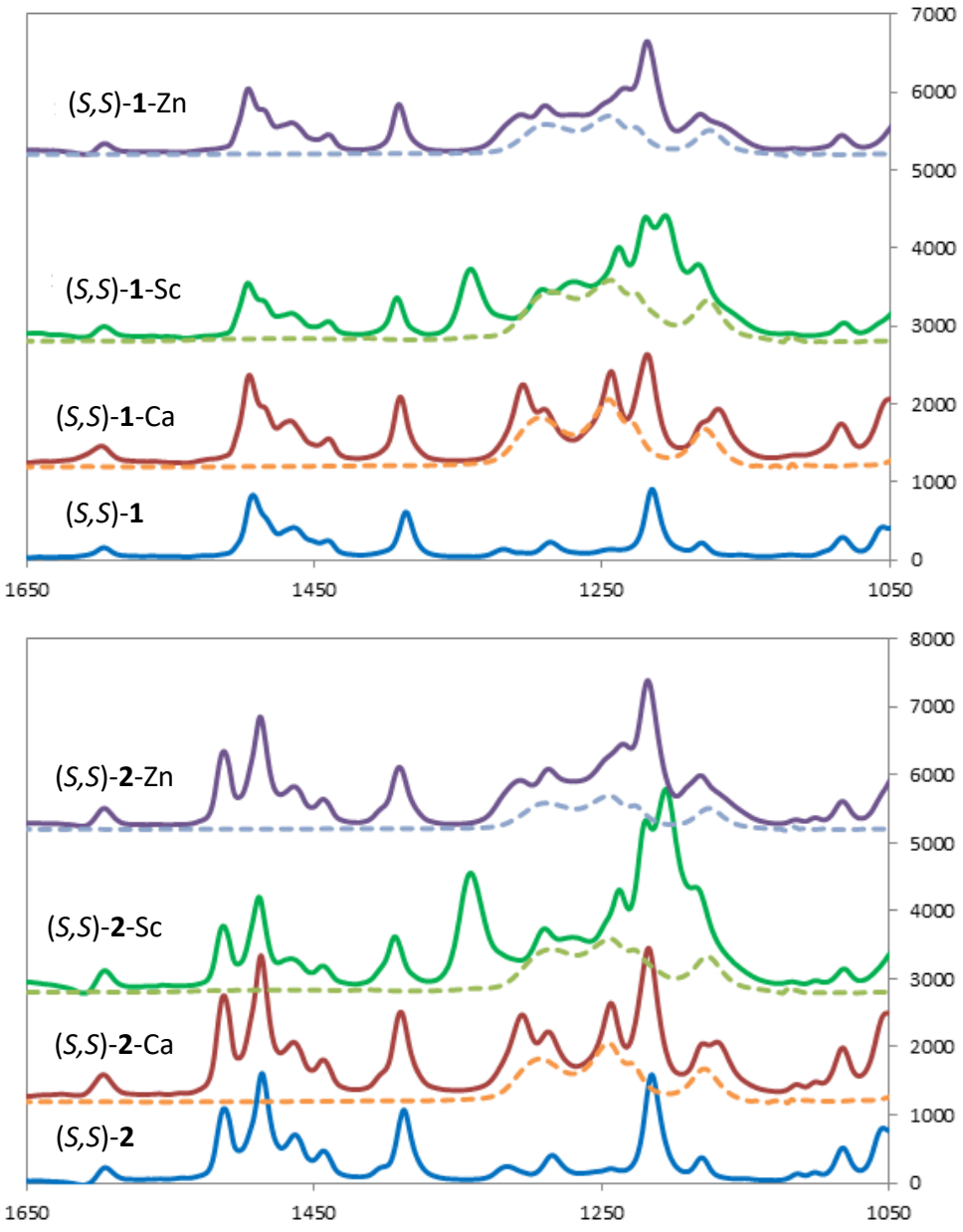
Raman spectra have been recorded on the same solutions and on the solid compound obtained after drying solvent with purged N_2.

FT-Raman spectra were recorded using a Nicolet NXR 9650 instrument equipped with Nd-YVO4 laser (1064 nm), and an InGaAs detector. The FT-Raman spectra were recorded in backscattering mode. The resolution is 4 cm−1 for all reported spectra. With reference to the reported FT-Raman spectra of solid powders (Fig. S26 (a) and (b)), power at the sample was kept low enough to avoid photo-induced degradation of the sample. With the adopted micro-FT-Raman setup the diameter of the laser spot on the solid samples is of about 50 μm. The solution samples were placed in borosilicate NMR tubes, which do not provide any appreciable background in the FT-Raman equipment.

All quantum chemical calculations have been carried out with the Gaussian code [Gaussian16][16]. Model structures, obtained starting from X ray geometry coordinates of the Ca complex of compound (*S,S*)-**1** and of the Zn complex of compound (*S,S*)-**2** (see discussion in the text) have been optimized at the B3LYP/6-31G** level, in order to calculate IR, VCD and Raman response. B3LYP is a functional widely used in the literature to calculate vibrational spectra. To describe the metal ions, we adopted the Stuttgart/Cologne energy-consistent pseudopotentials ECP10MDF (Zn) and ECP28MDF (Ag) and the associated basis sets ECP10MDF_VCD (Zn) and ECP28MDF_VDZ (Ag) [17,18]. We adopted ECP10MDF for Ca as well.[19]

Spectra have been simulated as superpositions of Lorentzian functions centered at the computed normal mode wavenumbers and with areas proportional to the calculated intensities. Lorentzian linewidth was assumed equal to 12 cm^{-1} for all transitions. To further facilitate comparison of observed and calculated spectra, 0.97 scaling factor was applied to the calculated wavenumbers.

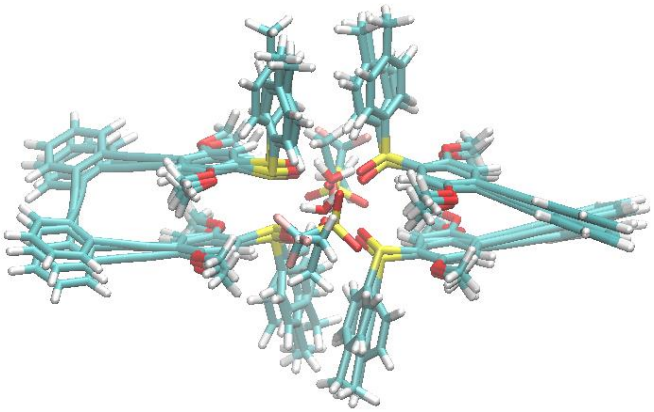
Figure S19. IR absorption spectra of compound (*S*,*S*)-**1** (top) and (*S*,*S*)-**2** (bottom) with salt excess of Ca, Sc and Zn triflate (full lines), absorption spectra of the corresponding salts are reported as broken lines.



VCD and IR spectra calculated on selected structures: compound (S,S)-1

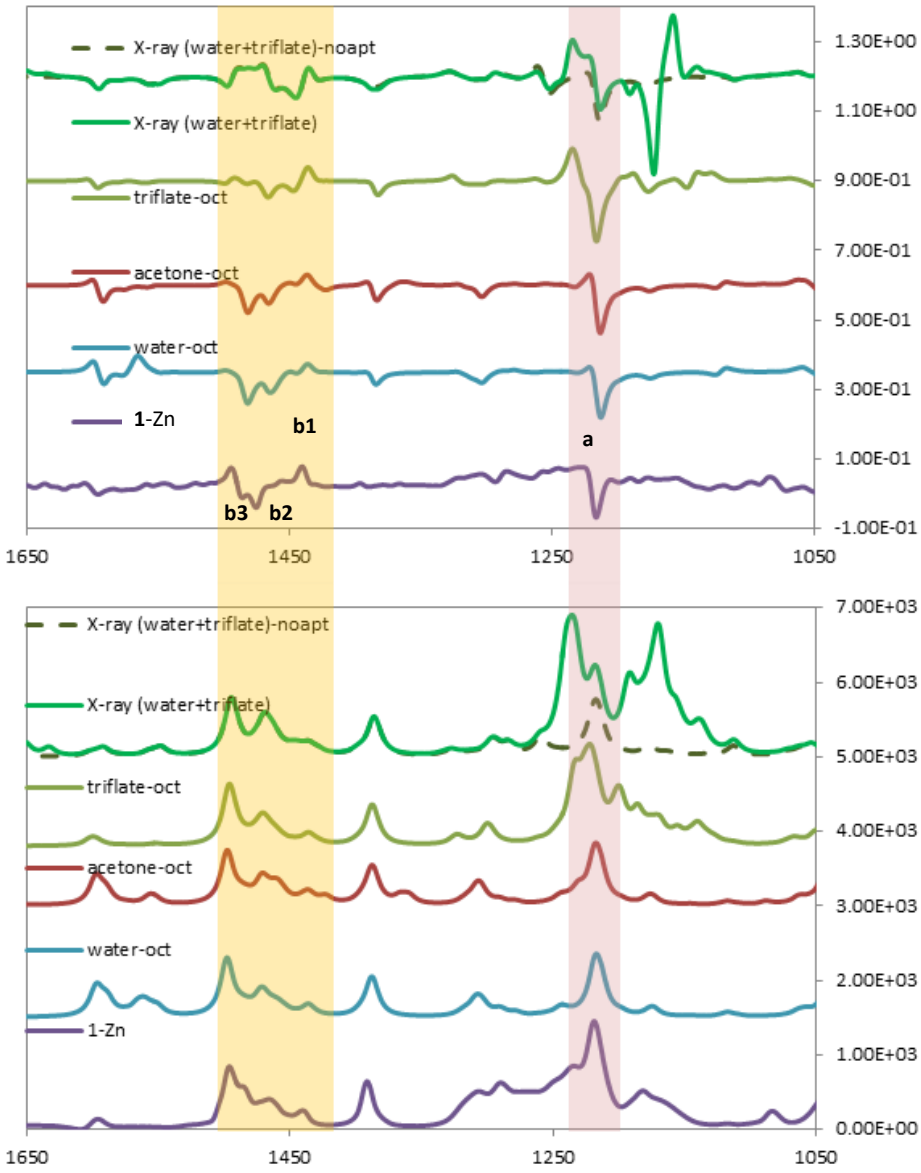
Calculated VCD and absorption spectra for model structures with octahedral coordination, two water or acetone molecules, or triflate anions have been assumed as extra-ligands, also a cluster extracted by the X-ray structure (three water molecules and four triflate anions symmetrically disposed) has been considered. As a test, this last structure has been considered also switching off the spectral contributions from to triflate and water molecules. This clarifies the contribution to the absorption spectrum due to triflates, while their VCD contribution is practically not observed.
The tested optimizations (no imaginary frequency) give quite similar structures only slight tilt of the phenyl rings of the sulfoxide moieties. This speaks of a quite rigid structure. This has a correspondence with quite similar spectra.

Figure S20. Optimized structure for (*S*,S)-**1**:Ca_2: octahedral complex with three water molecules and four triflate ions.



Also considering vibrational mode assignment (see below) we can say that the switch of VCD bands upon metal complexation is related to hampered internal rotation of the phenylsulfoxide groups.

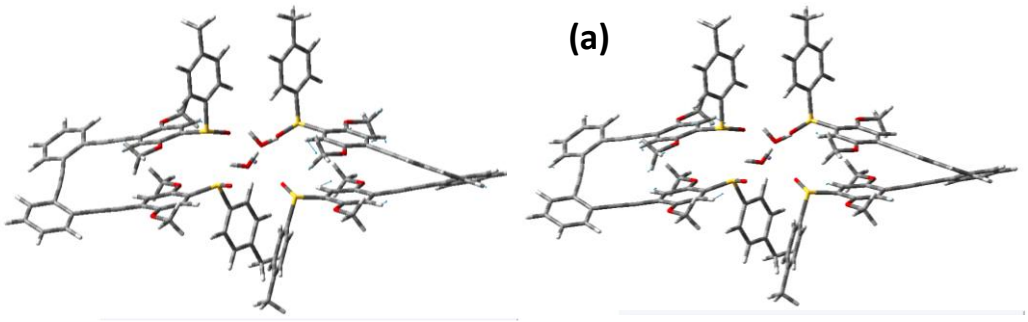
Figure S21. Calculated VCD and IR spectra of compound (*S*,*S*)-**1**, compared to experimental one (calculated wavenumbers scaled by 0.97): octahedral structure derived from X-ray data with Ca ion, optimized with three water molecules and four triflate ions (green trace), (optimized structures considering Ca ion or Zn ion give the same VCD and IR spectra); octahedral structure with two triflate ions (light green trace), two acetone molecules (red trace) or two water molecules (light blue trace) to complete coordination. Green broken trace is obtained after switching off APT of water and triflate molecules



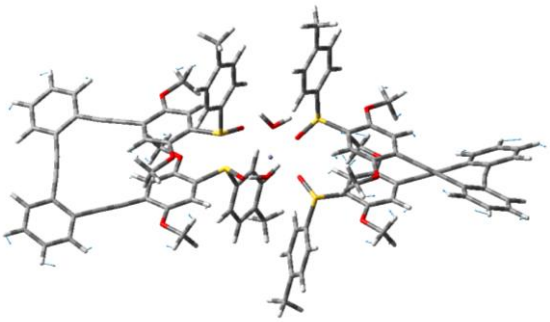
The most prominent VCD feature is the one observed at about 1200 cm^{-1} (**a**) attributed to in plane bendings associated with the extreme phenyl rings of the OPE backbone, adjacent the phenylsulfoxides. This feature is present also in case of the free molecules but with quite lower intensities. The feature at 1390 cm^{-1} is quite silent at VCD, other VCD signals are observed in the range 1440-1500 cm-1 (**b1**: in plane bendings of the phenyl far from the phenylsulfoxide group; **b**2: OCH_3 bendings and CC stretchings of adjacent rings; **b3**: aromatic CC stretchings delocalized on OPE backbone rings).

Normal modes responsable of the most intense VCD features

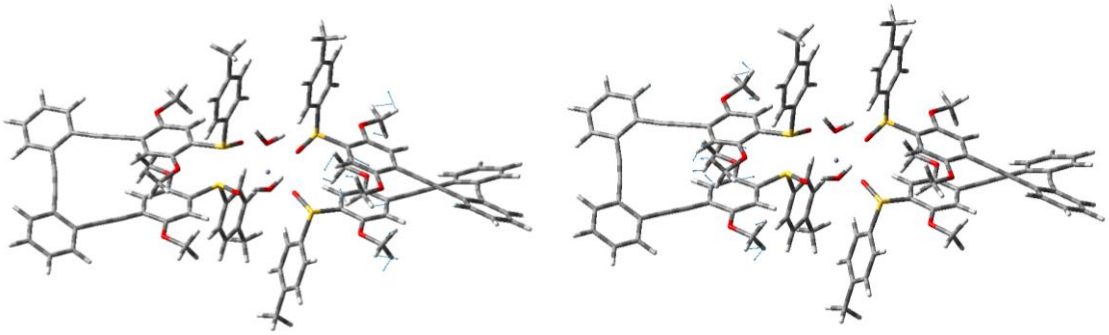
a	1250.55	192.7121	-947.6493
a	1251.11	70.5765	-334.4813



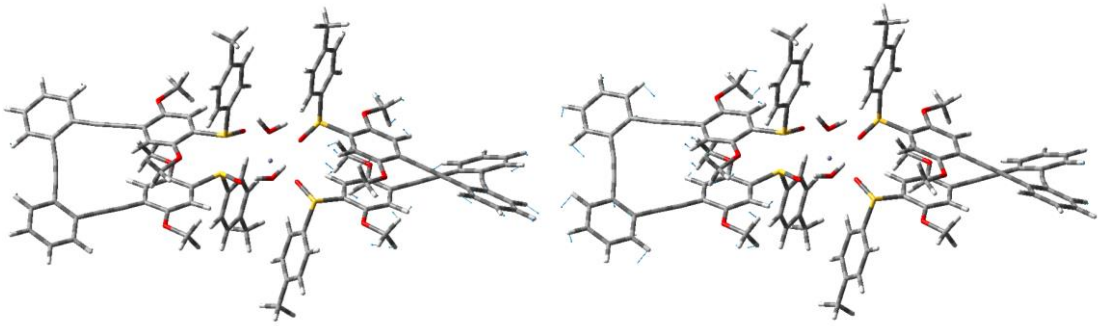
b1	1480.26	113.6378	365.5757



b2	1511.32	6.4288	-123.5887
b2	1511.52	5.8557	-105.7622



b3	1527.70	25.1005	-293.4861
b3	1527.86	20.0316	-294.0451



VCD and IR spectra calculated on selected structures for compound (S,S)-2

Analogously for compound (*S*,*S*)-**2** we considered octahedral coordination, starting from X-ray structure and considered just two water molecules or a cluster with two water molecules and four triflate anions as suggested by the measured structure. The calculated spectra, after optimization, are presented below; a test calculation excluding spectral contributions from triflate and water molecules is superimposed, this evidence the contribution to the absorption spectrum due to triflates and suggest also some possible VCD contribution in the measured spectra.
The tested optimized structures (no imaginary frequency) are similar but overall the system, being less compact, is less rigid. This probably causes a blurring out of signals at 1450-1500 cm-1 (the two calculated structures, that are just two possible examples, show a different profile in this region) and possibly favour the hosting triflate anions (with induced VCD). The feature at about 1200 cm-1 (a) resemble the one observed for compound **1** with the same assignment, some contribution at 1270 cm-1 (**a'**) is due to in plane bendings of para-phenyls groups not present in (*S*,*S*)-**1** .

Figure S22. Optimized structure for (*S*,*S*)-**2**: Ca_2: octahedral complex with two water molecules and two triflate anions.

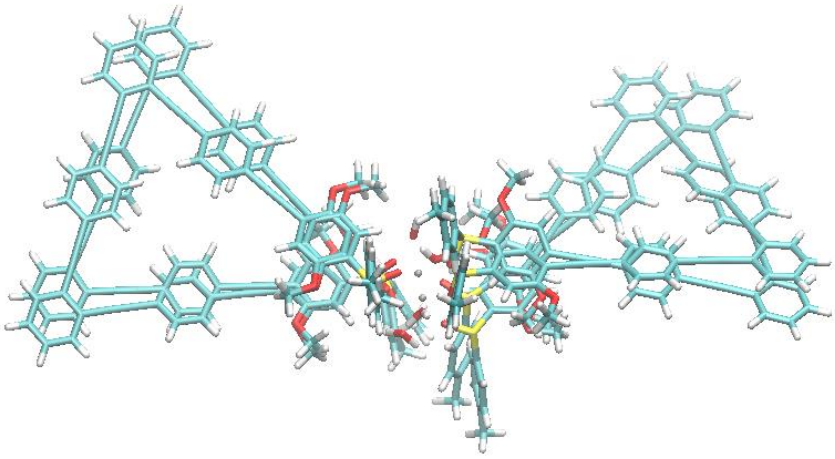
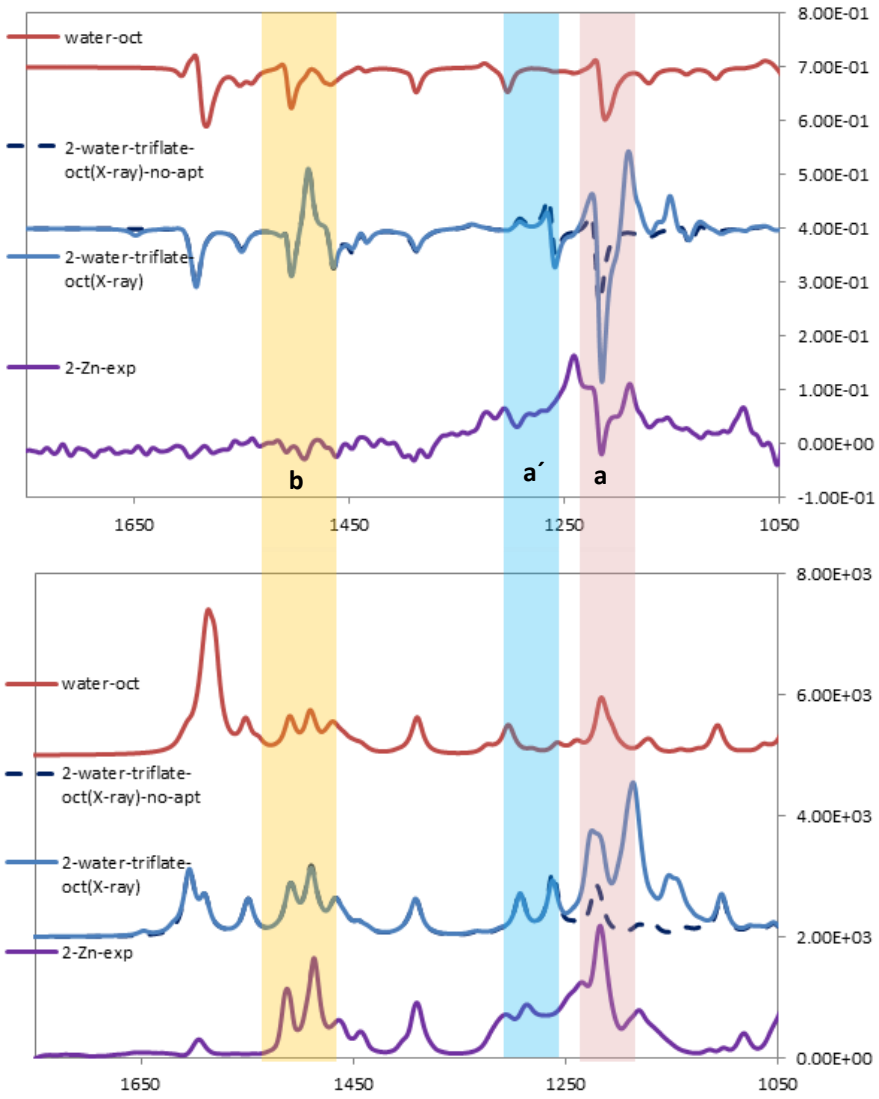
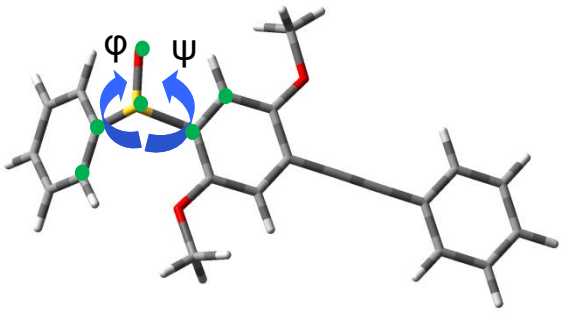


Figure S23. Calculated VCD and IR spectra of compound (*S*,*S*)-**2**, compared to the experimental one (calculated wavenumbers scaled by 0.97): Octahedral structure derived from X-ray data, optimized with two water molecules and two triflate ions (light blue trace) and with only two water molecules to complete octahedral coordination (red trace). Blue broken trace is obtained after switching off APT of water and triflate molecules.



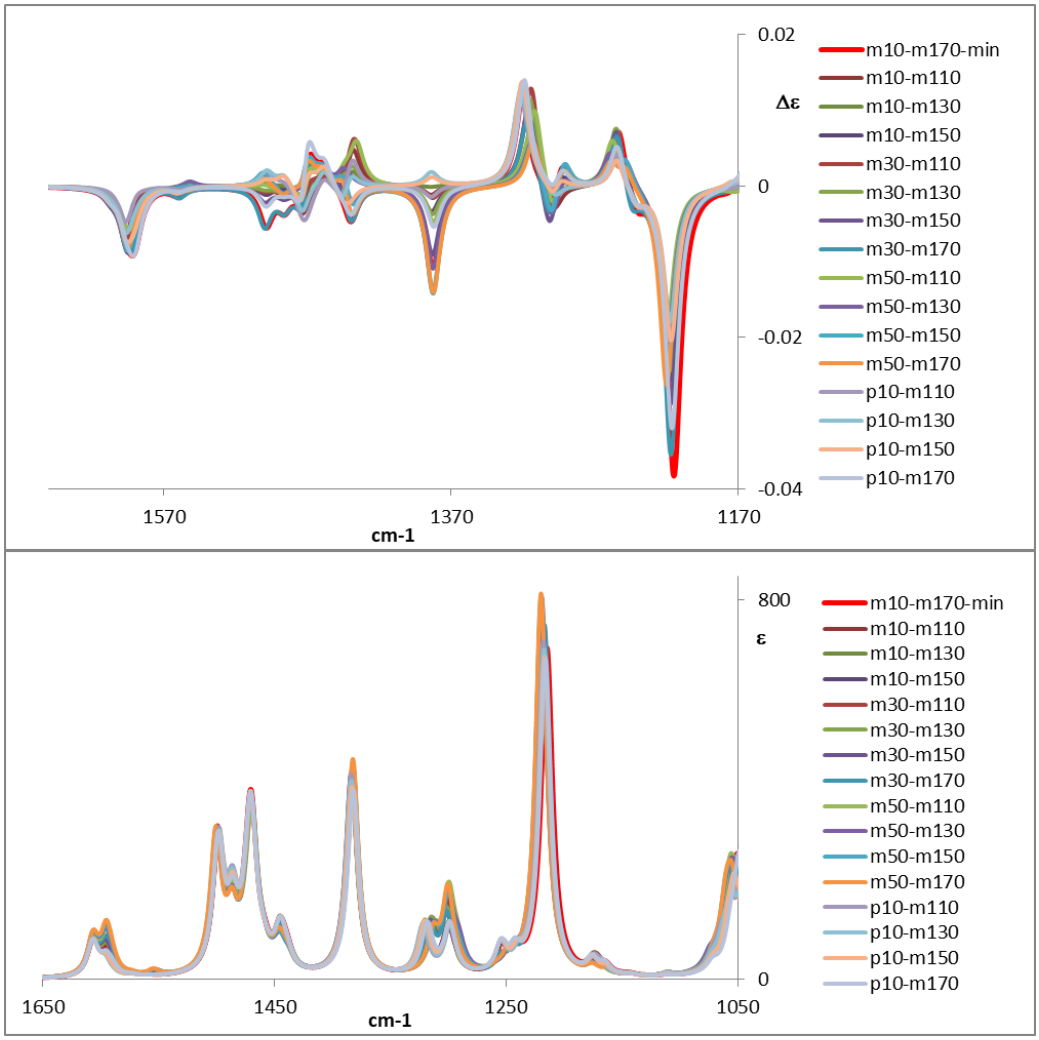
Model fragment

ψ and φ are the two dihedral angles O-S-C-C as indicated. The value obtained in the optimized structures are ψ=0 to -25° (cp. **1**); +10 to - 80 (cp. **2**) and φ = -100 to - 180 for both



Considering geometries obtained by varying the two dihedral angles (ψ, φ) VCD bands show sensitivity to these variations as illustrated in the plots below

Figure S24


0.02
Δε
0
-0.02
-0.04
1570
1370
1170
cm-1
m10-m170-min
m10-m110
m10-m130
m10-m150
m30-m110
m30-m130
m30-m150
m30-m170
m50-m110
m50-m130
m50-m150
m50-m170
p10-m110
p10-m130
p10-m150
p10-m170
800
ε
0
1650
1450
1250
1050
cm-1
m10-m170-min
m10-m110
m10-m130
m10-m150
m30-m110
m30-m130
m30-m150
m30-m170
m50-m110
m50-m130
m50-m150
m50-m170
p10-m110
p10-m130
p10-m150
p10-m170

Experimental Raman data

Figure S25. (a) Raman spectra of (*S*,*S*)-**1** in CH_2Cl_2 solution, with salt excess of $AgBF_4$ and Zn triflate (solvent subtracted). (b) Raman spectra of compound (*S*,*S*)-**2** in CH_2Cl_2 solution, with salt excess of $AgBF_4$ and Zn triflate (solvent subtracted).

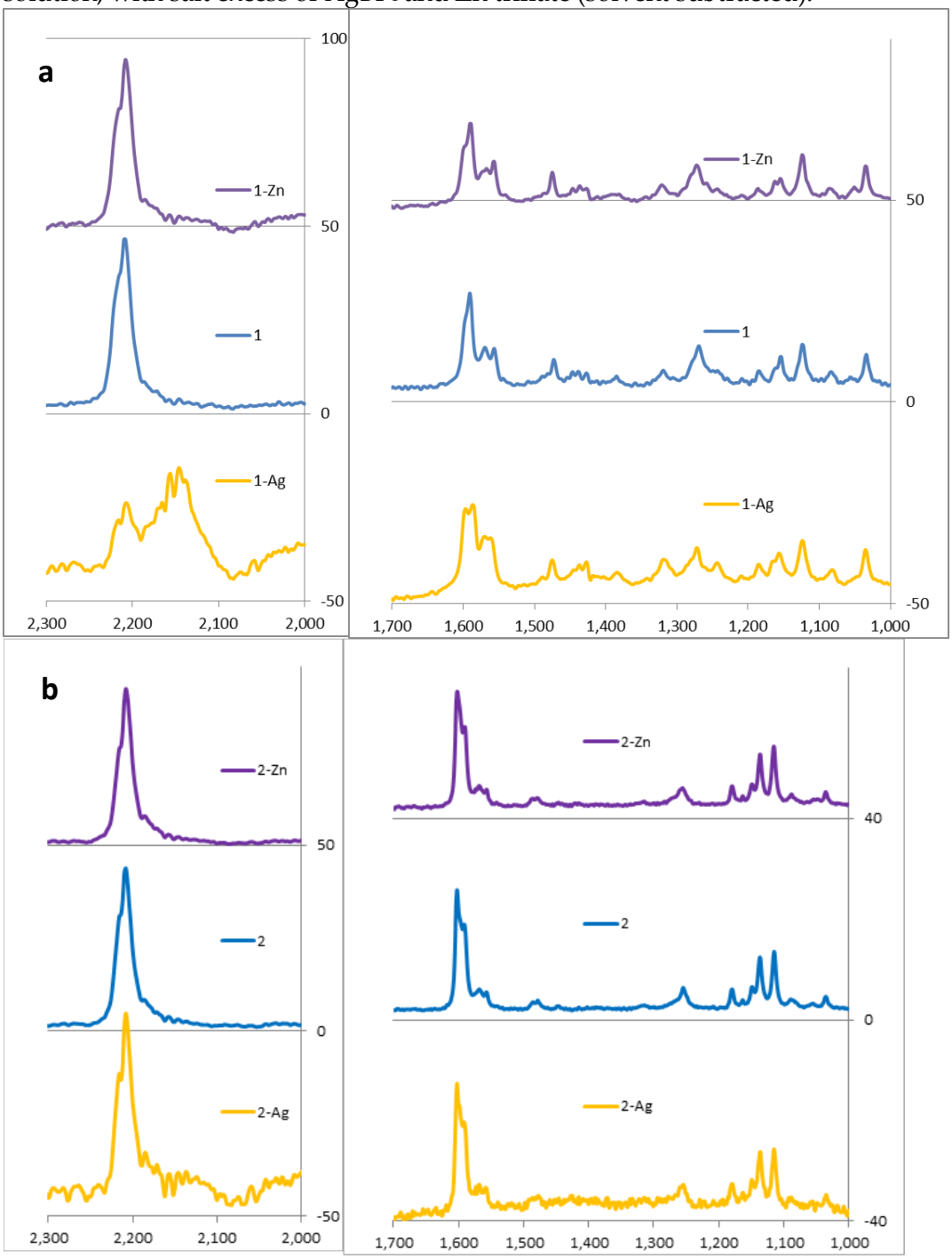
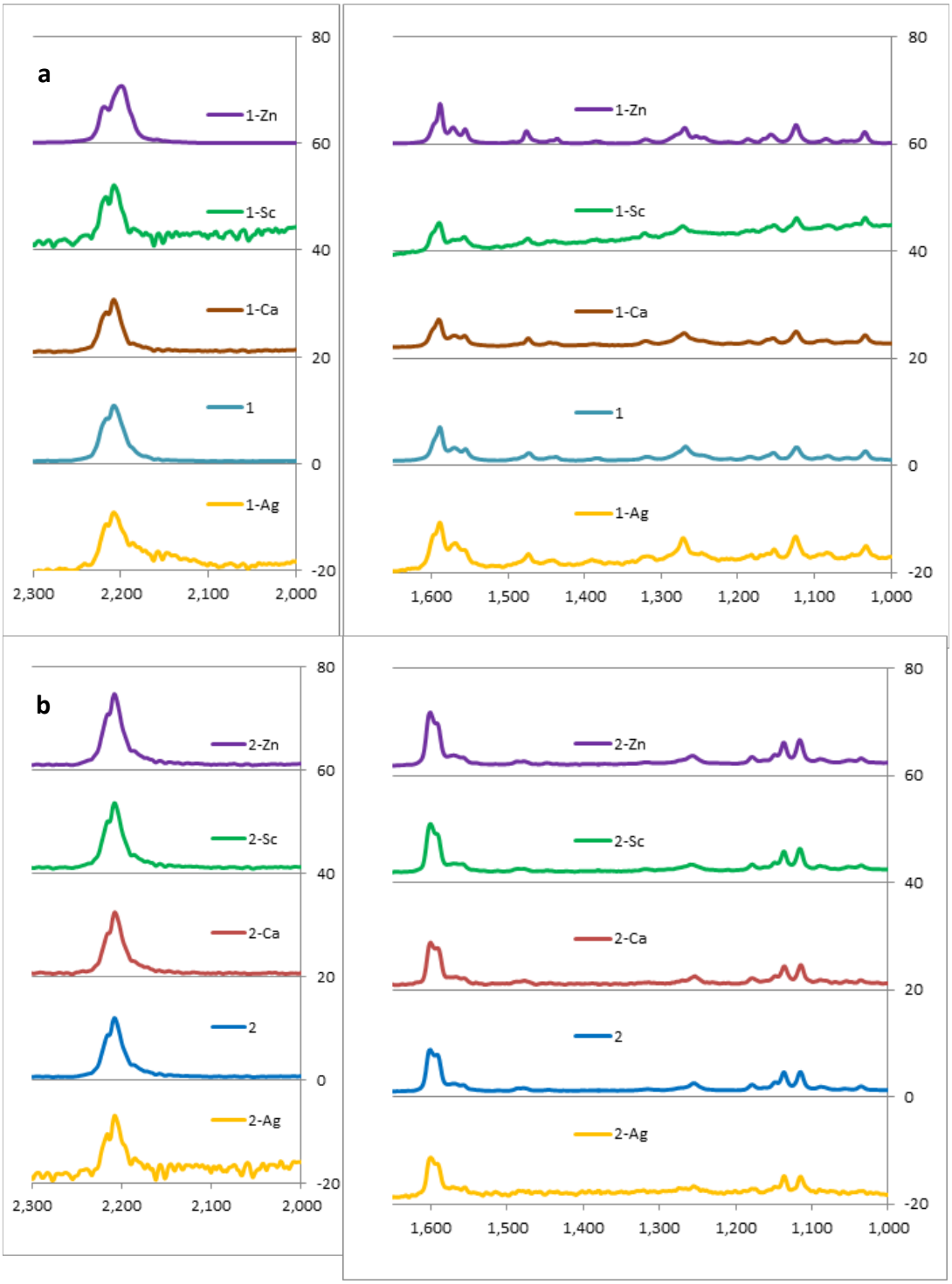
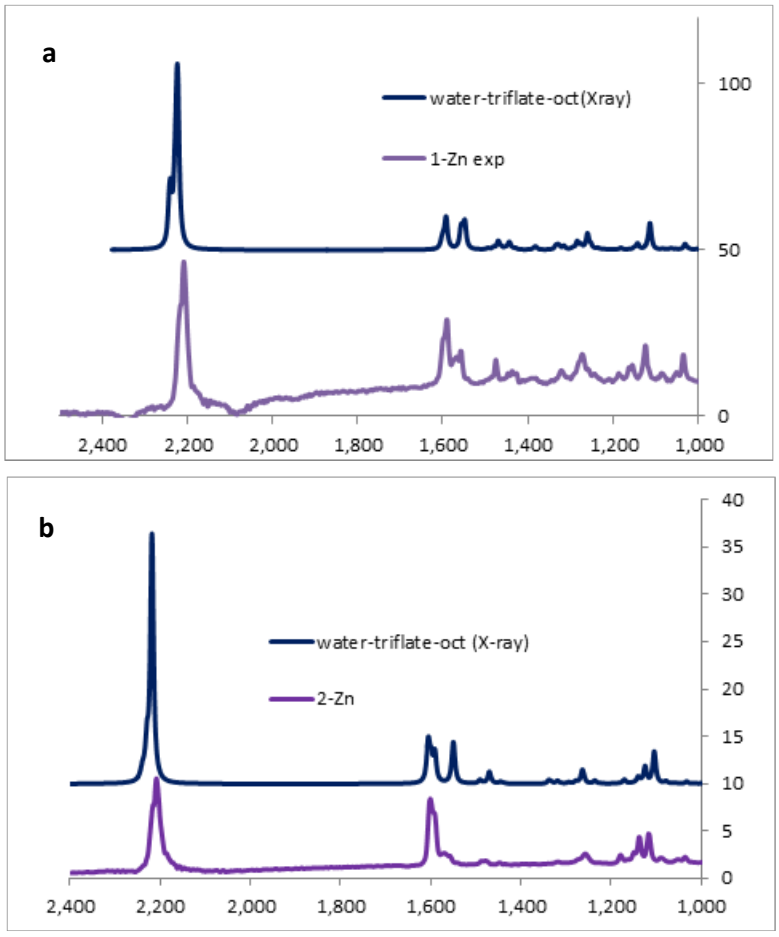


Figure S26. (a) Raman spectra of compound (*S*,*S*)-**1** , solid state, pure and dried after addition of salt excess of $AgBF_4$ and Zn , Sc and Ca triflate. (b) Raman spectra of compound (*S*,*S*)-**2** , solid state, pure and dried after addition of salt excess of $AgBF_4$ and Zn , Sc and Ca triflate.



Calculated Raman spectra

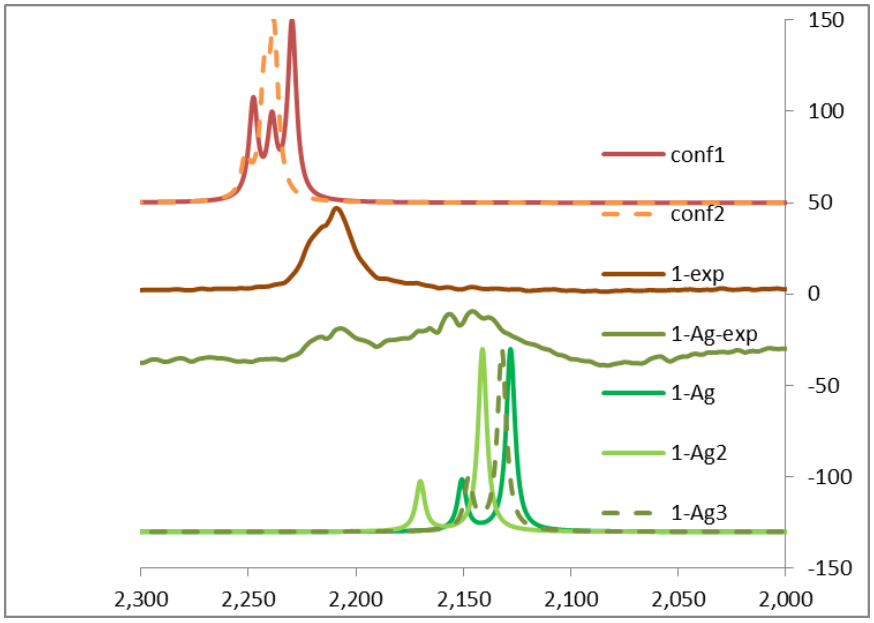
Figure S27. Raman spectra of compound (a) (*S*,*S*)-**1** and (b) (*S*,*S*)-**2** after addition of salt excess of Zn triflate. As can be seen, DFT calculations (blue lines) give a good representation of the experimental Raman data (purple lines).



Sensitivity of Raman to triple bond coordination: Ag complex

As can be seen in Figure S28 Raman is very sensitive to Ag complexation in the case of (*S*,*S*)-**1** due to the strong interaction between Ag and CC triple bonds. Calculations account well for the phenomenon.

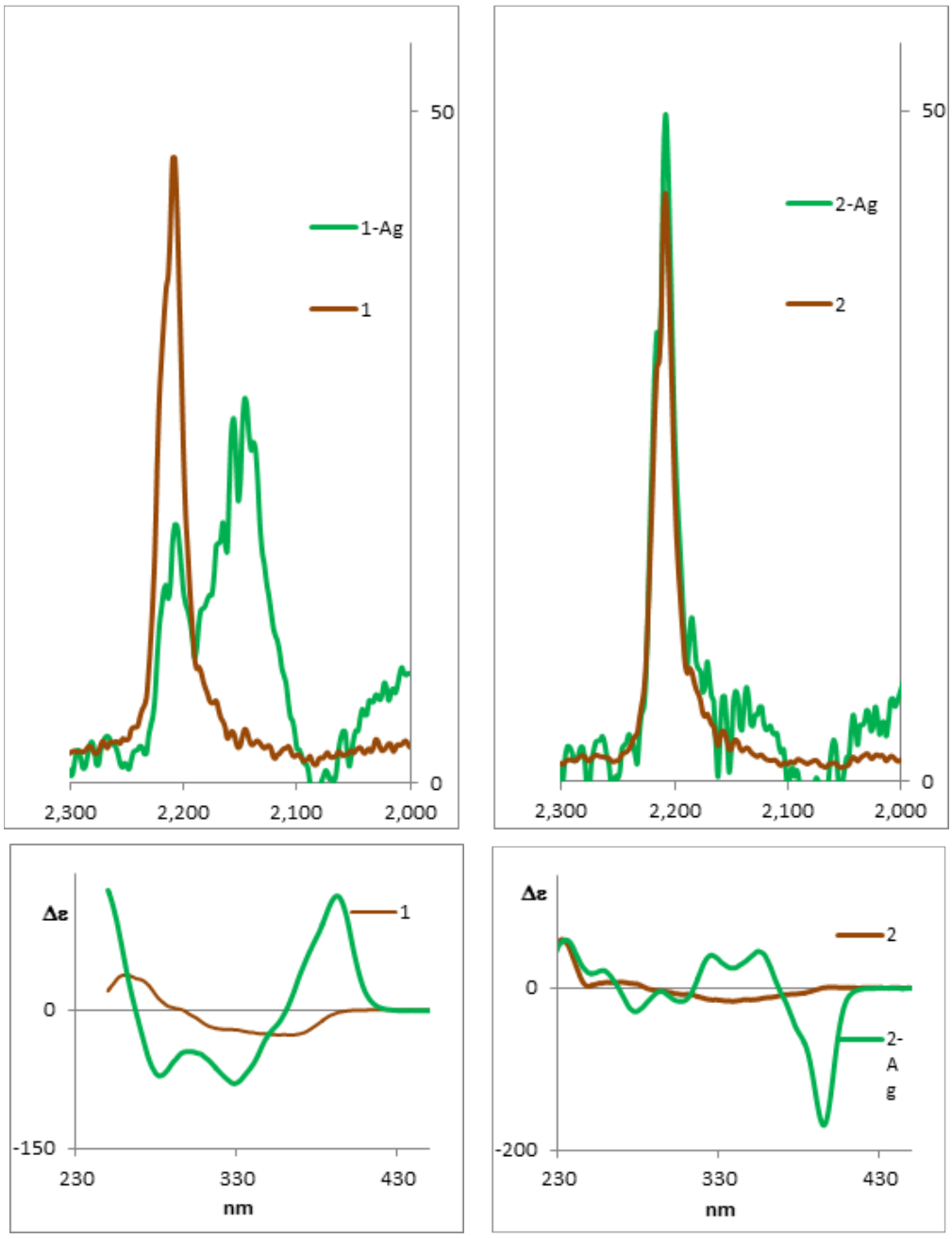
Figure S28. Experimental Raman spectra of compound (*S*,*S*)-**1** before (brown line) and after (green line) complexation with $AgBF_4$. These spectra are compared with those simulated by DFT on different conformations of pristine and Ag-complexed (*S*,*S*)-**1**.



Comparison of Ag complexes of compounds (S,S)-1 and (S,S)-2

Comparing the experimental Raman data of compounds (*S*,*S*)-**1** and (*S*,*S*)-**2** (Figure S29) it is clear that compound **1** offers the best cavity to host Ag strongly and simultaneously interacting with the three CC triple bonds. Compound (*S*,*S*)-**2**-Ag presents a CC band superimposable to that recorded for the solvated compound, as well as for complexes with oxophilic metals. Analogously, the CD spectrum of 1-Ag is completely different from the simple solvated compound and from complexes with oxophilic metals; on the contrary, the CD spectrum of the Ag complex of compound (*S*,*S*)-**2** is quite similar to the CD spectrum recorded for all the other complexes.

Figure S29. . Raman (up) and CD (down) spectra of compounds (*S*,*S*)-**1** (left) and (*S*,*S*)-**2** (right) in absence and presence of an excess of $AgBF_4$. Experiments in solution state (solvent CH_2Cl_2)..



THEORETICAL CALCULATIONS

Technical details

All quantum chemical calculations have been carried out with the Gaussian code.[16] Metal complexes of compounds (*S*,*S*)-**1** and (*S*,*S*)-**2** have been optimized at the M06/6-31g* level using the polarizable continuum model (PCM) approximation in order to take into account the solvent (dichloromethane). Additionally, for all metallic cations (with the exception of Ca(II), that was calculated with the previous M06/6-31g*) we used the LANL2DZ pseudopotential (Los Alamos ECP for the core plus DZ basis set for valence electrons).

Atomic coordinates of the DFT optimized complexes

[(S,S)-1]$_2$:Ca complex

Number	Label	X	Y	Z
1	S	2.3385	2.3381	-0.7767
2	S	2.6376	-1.7581	0.9104
3	O	1.6869	-1.1262	-0.1151
4	O	5.5894	-0.7762	-3.1923
5	O	5.3472	0.5608	3.064
6	O	4.8797	2.4677	-2.0851
7	O	1.3071	2.0067	0.3098
8	C	4.425	-0.3542	-3.8727
9	H	3.9245	0.4658	-3.3303
10	H	3.7226	-1.187	-4.0205
11	H	4.7581	0.0099	-4.8476
12	O	5.158	-2.4958	2.0312
13	C	10.945	-0.5439	2.0874
14	C	9.7558	-0.1889	2.7682
15	C	4.1996	0.3663	3.8642
16	H	3.4991	-0.3382	3.3913
17	H	3.6912	1.3199	4.0681
18	H	4.5557	-0.0578	4.8059
19	C	11.3349	-0.3493	-1.9446
20	C	3.963	1.4735	1.2872
21	H	3.0311	1.4034	1.8483
22	C	11.1678	-0.4102	-0.5347
23	C	10.2426	-0.5952	-2.8132
24	C	2.3339	4.8229	0.4286
25	H	2.2201	4.2788	1.3666
26	C	8.6144	0.3031	2.0802
27	C	5.1838	1.0737	1.8261
28	C	12.0429	-1.0029	2.8284
29	H	12.9543	-1.2707	2.2976
30	C	2.3623	6.2099	0.4069
31	H	2.2815	6.7662	1.3403
32	C	1.4418	-5.4985	-0.0819
33	H	1.1686	-6.0536	-0.9799
34	C	5.446	-1.2464	-1.9316
35	C	3.9227	1.9479	-0.0184
36	C	6.3558	1.1699	1.0409
37	C	2.4334	4.1307	-0.7744
38	C	6.5752	-1.9873	0.1021
39	H	7.513	-2.1643	0.6232
40	C	4.2212	-1.4043	-1.2961
41	H	3.277	-1.1532	-1.7761

42	C	2.4898	6.9106	-0.7981
43	C	11.9698	-1.1223	4.2081
44	H	12.8325	-1.481	4.7651
45	C	2.1334	-4.0973	2.2267
46	H	2.4074	-3.5374	3.1208
47	C	1.3903	-6.1436	1.1611
48	C	1.8425	-4.175	-0.1829
49	H	1.8996	-3.6752	-1.1498
50	C	8.9693	-0.9296	-2.281
51	C	2.5793	6.1871	-1.991
52	H	2.666	6.7231	-2.9358
53	C	6.6335	-1.5209	-1.2197
54	C	10.437	-0.513	-4.1981
55	H	9.5922	-0.703	-4.8571
56	C	11.0402	-0.4543	0.6725
57	C	6.2875	1.6553	-0.2698
58	H	7.2025	1.687	-0.8569
59	C	4.1913	-1.8321	0.0223
60	C	5.0667	2.0344	-0.8161
61	C	5.3491	-2.1316	0.7432
62	C	7.5886	0.7218	1.5807
63	C	12.7615	0.0294	-3.8658
64	H	13.7407	0.2695	-4.2744
65	C	2.1872	-3.4895	0.9786
66	C	12.5877	-0.0428	-2.4915
67	H	13.4215	0.1424	-1.8173
68	C	9.6985	-0.3241	4.1633
69	H	8.7759	-0.0521	4.6738
70	C	2.5499	4.797	-1.9894
71	H	2.615	4.2368	-2.9217
72	C	1.7435	-5.4291	2.3073
73	H	1.7076	-5.9231	3.2776
74	C	11.6844	-0.2039	-4.7201
75	H	11.8196	-0.1469	-5.798
76	C	6.0138	2.5362	-2.9366
77	H	5.6473	2.9105	-3.8951
78	H	6.4586	1.5401	-3.0763
79	H	6.7634	3.2312	-2.5369
80	C	7.8917	-1.2294	-1.8067
81	C	0.9421	-7.5683	1.2618
82	H	-0.1514	-7.624	1.3685
83	H	1.3789	-8.0687	2.1336
84	H	1.2088	-8.1403	0.3652
85	C	10.7934	-0.7859	4.8774
86	H	10.7321	-0.8819	5.9591
87	C	6.2989	-2.6598	2.859

88	H	5.9169	-2.928	3.8464
89	H	6.87	-1.7238	2.9267
90	H	6.942	-3.4686	2.4879
91	C	2.5394	8.4074	-0.8129
92	H	2.0027	8.8177	-1.6774
93	H	3.5763	8.7643	-0.8804
94	H	2.1061	8.8344	0.0989
95	C	-11.0083	0.2474	1.8679
96	S	-2.4103	-2.3085	-0.8533
97	S	-2.99	2.6351	1.2614
98	O	-1.9129	1.6092	0.9167
99	O	-5.2142	0.3468	-2.8143
100	O	-5.2335	-0.3892	3.0236
101	O	-5.0232	-2.7478	-1.9612
102	O	-1.351	-1.8401	0.1518
103	C	-3.9402	0.1398	-3.3874
104	H	-3.3096	-0.4931	-2.744
105	H	-3.4272	1.0933	-3.5805
106	H	-4.1138	-0.3771	-4.3343
107	O	-5.7562	3.0002	1.9954
108	C	-9.8549	0.1094	2.6797
109	C	-4.0285	-0.0717	3.6886
110	H	-3.3862	0.5813	3.0737
111	H	-3.4662	-0.9784	3.9541
112	H	-4.3118	0.4581	4.6007
113	C	-10.962	-0.7619	-2.062
114	C	-3.948	-1.3842	1.2257
115	H	-2.9844	-1.2056	1.699
116	C	-10.9728	-0.4032	-0.6866
117	C	-9.8096	-0.5313	-2.8548
118	C	-2.4561	-4.7842	0.4032
119	H	-2.585	-4.2441	1.341
120	C	-8.644	-0.4057	2.1466
121	C	-5.1456	-1.0117	1.8261
122	C	-12.1852	0.7519	2.4372
123	H	-13.0681	0.8512	1.8091
124	C	-2.3817	-6.1703	0.3873
125	H	-2.4644	-6.724	1.3226
126	C	-0.9299	5.4014	-0.8702
127	H	0.0258	5.4676	-1.3923
128	C	-5.2886	1.0275	-1.6498
129	C	-3.9685	-1.9739	-0.0298
130	C	-6.3604	-1.2542	1.1487
131	C	-2.3775	-4.0961	-0.8031
132	C	-6.776	1.8739	0.0916
133	H	-7.7896	1.974	0.4725

134	C	-4.199	1.5124	-0.9417
135	H	-3.1772	1.3705	-1.2925
136	C	-2.2192	-6.8723	-0.8127
137	C	-12.2246	1.1245	3.7728
138	H	-13.1469	1.5171	4.1954
139	C	-3.3671	5.2373	0.4614
140	H	-4.3237	5.1662	0.9801
141	C	-1.7567	6.5244	-0.818
142	C	-1.2911	4.2062	-0.2585
143	H	-0.6198	3.3482	-0.2753
144	C	-8.6724	0.1	-2.2879
145	C	-2.1313	-6.1517	-2.0077
146	H	-2.0068	-6.6885	-2.9478
147	C	-6.5891	1.2043	-1.1204
148	C	-9.808	-0.926	-4.1991
149	H	-8.9153	-0.7463	-4.7958
150	C	-10.9777	-0.1101	0.4924
151	C	-6.3544	-1.86	-0.1164
152	H	-7.3091	-2.0056	-0.6158
153	C	-4.409	2.1589	0.2734
154	C	-5.1558	-2.2051	-0.73
155	C	-5.6826	2.3539	0.8098
156	C	-7.5882	-0.8189	1.7096
157	C	-12.0669	-1.7353	-3.9856
158	H	-12.9467	-2.1998	-4.4256
159	C	-2.5145	4.1384	0.3925
160	C	-12.0835	-1.3599	-2.6499
161	H	-12.9668	-1.5323	-2.0385
162	C	-9.9141	0.4943	4.0267
163	H	-9.0214	0.3852	4.6403
164	C	-2.2057	-4.7656	-2.0107
165	H	-2.1462	-4.2069	-2.9445
166	C	-2.9812	6.4231	-0.1491
167	H	-3.6406	7.2894	-0.1054
168	C	-10.927	-1.5228	-4.7604
169	H	-10.9141	-1.8208	-5.8064
170	C	-6.179	-2.8207	-2.7838
171	H	-5.8402	-3.2264	-3.7395
172	H	-6.6109	-1.8212	-2.9359
173	H	-6.93	-3.4952	-2.3515
174	C	-7.7067	0.6347	-1.7808
175	C	-1.3119	7.8147	-1.436
176	H	-0.6298	8.3558	-0.7638
177	H	-2.1577	8.4789	-1.6473
178	H	-0.7664	7.643	-2.373
179	C	-11.0865	0.9989	4.5686

180	H	-11.1157	1.2925	5.6155
181	C	-6.9802	2.9212	2.7113
182	H	-6.8024	3.4143	3.6691
183	H	-7.2616	1.872	2.8775
184	H	-7.7881	3.4438	2.1821
185	C	-2.1402	-8.368	-0.8322
186	H	-1.1504	-8.7064	-1.1684
187	H	-2.873	-8.7938	-1.5294
188	H	-2.3238	-8.7993	0.1584
189	Ca	-0.1876	0.1818	0.3912
190	C	0.1642	0.8832	3.6747
191	O	0.287	0.1048	2.7307
192	C	0.0853	0.3772	5.0766
193	C	0.0852	2.3635	3.4756
194	H	-0.0199	-0.7107	5.0959
195	H	0.3771	2.6518	2.459
196	H	-0.7489	0.8513	5.6092
197	H	0.9996	0.6615	5.6163
198	H	0.706	2.8856	4.2144
199	H	-0.9496	2.6855	3.6655
200	C	0.0448	0.0415	-2.9917
201	O	-0.3817	0.5695	-1.966
202	C	0.281	-1.4325	-3.074
203	C	0.3352	0.8574	-4.2067
204	H	0.3007	-1.8856	-2.0762
205	H	-0.0979	1.8577	-4.1183
206	H	1.2083	-1.6597	-3.6158
207	H	-0.5365	-1.8751	-3.6633
208	H	-0.0233	0.3603	-5.1163
209	H	1.4269	0.9486	-4.31

[(S,S)-1]$_2$:Co complex

Number	Label	X	Y	Z
1	S	2.1326	2.1204	-0.9038
2	S	2.5112	-1.5766	0.863
3	O	1.6117	-1.0454	-0.2781
4	O	5.583	-0.9322	-3.2218
5	O	5.2228	0.7982	3.0324
6	O	4.6688	2.3441	-2.2307
7	O	1.1568	1.7514	0.2333
8	C	4.4321	-0.6011	-3.9709
9	H	3.869	0.213	-3.4858
10	H	3.7809	-1.4768	-4.1043
11	H	4.7886	-0.2652	-4.9476

12	O	5.0101	-2.2737	2.098
13	C	10.8435	-0.2107	2.1305
14	C	9.6387	0.1596	2.7754
15	C	4.0793	0.6172	3.8395
16	H	3.3787	-0.1039	3.3875
17	H	3.5639	1.5727	4.0166
18	H	4.4382	0.2207	4.7922
19	C	11.2754	-0.3142	-1.9008
20	C	3.8075	1.5384	1.205
21	H	2.8777	1.4721	1.7681
22	C	11.0945	-0.267	-0.4923
23	C	10.1974	-0.6519	-2.7569
24	C	2.0268	4.6512	0.1939
25	H	2.025	4.1498	1.1616
26	C	8.4916	0.5775	2.0497
27	C	5.0437	1.2304	1.7655
28	C	11.9446	-0.5899	2.9116
29	H	12.8684	-0.8695	2.409
30	C	1.9902	6.0355	0.1088
31	H	1.9672	6.6315	1.0214
32	C	1.4147	-5.4114	0.1711
33	H	1.1686	-6.0449	-0.6822
34	C	5.4028	-1.3	-1.9328
35	C	3.7409	1.9055	-0.133
36	C	6.2085	1.3204	0.9686
37	C	2.0732	3.9072	-0.9808
38	C	6.4734	-1.8795	0.1824
39	H	7.3954	-2.0181	0.7422
40	C	4.16	-1.4069	-1.3209
41	H	3.2328	-1.1781	-1.8421
42	C	1.9935	6.6814	-1.1335
43	C	11.8592	-0.6177	4.2959
44	H	12.7249	-0.9155	4.8837
45	C	2.0171	-3.799	2.3656
46	H	2.2596	-3.1625	3.217
47	C	1.4006	-5.9629	1.4604
48	C	1.7391	-4.0796	-0.0318
49	H	1.7542	-3.65	-1.0337
50	C	8.9244	-0.9702	-2.2149
51	C	2.0284	5.9057	-2.2968
52	H	2.0307	6.4001	-3.2681
53	C	6.5706	-1.512	-1.1673
54	C	10.4038	-0.6749	-4.1429
55	H	9.5689	-0.9343	-4.7909
56	C	10.951	-0.221	0.7137
57	C	6.1158	1.7164	-0.3714

58	H	7.0277	1.7485	-0.9632
59	C	4.0907	-1.7292	0.0273
60	C	4.8779	2.0022	-0.9383
61	C	5.2293	-1.9828	0.7975
62	C	7.4561	0.9422	1.5273
63	C	12.713	-0.0574	-3.8353
64	H	13.6912	0.1706	-4.2533
65	C	2.0506	-3.2905	1.0731
66	C	12.5271	-0.0248	-2.4606
67	H	13.3509	0.2309	-1.797
68	C	9.5689	0.1159	4.1762
69	H	8.6329	0.3963	4.6572
70	C	2.0661	4.5178	-2.231
71	H	2.1046	3.9155	-3.1384
72	C	1.6961	-5.1407	2.5488
73	H	1.6802	-5.5588	3.5548
74	C	11.6495	-0.3802	-4.6779
75	H	11.794	-0.405	-5.7559
76	C	5.8026	2.4251	-3.0809
77	H	5.4246	2.725	-4.0607
78	H	6.3017	1.4484	-3.1612
79	H	6.5125	3.1792	-2.7166
80	C	7.8418	-1.2519	-1.7395
81	C	1.0609	-7.4077	1.6584
82	H	-0.0255	-7.569	1.6002
83	H	1.3951	-7.7728	2.6361
84	H	1.5167	-8.0346	0.8819
85	C	10.667	-0.2687	4.9304
86	H	10.596	-0.2944	6.0156
87	C	6.1317	-2.4039	2.9573
88	H	5.7244	-2.5802	3.9555
89	H	6.7308	-1.4829	2.9644
90	H	6.7548	-3.2584	2.6618
91	C	1.9442	8.1752	-1.2296
92	H	0.9669	8.513	-1.6034
93	H	2.6988	8.5549	-1.93
94	H	2.1126	8.6506	-0.2562
95	C	-10.9238	-0.0094	1.9922
96	S	-2.1428	-2.0759	-0.8506
97	S	-2.6126	1.9658	0.9882
98	O	-1.6524	1.2936	-0.0053
99	O	-5.3932	0.6303	-3.1202
100	O	-5.2158	-0.6567	3.062
101	O	-4.6819	-2.4804	-2.1142
102	O	-1.1546	-1.6286	0.2461
103	C	-4.1779	0.3927	-3.8014

104	H	-3.5561	-0.3392	-3.2626
105	H	-3.6088	1.323	-3.9415
106	H	-4.4518	-0.016	-4.777
107	O	-5.2399	2.4375	2.0926
108	C	-9.734	-0.2455	2.7242
109	C	-4.0647	-0.3218	3.8083
110	H	-3.4776	0.4585	3.2997
111	H	-3.429	-1.2007	3.9876
112	H	-4.425	0.0646	4.7647
113	C	-11.0957	-0.3483	-2.0464
114	C	-3.8002	-1.4113	1.2431
115	H	-2.8643	-1.251	1.7778
116	C	-11.0125	-0.2327	-0.6326
117	C	-9.9869	-0.0168	-2.8651
118	C	-2.0837	-4.5605	0.3589
119	H	-2.1679	-4.0258	1.3044
120	C	-8.5368	-0.6611	2.0834
121	C	-5.0409	-1.1456	1.815
122	C	-12.0814	0.3786	2.6816
123	H	-12.9925	0.5559	2.1135
124	C	-2.0181	-5.9456	0.3335
125	H	-2.0672	-6.5021	1.2698
126	C	-1.3674	5.5277	-0.4669
127	H	-0.8589	5.9029	-1.3565
128	C	-5.3216	1.1305	-1.8667
129	C	-3.7427	-1.8673	-0.0672
130	C	-6.2142	-1.3539	1.0541
131	C	-2.0513	-3.8646	-0.8462
132	C	-6.5565	1.7773	0.1395
133	H	-7.516	1.8704	0.6425
134	C	-4.1316	1.4116	-1.2113
135	H	-3.1581	1.2373	-1.6671
136	C	-1.9043	-6.6433	-0.8752
137	C	-12.0665	0.5446	4.0587
138	H	-12.9745	0.8482	4.5755
139	C	-2.6551	4.5838	1.8194
140	H	-3.1609	4.2035	2.7064
141	C	-1.7366	6.4287	0.5394
142	C	-1.625	4.17	-0.3454
143	H	-1.3204	3.4629	-1.1171
144	C	-8.7821	0.4613	-2.2858
145	C	-1.8656	-5.9168	-2.0687
146	H	-1.7836	-6.4486	-3.0162
147	C	-6.5446	1.2976	-1.1784
148	C	-10.0932	-0.1616	-4.2553
149	H	-9.2349	0.0937	-4.874

150	C	-10.9535	-0.1441	0.5781
151	C	-6.1269	-1.8299	-0.2602
152	H	-7.048	-1.9519	-0.8253
153	C	-4.1704	1.843	0.1065
154	C	-4.8874	-2.0774	-0.84
155	C	-5.3623	2.0422	0.8046
156	C	-7.4742	-1.0077	1.6049
157	C	-12.3653	-0.9313	-4.0274
158	H	-13.2904	-1.2855	-4.4772
159	C	-2.2734	3.719	0.8008
160	C	-12.278	-0.7989	-2.6489
161	H	-13.1264	-1.0494	-2.0149
162	C	-9.737	-0.0649	4.1152
163	H	-8.8143	-0.2454	4.6647
164	C	-1.9389	-4.5288	-2.0632
165	H	-1.9296	-3.9719	-2.9997
166	C	-2.3853	5.9407	1.6764
167	H	-2.6771	6.6341	2.4645
168	C	-11.2707	-0.615	-4.8319
169	H	-11.3381	-0.7201	-5.9126
170	C	-5.8184	-2.6358	-2.9506
171	H	-5.4366	-2.9687	-3.9183
172	H	-6.3457	-1.6788	-3.0707
173	H	-6.5017	-3.3953	-2.5483
174	C	-7.7543	0.8801	-1.79
175	C	-1.4086	7.8838	0.4048
176	H	-0.3389	8.0612	0.5934
177	H	-1.9755	8.4962	1.115
178	H	-1.6175	8.2501	-0.6086
179	C	-10.8907	0.3269	4.7774
180	H	-10.8761	0.4603	5.8569
181	C	-6.4138	2.4707	2.8908
182	H	-6.0898	2.77	3.8901
183	H	-6.8816	1.477	2.9379
184	H	-7.1314	3.207	2.5051
185	C	-1.804	-8.1375	-0.8942
186	H	-0.7622	-8.4586	-1.0396
187	H	-2.3869	-8.5683	-1.7174
188	H	-2.1577	-8.5788	0.045
189	Co	-0.0403	0.0816	0.0919
190	C	0.1183	0.5372	3.2034
191	O	0.0947	-0.1606	2.1902
192	C	0.2402	-0.1051	4.5462
193	C	0.004	2.0259	3.1565
194	H	0.3919	-1.1831	4.444
195	H	0.0176	2.3912	2.1247

196	H	-0.6737	0.0839	5.1268
197	H	1.0622	0.3417	5.1201
198	H	0.8244	2.4918	3.7201
199	H	-0.9248	2.3301	3.6626
200	C	0.1474	-0.0935	-3.0973
201	O	-0.1722	0.3942	-2.0166
202	C	0.4307	-1.5492	-3.2638
203	C	0.2442	0.7773	-4.3058
204	H	0.6189	-2.0246	-2.2949
205	H	-0.2484	1.7384	-4.1286
206	H	1.271	-1.7167	-3.9487
207	H	-0.4468	-2.0118	-3.7413
208	H	-0.1737	0.2851	-5.1923
209	H	1.3081	0.9615	-4.5186

[(S,S)-1]$_2$:Ga complex

Number	Label	X	Y	Z
1	S	-2.1533	2.135	0.7471
2	S	-2.4437	-1.6211	-0.8002
3	O	-1.5027	-0.9818	0.2835
4	O	-5.4531	-0.7421	3.3115
5	O	-5.2516	0.648	-3.1548
6	O	-4.6392	2.4256	2.0239
7	O	-1.124	1.6677	-0.3438
8	C	-4.3014	-0.4138	4.0607
9	H	-3.7103	0.3672	3.5551
10	H	-3.6757	-1.3012	4.2331
11	H	-4.6599	-0.0331	5.0197
12	O	-4.9147	-2.3292	-1.9403
13	C	-10.8246	-0.4284	-2.0569
14	C	-9.6408	-0.1036	-2.7624
15	C	-4.1262	0.3032	-3.9339
16	H	-3.5091	-0.452	-3.42
17	H	-3.5178	1.1866	-4.1774
18	H	-4.5185	-0.1233	-4.8601
19	C	-11.1501	-0.131	1.9742
20	C	-3.8084	1.4651	-1.3816
21	H	-2.8953	1.3851	-1.9673
22	C	-11.0007	-0.2286	0.5648
23	C	-10.0571	-0.3868	2.8394
24	C	-2.0417	4.6195	-0.4662
25	H	-2.0888	4.0975	-1.4215
26	C	-8.4881	0.3947	-2.0999
27	C	-5.0512	1.1291	-1.9108

28	C	-11.9366	-0.8937	-2.7726
29	H	-12.8444	-1.139	-2.225
30	C	-2.0159	6.0053	-0.416
31	H	-2.034	6.5783	-1.3428
32	C	-1.5864	-5.4756	0.0765
33	H	-1.5229	-6.1224	0.9517
34	C	-5.2792	-1.1628	2.0402
35	C	-3.73	1.8889	-0.0581
36	C	-6.2075	1.248	-1.1022
37	C	-2.0247	3.9098	0.7315
38	C	-6.3681	-1.8419	-0.0374
39	H	-7.2927	-2.0052	-0.5859
40	C	-4.0405	-1.3015	1.4277
41	H	-3.1156	-1.0523	1.9412
42	C	-1.9923	6.6841	0.8096
43	C	-11.8807	-1.048	-4.1502
44	H	-12.754	-1.4111	-4.6877
45	C	-1.7631	-3.8368	-2.1746
46	H	-1.8472	-3.1864	-3.046
47	C	-1.4241	-6.0301	-1.2017
48	C	-1.8621	-4.1277	0.2419
49	H	-2.0244	-3.7074	1.2348
50	C	-8.7948	-0.7617	2.3091
51	C	-1.9669	5.9405	1.9944
52	H	-1.9481	6.461	2.9513
53	C	-6.454	-1.4002	1.2892
54	C	-10.2355	-0.27	4.2247
55	H	-9.3894	-0.4683	4.8796
56	C	-10.8969	-0.3035	-0.6437
57	C	-6.1043	1.7147	0.212
58	H	-7.0081	1.7698	0.8145
59	C	-3.9844	-1.689	0.094
60	C	-4.8612	2.0275	0.7527
61	C	-5.1285	-1.9793	-0.6553
62	C	-7.4546	0.8177	-1.6196
63	C	-12.547	0.3301	3.9001
64	H	-13.515	0.6083	4.3114
65	C	-1.9624	-3.3269	-0.8954
66	C	-12.3888	0.2227	2.5257
67	H	-13.2237	0.4168	1.8554
68	C	-9.5997	-0.2751	-4.1541
69	H	-8.6797	-0.0269	-4.6815
70	C	-1.9801	4.5521	1.9664
71	H	-1.9781	3.9716	2.8883
72	C	-1.4954	-5.1926	-2.3181
73	H	-1.3636	-5.6154	-3.3133

74	C	-11.4692	0.0848	4.7508
75	H	-11.5931	0.169	5.8282
76	C	-5.7642	2.5424	2.8878
77	H	-5.3719	2.8917	3.8451
78	H	-6.2559	1.5679	3.0232
79	H	-6.48	3.2763	2.4966
80	C	-7.7187	-1.0921	1.8506
81	C	-1.1784	-7.4968	-1.3714
82	H	-0.1019	-7.7149	-1.4302
83	H	-1.6301	-7.8739	-2.2962
84	H	-1.5826	-8.0724	-0.5306
85	C	-10.7088	-0.7426	-4.8428
86	H	-10.6625	-0.867	-5.9225
87	C	-6.0429	-2.5541	-2.7767
88	H	-5.6396	-2.7909	-3.7634
89	H	-6.6676	-1.6529	-2.8407
90	H	-6.6347	-3.4024	-2.4104
91	C	-1.9981	8.1801	0.866
92	H	-1.0505	8.5652	1.2678
93	H	-2.7921	8.5453	1.5297
94	H	-2.1519	8.6253	-0.1236
95	C	10.8988	-0.1044	-1.9451
96	S	2.1362	-1.982	0.9519
97	S	2.5799	1.9142	-1.1036
98	O	1.5943	1.2263	-0.1193
99	O	5.3098	0.7403	3.1114
100	O	5.2133	-0.822	-3.0656
101	O	4.6158	-2.3397	2.1967
102	O	1.1072	-1.5034	-0.123
103	C	4.1006	0.5661	3.8223
104	H	3.4681	-0.2029	3.3496
105	H	3.5436	1.5103	3.8985
106	H	4.3834	0.231	4.8228
107	O	5.1787	2.3081	-2.1763
108	C	9.7254	-0.3838	-2.6881
109	C	4.0784	-0.48	-3.8332
110	H	3.5335	0.3595	-3.3729
111	H	3.3988	-1.3349	-3.9607
112	H	4.4553	-0.1688	-4.81
113	C	11.0235	-0.262	2.1061
114	C	3.7724	-1.4628	-1.2253
115	H	2.8498	-1.3202	-1.7858
116	C	10.9514	-0.2096	0.688
117	C	9.9058	0.0938	2.9018
118	C	1.8789	-4.4562	-0.2421
119	H	1.9145	-3.9322	-1.1963

120	C	8.5199	-0.7791	-2.0511
121	C	5.0204	-1.2467	-1.7994
122	C	12.065	0.2641	-2.6303
123	H	12.9638	0.4761	-2.0546
124	C	1.7936	-5.8378	-0.1959
125	H	1.7772	-6.4033	-1.1277
126	C	1.3373	5.4838	0.3258
127	H	0.8655	5.8812	1.225
128	C	5.237	1.1795	1.8372
129	C	3.7049	-1.8333	0.1136
130	C	6.1877	-1.4273	-1.0178
131	C	1.9269	-3.7519	0.9591
132	C	6.486	1.7305	-0.1913
133	H	7.4496	1.8093	-0.6884
134	C	4.0498	1.4354	1.1673
135	H	3.0783	1.2984	1.6391
136	C	1.7546	-6.523	1.0266
137	C	12.0733	0.3681	-4.0136
138	H	12.9879	0.6575	-4.5268
139	C	2.5545	4.4935	-1.9805
140	H	3.0439	4.1004	-2.871
141	C	1.6818	6.364	-0.7084
142	C	1.5816	4.1228	0.2239
143	H	1.3017	3.4346	1.0227
144	C	8.7016	0.5356	2.2942
145	C	1.7966	-5.7857	2.2126
146	H	1.7726	-6.3074	3.1684
147	C	6.4647	1.311	1.1446
148	C	10.0012	0.0122	4.2979
149	H	9.1354	0.2857	4.8981
150	C	10.9055	-0.1764	-0.5261
151	C	6.0884	-1.8288	0.3193
152	H	7.004	-1.9313	0.8973
153	C	4.1003	1.7944	-0.1749
154	C	4.8416	-2.0187	0.905
155	C	5.2958	1.9638	-0.8758
156	C	7.4523	-1.1109	-1.5734
157	C	12.2822	-0.7428	4.1209
158	H	13.2073	-1.0663	4.5932
159	C	2.1919	3.6503	-0.9358
160	C	12.2052	-0.6733	2.7372
161	H	13.0613	-0.9426	2.1218
162	C	9.7513	-0.266	-4.0856
163	H	8.8406	-0.4799	-4.6429
164	C	1.887	-4.399	2.1902
165	H	1.953	-3.8328	3.1187

166	C	2.2945	5.853	-1.8548
167	H	2.5705	6.5295	-2.6624
168	C	11.1785	-0.4024	4.9028
169	H	11.239	-0.4582	5.9875
170	C	5.7373	-2.5034	3.0554
171	H	5.3274	-2.7268	4.0427
172	H	6.328	-1.5788	3.1049
173	H	6.3641	-3.3397	2.7213
174	C	7.6723	0.9257	1.7785
175	C	1.3681	7.8225	-0.5925
176	H	0.3133	8.0121	-0.8429
177	H	1.9802	8.4263	-1.2715
178	H	1.5251	8.1861	0.4307
179	C	10.9137	0.1063	-4.7436
180	H	10.9189	0.1905	-5.828
181	C	6.3586	2.3253	-2.9713
182	H	6.0376	2.5986	-3.9784
183	H	6.8281	1.3319	-2.9897
184	H	7.0693	3.074	-2.5988
185	C	1.6522	-8.0161	1.0633
186	H	0.6006	-8.3358	1.104
187	H	2.1483	-8.4316	1.9479
188	H	2.096	-8.4727	0.1707
189	Ga	0.0359	0.1122	-0.1115
190	C	-0.0211	0.3545	-3.1783
191	O	-0.0443	-0.2364	-2.0863
192	C	0.0015	-0.4531	-4.4236
193	C	-0.014	1.8346	-3.2981
194	H	0.2183	-1.502	-4.2062
195	H	-0.1495	2.3365	-2.3349
196	H	0.7307	-0.0463	-5.1354
197	H	-0.9793	-0.3769	-4.9154
198	H	-0.8015	2.1522	-3.9956
199	H	0.9328	2.1432	-3.7666
200	C	-0.0946	0.1424	3.0066
201	O	0.1485	0.5422	1.86
202	C	-0.3186	-1.2903	3.3224
203	C	-0.1451	1.1375	4.1058
204	H	-0.5622	-1.8739	2.4271
205	H	0.2623	2.0985	3.7783
206	H	-1.0972	-1.4076	4.0858
207	H	0.6081	-1.6741	3.7767
208	H	0.376	0.772	4.9989
209	H	-1.1985	1.273	4.3951

[(S,S)-1]$_2$:Mn complex

Number	Label	X	Y	Z
1	S	2.2289	2.1842	-0.7381
2	S	2.5048	-1.6499	0.7281
3	O	1.5899	-0.9795	-0.3193
4	O	5.5504	-0.7303	-3.3228
5	O	5.1858	0.4908	3.1724
6	O	4.7935	2.4022	-1.9829
7	O	1.1847	1.8467	0.344
8	C	4.4006	-0.357	-4.0526
9	H	3.8359	0.431	-3.5285
10	H	3.7444	-1.2212	-4.231
11	H	4.7586	0.0292	-5.0098
12	O	4.987	-2.476	1.8796
13	C	10.8302	-0.5553	2.165
14	C	9.6365	-0.2567	2.8661
15	C	4.0196	0.2209	3.9192
16	H	3.3717	-0.5027	3.3974
17	H	3.4614	1.1449	4.13
18	H	4.3553	-0.2144	4.8633
19	C	11.2417	-0.1475	-1.8494
20	C	3.8252	1.3719	1.3627
21	H	2.8787	1.2721	1.8919
22	C	11.0554	-0.2854	-0.4472
23	C	10.1753	-0.3856	-2.7522
24	C	2.2044	4.6675	0.4589
25	H	2.0901	4.1229	1.3965
26	C	8.4871	0.2517	2.2048
27	C	5.0423	1.0027	1.9312
28	C	11.938	-1.0328	2.8799
29	H	12.8526	-1.2575	2.3346
30	C	2.2428	6.0538	0.4362
31	H	2.1684	6.612	1.3694
32	C	1.4088	-5.4323	-0.2322
33	H	1.2103	-6.0238	-1.1267
34	C	5.3725	-1.1969	-2.0659
35	C	3.8025	1.8404	0.0554
36	C	6.228	1.124	1.1707
37	C	2.2957	3.9746	-0.745
38	C	6.4465	-1.9474	-0.0067
39	H	7.3688	-2.1322	0.5388
40	C	4.1311	-1.3504	-1.4609
41	H	3.2036	-1.0817	-1.9629
42	C	2.3768	6.7529	-0.7701
43	C	11.8704	-1.2248	4.252

44	H	12.7408	-1.597	4.7882
45	C	1.9159	-3.94	2.0669
46	H	2.123	-3.3454	2.9572
47	C	1.3456	-6.0523	1.0241
48	C	1.7398	-4.0915	-0.3519
49	H	1.8078	-3.6131	-1.3297
50	C	8.9011	-0.7838	-2.2692
51	C	2.452	6.0287	-1.9634
52	H	2.5439	6.5635	-2.9085
53	C	6.5412	-1.4618	-1.3188
54	C	10.3928	-0.2256	-4.1275
55	H	9.5672	-0.4092	-4.8123
56	C	10.9226	-0.392	0.7563
57	C	6.1794	1.6166	-0.1391
58	H	7.106	1.6672	-0.7068
59	C	4.0641	-1.7778	-0.1422
60	C	4.9628	1.9673	-0.7137
61	C	5.2042	-2.0965	0.6016
62	C	7.4567	0.6778	1.7204
63	C	12.6897	0.3807	-3.7203
64	H	13.6665	0.6784	-4.0953
65	C	2.0077	-3.364	0.8059
66	C	12.4929	0.2305	-2.3551
67	H	13.3068	0.4093	-1.6551
68	C	9.5845	-0.4661	4.2524
69	H	8.6582	-0.2377	4.7775
70	C	2.4117	4.6384	-1.9613
71	H	2.4767	4.0786	-2.8936
72	C	1.5901	-5.2885	2.1666
73	H	1.5348	-5.7598	3.1473
74	C	11.6376	0.1544	-4.6077
75	H	11.7904	0.2727	-5.6783
76	C	5.9457	2.5104	-2.8065
77	H	5.5916	2.8865	-3.7691
78	H	6.4199	1.5279	-2.9476
79	H	6.6665	3.2209	-2.3815
80	C	7.8134	-1.1327	-1.8533
81	C	1.0168	-7.5089	1.1371
82	H	-0.0697	-7.6739	1.1002
83	H	1.3772	-7.931	2.0822
84	H	1.4572	-8.0842	0.3131
85	C	10.6894	-0.9453	4.9399
86	H	10.6324	-1.0987	6.0153
87	C	6.1127	-2.6865	2.718
88	H	5.7107	-2.9353	3.7027
89	H	6.7228	-1.7757	2.7895

90	H	6.7227	-3.5231	2.3524
91	C	2.4578	8.2484	-0.783
92	H	1.962	8.6709	-1.6657
93	H	3.5046	8.5814	-0.8109
94	H	2.0017	8.6859	0.1132
95	C	-10.9484	0.0504	1.9659
96	S	-2.2161	-2.0587	-0.8594
97	S	-2.8596	2.2452	1.3438
98	O	-1.852	1.2321	0.7925
99	O	-5.2816	0.564	-2.8969
100	O	-5.2192	-0.6427	3.0926
101	O	-4.7767	-2.5517	-2.0625
102	O	-1.1985	-1.6793	0.232
103	C	-4.0234	0.364	-3.506
104	H	-3.406	-0.3374	-2.9238
105	H	-3.4859	1.316	-3.6277
106	H	-4.2247	-0.0674	-4.4895
107	O	-5.5756	2.758	2.1605
108	C	-9.7745	-0.1686	2.7293
109	C	-4.0595	-0.4792	3.8794
110	H	-3.3584	0.2377	3.4244
111	H	-3.5419	-1.437	4.0326
112	H	-4.3953	-0.0876	4.8421
113	C	-11.0369	-0.4801	-2.0559
114	C	-3.8392	-1.4274	1.2605
115	H	-2.8948	-1.2361	1.7677
116	C	-10.9926	-0.2902	-0.648
117	C	-9.9083	-0.1771	-2.859
118	C	-2.1951	-4.6554	0.1046
119	H	-2.366	-4.2257	1.0916
120	C	-8.5687	-0.6126	2.1243
121	C	-5.0694	-1.1495	1.8483
122	C	-12.1153	0.4733	2.6182
123	H	-13.0138	0.6374	2.0266
124	C	-2.0814	-6.0277	-0.0639
125	H	-2.1838	-6.6843	0.8003
126	C	-1.0215	5.1504	-0.7984
127	H	-0.2662	5.2256	-1.5821
128	C	-5.3026	1.1143	-1.6631
129	C	-3.8034	-1.9048	-0.0417
130	C	-6.2546	-1.3505	1.1059
131	C	-2.0998	-3.8348	-1.0158
132	C	-6.7022	1.8508	0.1984
133	H	-7.6996	1.9601	0.6178
134	C	-4.1717	1.4622	-0.9384
135	H	-3.1645	1.2929	-1.3187

136	C	-1.8551	-6.5867	-1.3281
137	C	-12.1255	0.6887	3.9885
138	H	-13.0404	1.0196	4.4754
139	C	-2.9545	4.9802	1.201
140	H	-3.7196	4.8996	1.9739
141	C	-1.6089	6.3193	-0.3095
142	C	-1.374	3.9004	-0.301
143	H	-0.8977	2.9875	-0.6595
144	C	-8.7333	0.3543	-2.2663
145	C	-1.7552	-5.736	-2.4327
146	H	-1.5892	-6.1616	-3.4221
147	C	-6.5788	1.287	-1.0765
148	C	-9.9674	-0.4026	-4.241
149	H	-9.0939	-0.1682	-4.8467
150	C	-10.954	-0.1425	0.5579
151	C	-6.1902	-1.8491	-0.2026
152	H	-7.1203	-1.9706	-0.7524
153	C	-4.3213	1.9854	0.3416
154	C	-4.962	-2.1214	-0.7941
155	C	-5.569	2.2104	0.9248
156	C	-7.5053	-0.9779	1.6614
157	C	-12.235	-1.1925	-4.0385
158	H	-13.1408	-1.5852	-4.4956
159	C	-2.3432	3.8375	0.6909
160	C	-12.1935	-0.9816	-2.6676
161	H	-13.0575	-1.2107	-2.0469
162	C	-9.8041	0.0592	4.1133
163	H	-8.8952	-0.1121	4.6879
164	C	-1.8755	-4.3596	-2.2842
165	H	-1.8182	-3.7013	-3.1509
166	C	-2.5807	6.2166	0.6928
167	H	-3.0474	7.1223	1.0798
168	C	-11.1199	-0.9063	-4.8261
169	H	-11.1521	-1.0742	-5.9005
170	C	-5.9193	-2.6682	-2.8966
171	H	-5.5519	-3.0264	-3.8608
172	H	-6.4082	-1.6916	-3.0253
173	H	-6.6325	-3.3965	-2.4884
174	C	-7.736	0.8144	-1.7458
175	C	-1.1867	7.661	-0.8253
176	H	-0.475	8.1399	-0.1364
177	H	-2.0404	8.3425	-0.9258
178	H	-0.6928	7.5795	-1.8015
179	C	-10.9667	0.4846	4.738
180	H	-10.9726	0.655	5.8124
181	C	-6.784	2.6865	2.9023

182	H	-6.5411	3.0282	3.9107
183	H	-7.1534	1.6519	2.9392
184	H	-7.5523	3.3432	2.4733
185	C	-1.6948	-8.0669	-1.4913
186	H	-0.6307	-8.3463	-1.4842
187	H	-2.1116	-8.4163	-2.4434
188	H	-2.1814	-8.618	-0.6779
189	Mn	-0.1257	0.1605	0.2867
190	C	0.2172	0.4577	3.4006
191	O	0.2676	-0.2572	2.3981
192	C	0.3171	-0.1528	4.7589
193	C	0.0413	1.9394	3.3223
194	H	0.6592	-1.1899	4.6973
195	H	0.0256	2.2898	2.2858
196	H	-0.6783	-0.1343	5.2263
197	H	0.9729	0.4334	5.414
198	H	0.8528	2.4403	3.868
199	H	-0.888	2.2221	3.839
200	C	-0.0188	0.4199	-2.905
201	O	-0.5157	0.6688	-1.8049
202	C	0.3391	-0.976	-3.2925
203	C	0.1988	1.5114	-3.8956
204	H	0.5882	-1.5678	-2.4028
205	H	-0.1665	2.4667	-3.5044
206	H	1.1512	-1.0091	-4.0276
207	H	-0.5447	-1.4201	-3.7762
208	H	-0.3042	1.2718	-4.8424
209	H	1.2713	1.587	-4.1264

[(S,S)-1]$_2$:Sc complex

Number	Label	X	Y	Z
1	S	2.2178	2.2014	-1.0164
2	S	2.6682	-1.792	1.0825
3	O	1.6987	-1.1238	0.068
4	O	5.5032	-0.8226	-3.1238
5	O	5.2081	0.776	2.9877
6	O	4.7315	2.4696	-2.2338
7	O	1.1575	1.7823	0.0467
8	C	4.3184	-0.4884	-3.8173
9	H	3.7923	0.3394	-3.3136
10	H	3.648	-1.3544	-3.9125
11	H	4.6303	-0.1634	-4.8125
12	O	5.2099	-2.3777	2.1582
13	C	10.8568	-0.1584	2.074

14	C	9.659	0.1825	2.7486
15	C	4.0785	0.6915	3.8289
16	H	3.3419	-0.0319	3.4435
17	H	3.6013	1.6745	3.9534
18	H	4.4452	0.3422	4.7966
19	C	11.232	-0.12	-1.9639
20	C	3.8122	1.5494	1.1567
21	H	2.8766	1.4542	1.7062
22	C	11.0713	-0.1266	-0.5522
23	C	10.146	-0.4435	-2.8157
24	C	2.2423	4.7542	0.0597
25	H	2.4293	4.2901	1.028
26	C	8.4988	0.6047	2.0472
27	C	5.0408	1.2327	1.729
28	C	11.9735	-0.5486	2.8267
29	H	12.8913	-0.8065	2.3019
30	C	2.1457	6.1333	-0.0591
31	H	2.2647	6.7583	0.826
32	C	1.2682	-5.418	-0.0259
33	H	0.8198	-5.8802	-0.9067
34	C	5.3881	-1.2494	-1.8475
35	C	3.7749	1.9616	-0.172
36	C	6.2204	1.3413	0.9525
37	C	2.109	3.9762	-1.0876
38	C	6.5781	-1.866	0.1958
39	H	7.5298	-1.9931	0.7058
40	C	4.1786	-1.4355	-1.1923
41	H	3.2243	-1.2439	-1.6785
42	C	1.9195	6.7389	-1.3018
43	C	11.9107	-0.6138	4.2109
44	H	12.7881	-0.9196	4.7766
45	C	2.3835	-4.2402	2.2444
46	H	2.8158	-3.7724	3.1285
47	C	1.482	-6.1931	1.1226
48	C	1.6143	-4.0767	-0.0598
49	H	1.4322	-3.473	-0.9485
50	C	8.8914	-0.8065	-2.2603
51	C	1.7852	5.9286	-2.4342
52	H	1.6156	6.3916	-3.4057
53	C	6.5971	-1.4466	-1.1407
54	C	10.3284	-0.4122	-4.2046
55	H	9.4873	-0.6616	-4.8485
56	C	10.9433	-0.1243	0.6564
57	C	6.1534	1.7685	-0.3781
58	H	7.076	1.8149	-0.9521
59	C	4.1898	-1.8062	0.1474

60	C	4.926	2.0789	-0.9555
61	C	5.3673	-2.0385	0.8615
62	C	7.4608	0.9633	1.5255
63	C	12.6324	0.2307	-3.91
64	H	13.5997	0.4905	-4.3348
65	C	2.1754	-3.507	1.081
66	C	12.4694	0.2104	-2.532
67	H	13.3001	0.4556	-1.8732
68	C	9.6129	0.1035	4.1488
69	H	8.6843	0.365	4.6541
70	C	1.8765	4.5465	-2.3367
71	H	1.7914	3.9197	-3.2237
72	C	2.0392	-5.5875	2.2508
73	H	2.2051	-6.1797	3.1496
74	C	11.5607	-0.0783	-4.7475
75	H	11.6887	-0.0614	-5.8276
76	C	5.8666	2.5408	-3.0865
77	H	5.4923	2.8675	-4.0588
78	H	6.3394	1.5536	-3.1836
79	H	6.5928	3.2719	-2.709
80	C	7.8319	-1.1286	-1.7595
81	C	1.0918	-7.6379	1.1421
82	H	0.0106	-7.7472	1.3139
83	H	1.607	-8.1862	1.9384
84	H	1.3143	-8.1261	0.185
85	C	10.7269	-0.2907	4.8743
86	H	10.675	-0.3438	5.9595
87	C	6.3642	-2.4085	2.9876
88	H	6.0073	-2.6582	3.9888
89	H	6.856	-1.4262	3.0037
90	H	7.0681	-3.1798	2.6496
91	C	1.8052	8.2263	-1.4268
92	H	0.765	8.522	-1.6257
93	H	2.406	8.6013	-2.2645
94	H	2.1305	8.7386	-0.5145
95	C	-10.8406	0.1573	2.0779
96	S	-2.235	-2.2402	-1.0362
97	S	-2.6802	1.8908	1.0673
98	O	-1.7069	1.2027	0.0714
99	O	-5.4725	0.7326	-3.107
100	O	-5.1342	-0.6599	2.9811
101	O	-4.7748	-2.4888	-2.2035
102	O	-1.1495	-1.7642	-0.0269
103	C	-4.2747	0.4781	-3.8115
104	H	-3.6676	-0.2883	-3.3017
105	H	-3.6851	1.3976	-3.9336

106	H	-4.5736	0.1051	-4.7938
107	O	-5.2238	2.4784	2.1162
108	C	-9.6382	-0.126	2.7716
109	C	-3.9882	-0.5633	3.7988
110	H	-3.2497	0.1418	3.3833
111	H	-3.5171	-1.5466	3.9402
112	H	-4.3353	-0.1857	4.7632
113	C	-11.1749	-0.0853	-1.9567
114	C	-3.7795	-1.4888	1.1441
115	H	-2.8345	-1.3908	1.6779
116	C	-11.0322	-0.0039	-0.5455
117	C	-10.0885	0.2301	-2.8113
118	C	-2.1945	-4.696	0.2398
119	H	-2.27	-4.1506	1.1801
120	C	-8.4677	-0.5526	2.0899
121	C	-4.9951	-1.1537	1.7331
122	C	-11.9693	0.5557	2.8077
123	H	-12.8901	0.7695	2.2685
124	C	-2.1408	-6.0817	0.2312
125	H	-2.1849	-6.6255	1.1748
126	C	-1.3459	5.5292	-0.085
127	H	-0.9749	6.0135	-0.9892
128	C	-5.3724	1.2172	-1.8502
129	C	-3.7719	-1.9328	-0.1753
130	C	-6.1923	-1.2911	0.9891
131	C	-2.156	-4.0193	-0.9768
132	C	-6.5813	1.8795	0.1687
133	H	-7.535	1.9997	0.6768
134	C	-4.1696	1.4564	-1.202
135	H	-3.2101	1.2665	-1.6791
136	C	-2.0543	-6.7962	-0.9704
137	C	-11.9148	0.6841	4.1878
138	H	-12.8013	0.9955	4.736
139	C	-2.2871	4.3065	2.239
140	H	-2.654	3.8199	3.1423
141	C	-1.4553	6.2766	1.0969
142	C	-1.7089	4.1929	-0.124
143	H	-1.6105	3.6116	-1.0408
144	C	-8.8527	0.659	-2.2609
145	C	-2.0127	-6.0866	-2.1753
146	H	-1.9496	-6.6334	-3.1154
147	C	-6.5873	1.4113	-1.1522
148	C	-10.2515	0.1221	-4.1989
149	H	-9.4104	0.3656	-4.8452
150	C	-10.9181	0.056	0.663
151	C	-6.1547	-1.7546	-0.3302

152	H	-7.092	-1.8273	-0.8766
153	C	-4.1928	1.8735	0.1238
154	C	-4.9398	-2.0699	-0.9307
155	C	-5.3756	2.1016	0.8291
156	C	-7.4256	-0.9102	1.5755
157	C	-12.537	-0.5813	-3.8984
158	H	-13.4892	-0.8961	-4.32
159	C	-2.1841	3.6009	1.0455
160	C	-12.3933	-0.4848	-2.5215
161	H	-13.2241	-0.7238	-1.8605
162	C	-9.6013	0.015	4.167
163	H	-8.671	-0.2052	4.6883
164	C	-2.0584	-4.6983	-2.1887
165	H	-2.0372	-4.1505	-3.1302
166	C	-1.9261	5.6496	2.2518
167	H	-2.0084	6.2206	3.1755
168	C	-11.4648	-0.2801	-4.7381
169	H	-11.5777	-0.3569	-5.8173
170	C	-5.9293	-2.5844	-3.0277
171	H	-5.5747	-2.9242	-4.0028
172	H	-6.4141	-1.6038	-3.129
173	H	-6.639	-3.3169	-2.6224
174	C	-7.8097	1.0366	-1.7639
175	C	-1.0528	7.7178	1.1156
176	H	0.0421	7.8161	1.0857
177	H	-1.4064	8.2264	2.0189
178	H	-1.4435	8.2533	0.2412
179	C	-10.7275	0.4164	4.8695
180	H	-10.6822	0.5182	5.9515
181	C	-6.377	2.4995	2.9472
182	H	-6.0254	2.7842	3.9409
183	H	-6.8408	1.5047	2.9886
184	H	-7.1027	3.2419	2.5908
185	C	-1.9942	-8.292	-0.9754
186	H	-0.9878	-8.642	-1.2453
187	H	-2.6861	-8.7147	-1.7143
188	H	-2.2419	-8.7127	0.0058
189	Sc	-0.0236	0.0191	0.0592
190	C	0.0529	0.072	3.4055
191	O	-0.0774	-0.0762	2.1851
192	C	0.077	-1.1143	4.2992
193	C	0.1714	1.4333	3.9899
194	H	0.0299	-2.0429	3.7212
195	H	0.3381	2.1853	3.2114
196	H	-0.7686	-1.0637	4.9999
197	H	0.983	-1.0983	4.9193

198	H	0.9698	1.4689	4.7411
199	H	-0.7608	1.6706	4.5253
200	C	-0.0812	0.003	-3.3027
201	O	-0.0661	0.1124	-2.0724
202	C	0.0574	-1.3276	-3.9457
203	C	-0.2335	1.2071	-4.156
204	H	0.4014	-2.0797	-3.2277
205	H	-0.5325	2.0769	-3.5628
206	H	0.7291	-1.2796	-4.8115
207	H	-0.9266	-1.6246	-4.3402
208	H	-0.9454	1.0249	-4.9704
209	H	0.7335	1.4168	-4.6367

[(S,S)-1]$_2$:Zn complex

Number	Label	X	Y	Z
1	S	2.1695	2.0809	-0.8902
2	S	2.5284	-1.6223	0.8125
3	O	1.6463	-1.081	-0.3295
4	O	5.6688	-0.8809	-3.1996
5	O	5.2326	0.7958	3.09
6	O	4.7117	2.3641	-2.1695
7	O	1.1585	1.7151	0.2132
8	C	4.5264	-0.5511	-3.9613
9	H	3.954	0.2587	-3.4786
10	H	3.8792	-1.4285	-4.1069
11	H	4.8928	-0.2087	-4.9319
12	O	5.0276	-2.2684	2.1022
13	C	10.8757	-0.1343	2.2243
14	C	9.6614	0.2114	2.8653
15	C	4.0809	0.516	3.8559
16	H	3.4728	-0.2671	3.3762
17	H	3.4705	1.4183	4.0094
18	H	4.4376	0.156	4.8238
19	C	11.3307	-0.1861	-1.8056
20	C	3.8217	1.5045	1.2455
21	H	2.8877	1.4023	1.7961
22	C	11.1428	-0.1578	-0.3975
23	C	10.2614	-0.5293	-2.6703
24	C	2.0762	4.6329	0.1655
25	H	2.1035	4.1513	1.1428
26	C	8.5131	0.6203	2.1363
27	C	5.0582	1.2229	1.8207
28	C	11.9772	-0.5061	3.0083
29	H	12.9082	-0.7667	2.5087

30	C	2.027	6.0149	0.0534
31	H	2.0255	6.6284	0.9546
32	C	1.4072	-5.4276	0.0034
33	H	1.1349	-6.0264	-0.8671
34	C	5.4733	-1.2639	-1.9169
35	C	3.7646	1.8887	-0.0883
36	C	6.2305	1.3402	1.0388
37	C	2.0997	3.866	-0.995
38	C	6.5139	-1.8429	0.2126
39	H	7.4271	-1.9693	0.7894
40	C	4.2224	-1.3988	-1.3286
41	H	3.3007	-1.1796	-1.8633
42	C	1.9929	6.6357	-1.2014
43	C	11.8834	-0.5505	4.3916
44	H	12.7495	-0.8426	4.9817
45	C	2.075	-3.9047	2.2428
46	H	2.3395	-3.2995	3.1104
47	C	1.421	-6.0285	1.2707
48	C	1.7382	-4.0917	-0.1561
49	H	1.7304	-3.6248	-1.1408
50	C	8.9903	-0.8735	-2.1397
51	C	2.0018	5.837	-2.3496
52	H	1.9734	6.3117	-3.3302
53	C	6.6305	-1.4638	-1.1323
54	C	10.4735	-0.532	-4.0555
55	H	9.6449	-0.7952	-4.7101
56	C	10.9922	-0.1273	0.8082
57	C	6.1467	1.7449	-0.299
58	H	7.0645	1.7949	-0.8805
59	C	4.132	-1.735	0.0146
60	C	4.9111	2.0142	-0.8777
61	C	5.2609	-1.9708	0.8049
62	C	7.4776	0.9763	1.608
63	C	12.7722	0.1152	-3.7309
64	H	13.7485	0.3633	-4.1419
65	C	2.0827	-3.3479	0.9703
66	C	12.5803	0.1283	-2.3567
67	H	13.3976	0.3879	-1.6866
68	C	9.5835	0.1513	4.265
69	H	8.6407	0.413	4.7432
70	C	2.0528	4.4511	-2.2561
71	H	2.073	3.8285	-3.1506
72	C	1.7496	-5.2509	2.3821
73	H	1.7542	-5.7069	3.3715
74	C	11.7168	-0.2124	-4.5819
75	H	11.8659	-0.2215	-5.6595

76	C	5.8519	2.4634	-3.0094
77	H	5.4795	2.7737	-3.9882
78	H	6.3572	1.4904	-3.0989
79	H	6.5543	3.2172	-2.6304
80	C	7.9072	-1.1783	-1.68
81	C	1.0774	-7.4785	1.4194
82	H	-0.0074	-7.6389	1.3346
83	H	1.3943	-7.8732	2.3913
84	H	1.5487	-8.081	0.6326
85	C	10.6822	-0.2258	5.0221
86	H	10.6047	-0.2644	6.1065
87	C	6.1422	-2.4085	2.9692
88	H	5.7277	-2.6068	3.9602
89	H	6.7364	-1.4844	2.999
90	H	6.7729	-3.2535	2.6632
91	C	1.9289	8.1271	-1.3247
92	H	0.9287	8.4514	-1.6463
93	H	2.6397	8.4969	-2.0742
94	H	2.1476	8.6223	-0.3716
95	C	-10.8503	-0.0174	2.1845
96	S	-2.1895	-2.1374	-1.0724
97	S	-2.6547	1.9065	1.0064
98	O	-1.7238	1.2276	-0.0027
99	O	-5.5757	0.7759	-3.0775
100	O	-5.1441	-0.7532	2.9491
101	O	-4.7619	-2.4799	-2.2741
102	O	-1.1584	-1.7154	-0.0134
103	C	-4.3857	0.4908	-3.7861
104	H	-3.8177	-0.3127	-3.2914
105	H	-3.7536	1.3843	-3.8866
106	H	-4.6966	0.1542	-4.778
107	O	-5.2406	2.4209	2.1809
108	C	-9.6255	-0.3148	2.8312
109	C	-3.9879	-0.6448	3.7513
110	H	-3.2702	0.0767	3.3318
111	H	-3.4918	-1.6185	3.8734
112	H	-4.3263	-0.2851	4.7258
113	C	-11.2623	-0.0975	-1.8499
114	C	-3.7842	-1.5028	1.0832
115	H	-2.8324	-1.3821	1.6
116	C	-11.0997	-0.0721	-0.4386
117	C	-10.1881	0.2556	-2.705
118	C	-2.1092	-4.6318	0.1177
119	H	-2.1842	-4.1055	1.0688
120	C	-8.469	-0.6994	2.1023
121	C	-5.0044	-1.2162	1.6878

122	C	-11.9622	0.3377	2.9612
123	H	-12.9004	0.5615	2.4571
124	C	-2.0258	-6.0155	0.0814
125	H	-2.0551	-6.5797	1.014
126	C	-1.3467	5.4706	-0.3896
127	H	-0.8398	5.8516	-1.2779
128	C	-5.4554	1.2259	-1.8083
129	C	-3.7669	-1.9224	-0.2406
130	C	-6.1991	-1.3673	0.9458
131	C	-2.1	-3.9268	-1.0826
132	C	-6.6208	1.8373	0.2486
133	H	-7.5662	1.941	0.7756
134	C	-4.2414	1.4564	-1.1757
135	H	-3.2853	1.2816	-1.6662
136	C	-1.9159	-6.7029	-1.1339
137	C	-11.8701	0.4111	4.3434
138	H	-12.7439	0.6904	4.9283
139	C	-2.6278	4.5088	1.8933
140	H	-3.1339	4.1238	2.7779
141	C	-1.6906	6.3601	0.6357
142	C	-1.6299	4.1161	-0.2894
143	H	-1.3506	3.4174	-1.0779
144	C	-8.9454	0.6702	-2.1579
145	C	-1.9029	-5.9676	-2.3223
146	H	-1.8234	-6.4913	-3.2746
147	C	-6.6551	1.3989	-1.0826
148	C	-10.37	0.1985	-4.0934
149	H	-9.538	0.4689	-4.7409
150	C	-10.9633	-0.0607	0.769
151	C	-6.1536	-1.8028	-0.385
152	H	-7.0908	-1.8795	-0.9315
153	C	-4.2343	1.8467	0.1558
154	C	-4.9333	-2.0811	-0.9928
155	C	-5.4035	2.0554	0.8891
156	C	-7.4356	-1.0253	1.5506
157	C	-12.6492	-0.5249	-3.7909
158	H	-13.6057	-0.8274	-4.2118
159	C	-2.2746	3.6555	0.8548
160	C	-12.4869	-0.4799	-2.4136
161	H	-13.3079	-0.747	-1.751
162	C	-9.551	-0.2288	4.2298
163	H	-8.6024	-0.4558	4.714
164	C	-1.9948	-4.5803	-2.3056
165	H	-1.9992	-4.0134	-3.2359
166	C	-2.3346	5.8628	1.7713
167	H	-2.6061	6.547	2.5746

168	C	-11.5886	-0.1886	-4.632
169	H	-11.7145	-0.2259	-5.712
170	C	-5.9143	-2.5774	-3.0957
171	H	-5.5598	-2.8993	-4.0772
172	H	-6.4104	-1.6008	-3.1832
173	H	-6.6184	-3.3213	-2.7001
174	C	-7.8921	1.0356	-1.6737
175	C	-1.3459	7.8132	0.5222
176	H	-0.2773	7.9792	0.726
177	H	-1.9141	8.4223	1.2342
178	H	-1.5414	8.1941	-0.4884
179	C	-10.6607	0.131	4.9795
180	H	-10.585	0.1909	6.063
181	C	-6.3854	2.415	3.0193
182	H	-6.0296	2.677	4.018
183	H	-6.845	1.4171	3.0402
184	H	-7.1203	3.1607	2.6882
185	C	-1.7869	-8.1948	-1.1621
186	H	-0.7349	-8.4941	-1.279
187	H	-2.3373	-8.6311	-2.0043
188	H	-2.1573	-8.6501	-0.236
189	Zn	-0.065	0.0347	0.0039
190	C	0.0369	0.2687	3.1867
191	O	0.0098	-0.3235	2.1082
192	C	0.0564	-0.507	4.4606
193	C	0.0391	1.7594	3.2793
194	H	-0.1217	-1.5693	4.271
195	H	0.3951	2.2159	2.3474
196	H	-0.6864	-0.1106	5.1654
197	H	1.0349	-0.3801	4.9465
198	H	0.635	2.102	4.1336
199	H	-0.9938	2.0923	3.4704
200	C	0.2604	-0.0117	-3.1812
201	O	-0.1515	0.4177	-2.1055
202	C	0.5993	-1.4504	-3.3867
203	C	0.4172	0.9154	-4.3409
204	H	0.7011	-1.9696	-2.4278
205	H	-0.096	1.8631	-4.1498
206	H	1.5126	-1.5618	-3.9851
207	H	-0.209	-1.9118	-3.973
208	H	0.0555	0.4598	-5.2707
209	H	1.4892	1.1176	-4.4871

[(S,S)-2]$_2$:Zn complex

Number	Label	X	Y	Z
1	S	-2.0527	0.0563	-2.014
2	S	-2.781	-0.8029	2.3231
3	O	-1.7298	-0.1476	1.4288
4	O	-5.2057	3.1491	0.0652
5	O	-5.2106	-3.3745	0.2489
6	O	-4.5549	1.2311	-2.7097
7	O	-1.0603	-0.8908	-1.3178
8	C	-3.9412	3.6046	-0.3764
9	H	-3.4586	2.8581	-1.028
10	H	-3.2774	3.8376	0.4691
11	H	-4.1322	4.5153	-0.949
12	O	-5.486	-1.5431	2.9582
13	C	-11.0097	-2.2838	-0.3257
14	C	-9.8392	-2.9058	0.1415
15	C	-4.0795	-4.0914	0.6969
16	H	-3.4169	-3.4539	1.303
17	H	-3.5108	-4.5088	-0.1461
18	H	-4.4602	-4.9061	1.3168
19	C	-11.0478	2.5333	-0.4647
20	C	-3.7493	-1.8146	-0.9029
21	H	-2.8229	-2.3053	-0.6073
22	C	-9.8621	3.2754	-0.3268
23	C	-1.9228	-1.7205	-4.1246
24	H	-1.9763	-2.5046	-3.3701
25	C	-8.5574	-2.4339	-0.2481
26	C	-5.0032	-2.2917	-0.5297
27	C	-12.2533	-2.7606	0.0484
28	H	-13.1603	-2.2854	-0.3209
29	C	-1.8421	-2.0335	-5.4736
30	H	-1.8496	-3.079	-5.783
31	C	-1.359	1.4737	5.3456
32	H	-0.7328	2.3606	5.4553
33	C	-5.2394	2.0202	0.8083
34	C	-3.6631	-0.6455	-1.647
35	C	-6.1604	-1.5953	-0.9493
36	C	-1.9436	-0.3809	-3.7482
37	C	-6.6337	0.3276	1.8818
38	H	-7.6313	-0.0481	2.0957
39	C	-4.1066	1.3275	1.2171
40	H	-3.102	1.6475	0.9446
41	C	-1.7624	-1.0297	-6.4464
42	C	-12.3637	-3.874	0.8991
43	C	-2.92	-0.8221	5.0763

44	H	-3.5257	-1.7207	4.9618
45	C	-1.8441	0.8321	6.4896
46	C	-1.6455	0.9914	4.0751
47	H	-1.2577	1.4788	3.1796
48	C	-8.688	2.666	0.1923
49	C	-1.7777	0.3067	-6.0363
50	H	-1.7217	1.0963	-6.7854
51	C	-6.5165	1.5083	1.1336
52	C	-9.8518	4.6265	-0.713
53	H	-8.9337	5.2014	-0.609
54	C	-6.0425	-0.4195	-1.7025
55	H	-6.9528	0.1067	-1.9797
56	C	-4.2532	0.1502	1.9345
57	C	-4.7902	0.0792	-2.0409
58	C	-5.4992	-0.3735	2.2805
59	C	-7.447	-2.0575	-0.5715
60	C	-12.1814	4.4806	-1.3509
61	C	-2.4275	-0.1519	3.9609
62	C	-12.1883	3.1268	-0.9732
63	H	-13.1048	2.5516	-1.0933
64	C	-9.9496	-4.0156	0.9973
65	H	-9.0435	-4.5004	1.3569
66	C	-1.8686	0.6394	-4.6901
67	H	-1.8991	1.6827	-4.3789
68	C	-2.6301	-0.315	6.3369
69	H	-3.0107	-0.823	7.2229
70	C	-10.9952	5.2212	-1.2155
71	H	-10.9864	6.2693	-1.508
72	C	-5.6646	2.0593	-3.0228
73	H	-5.252	2.9346	-3.5297
74	H	-6.1858	2.3796	-2.1084
75	H	-6.3619	1.5457	-3.6973
76	C	-7.6836	2.1467	0.6397
77	C	-1.5025	1.3386	7.8574
78	H	-0.7122	0.727	8.3162
79	H	-2.3684	1.2983	8.5298
80	H	-1.1409	2.3739	7.8262
81	C	-11.1928	-4.492	1.3709
82	H	-11.2752	-5.3547	2.0291
83	C	-6.7241	-2.208	3.1515
84	H	-6.4838	-3.1691	3.6112
85	H	-7.2298	-2.3757	2.1899
86	H	-7.3776	-1.6345	3.8225
87	C	-1.641	-1.3728	-7.8994
88	H	-0.6089	-1.2283	-8.2504
89	H	-2.2802	-0.7308	-8.518

90	H	-1.9123	-2.4169	-8.0937
91	S	2.1114	1.1602	2.1832
92	S	2.6412	-1.3925	-1.0667
93	O	1.7056	-0.1951	-0.7965
94	O	5.7061	2.75	-1.2562
95	O	5.2022	-2.9772	1.8017
96	O	4.647	2.495	2.2041
97	O	1.1235	-0.0169	2.0882
98	C	4.5524	3.5606	-1.1784
99	H	3.9364	3.2927	-0.3051
100	H	3.9485	3.4796	-2.0937
101	H	4.9076	4.588	-1.0694
102	O	5.1395	-2.7323	-1.4397
103	C	4.0617	-3.8069	1.7343
104	H	3.4129	-3.5251	0.8885
105	H	3.4897	-3.7738	2.6732
106	H	4.4341	-4.8219	1.577
107	C	3.778	-1.0317	2.1002
108	H	2.8436	-1.5914	2.1202
109	C	2.0436	0.7365	4.9165
110	H	2.0845	-0.327	4.6796
111	C	8.4967	-1.9406	1.286
112	C	5.0179	-1.6478	1.9516
113	C	1.9865	1.176	6.2315
114	H	1.9938	0.4492	7.0436
115	C	1.5865	-1.5877	-4.9757
116	H	1.3188	-0.9051	-5.7838
117	C	5.5278	1.4127	-1.3457
118	C	3.7138	0.354	2.1812
119	C	6.1829	-0.8507	1.9017
120	C	2.0374	1.6807	3.8938
121	C	6.602	-0.7747	-1.4652
122	H	7.5227	-1.3529	-1.4807
123	C	4.284	0.7919	-1.3409
124	H	3.355	1.3519	-1.2584
125	C	1.9283	2.542	6.5351
126	C	2.2408	-3.3492	-2.9156
127	H	2.5085	-4.0238	-2.1015
128	C	1.6262	-2.9662	-5.2296
129	C	1.8861	-1.0836	-3.7194
130	H	1.867	-0.0109	-3.525
131	C	9.0237	1.8149	-1.0584
132	C	1.9037	3.4656	5.4849
133	H	1.8473	4.5303	5.7103
134	C	6.6982	0.6215	-1.3866
135	C	6.0927	0.5423	2.0211

136	H	7.0114	1.1213	1.9682
137	C	4.2167	-0.5935	-1.3724
138	C	4.8541	1.1599	2.144
139	C	5.3577	-1.3982	-1.4417
140	C	7.438	-1.4463	1.6208
141	C	2.222	-1.9764	-2.7041
142	C	1.9548	3.0431	4.1616
143	H	1.9408	3.7652	3.3454
144	C	1.9487	-3.8356	-4.1859
145	H	1.976	-4.9086	-4.3733
146	C	5.7816	3.3406	2.0957
147	H	5.4015	4.3637	2.1361
148	H	6.2996	3.1764	1.1391
149	H	6.4761	3.1756	2.9296
150	C	7.964	1.2474	-1.2433
151	C	1.3123	-3.4932	-6.5957
152	H	0.2254	-3.5573	-6.7535
153	H	1.7241	-4.4976	-6.7457
154	H	1.7099	-2.8361	-7.3791
155	C	6.2549	-3.5922	-1.2592
156	H	5.8532	-4.6082	-1.2618
157	H	6.745	-3.3896	-0.2964
158	H	6.9742	-3.4868	-2.0821
159	C	1.9051	3.0145	7.9564
160	H	1.1599	3.807	8.1033
161	H	2.8782	3.4356	8.2441
162	H	1.6815	2.1978	8.6524
163	Zn	0.0035	-0.3645	0.3757
164	C	-13.6412	-4.3794	1.2597
165	C	-14.7356	-4.8244	1.5465
166	C	-16.0106	-5.3668	1.8572
167	C	-16.1116	-6.6306	2.4551
168	H	-15.1974	-7.1716	2.6921
169	H	-17.4126	-8.1694	3.1956
170	C	-17.352	-7.1863	2.7335
171	C	-18.5171	-6.4883	2.4169
172	H	-19.4909	-6.9242	2.6299
173	H	-19.3418	-4.6797	1.5829
174	C	-18.438	-5.2338	1.829
175	C	-17.1948	-4.6525	1.545
176	C	-16.8297	4.0708	-2.2116
177	C	-16.8669	2.9546	-1.731
178	C	-16.921	1.6486	-1.1733
179	C	-15.9118	1.2004	-0.3041
180	H	-15.096	1.8732	-0.0457
181	H	-15.1812	-0.4162	0.9102

182	C	-15.9615	-0.0735	0.2331
183	C	-17.0258	-0.9366	-0.0774
184	H	-18.868	-1.1498	-1.1791
185	C	-18.0401	-0.4858	-0.9389
186	C	-17.9873	0.7863	-1.48
187	C	-13.3643	5.0803	-1.8583
188	C	-14.3919	5.569	-2.286
189	C	-15.5949	6.1269	-2.7924
190	C	-16.7996	5.3785	-2.7659
191	H	-18.8882	5.367	-3.2667
192	C	-17.9684	5.9483	-3.2888
193	C	-17.9563	7.2295	-3.8214
194	H	-18.8741	7.6558	-4.2209
195	H	-16.7624	8.9728	-4.2575
196	C	-16.7731	7.9674	-3.8419
197	C	-15.6041	7.42	-3.3331
198	H	-10.928	-1.4286	-0.9938
199	H	-11.0572	1.4862	-0.1686
200	C	-17.0788	-2.2437	0.4793
201	C	-17.1273	-3.3583	0.962
202	H	-18.7723	1.1305	-2.1505
203	H	-14.6754	7.9874	-3.3478
204	C	11.4805	2.0536	-1.1632
205	C	10.2148	2.5483	-0.8058
206	C	10.707	-1.7739	0.2332
207	C	9.6959	-2.5471	0.8284
208	C	12.621	2.7941	-0.9019
209	H	13.6005	2.4145	-1.19
210	C	12.5301	4.0481	-0.273
211	C	9.8665	-3.9381	0.932
212	H	9.0809	-4.5367	1.39
213	C	12.0332	-3.7662	-0.1358
214	C	11.8592	-2.3754	-0.2429
215	H	12.6356	-1.776	-0.715
216	C	10.1247	3.8051	-0.1817
217	H	9.1444	4.1901	0.0936
218	C	11.0183	-4.5375	0.4583
219	H	11.1513	-5.6144	0.5403
220	C	11.2635	4.5426	0.0819
221	H	11.1887	5.514	0.5667
222	C	13.6977	4.8103	-0.0017
223	C	14.6909	5.4723	0.2289
224	C	15.8786	6.2113	0.4754
225	C	15.8241	7.5744	0.7938
226	H	14.8515	8.0581	0.8622
227	H	16.9299	9.3538	1.2627

228	C	16.9887	8.2958	1.0161
229	C	18.2301	7.6673	0.9212
230	H	19.1433	8.2326	1.0946
231	H	19.2701	5.8183	0.5383
232	C	18.3053	6.3168	0.6096
233	C	17.1418	5.5704	0.3866
234	C	16.696	-3.718	-1.4864
235	C	16.8252	-2.5328	-1.2503
236	C	16.9403	-1.147	-0.9645
237	C	15.9158	-0.4896	-0.2618
238	H	15.0521	-1.063	0.0711
239	H	15.218	1.3754	0.5533
240	C	16.0091	0.8634	0.0068
241	C	17.1293	1.5986	-0.4191
242	H	19.0294	1.5051	-1.4342
243	C	18.159	0.9389	-1.109
244	C	18.0654	-0.4151	-1.3784
245	C	13.2049	-4.4077	-0.6218
246	C	14.1796	-5.0126	-1.0255
247	C	15.2989	-5.7446	-1.5062
248	C	16.5409	-5.1042	-1.7467
249	H	18.5671	-5.3587	-2.4129
250	C	17.6175	-5.8589	-2.2324
251	C	17.4798	-7.2184	-2.4723
252	H	18.3269	-7.7891	-2.8468
253	H	16.1501	-8.9166	-2.4154
254	C	16.2603	-7.8502	-2.2301
255	C	15.1819	-7.1198	-1.7521
256	H	11.5571	1.0862	-1.6579
257	H	10.5661	-0.6969	0.1482
258	C	17.1947	2.9925	-0.1529
259	C	17.2047	4.1831	0.0903
260	H	18.8621	-0.9241	-1.9174
261	H	14.2256	-7.6045	-1.5642
262	C	0.1926	-3.2757	1.5852
263	O	0.2702	-2.4652	0.6614
264	C	-0.0201	-2.8593	3.0045
265	C	0.2932	-4.7379	1.3032
266	H	0.0645	-1.774	3.1233
267	H	0.5471	-4.9157	0.2542
268	H	0.7077	-3.3596	3.657
269	H	-1.0112	-3.2041	3.3377
270	H	-0.6704	-5.2156	1.5314
271	H	1.0315	-5.2124	1.9621
272	C	0.1551	2.7502	-0.4173
273	O	-0.2097	1.7859	0.2522

274	C	0.2466	4.1024	0.2078
275	C	0.5123	2.6279	-1.8604
276	H	-0.2777	4.1204	1.1685
277	H	0.6952	1.5823	-2.1311
278	H	-0.1403	4.881	-0.461
279	H	1.3097	4.333	0.3789
280	H	1.382	3.2491	-2.1087
281	H	-0.3261	3.0238	-2.4523

[(S,S)-2]$_2$:Zn complex

Number	Label	X	Y	Z
1	S	-2.1333	0.3945	-2.1418
2	S	-2.8324	-0.9526	2.3926
3	O	-1.7805	-0.3017	1.4537
4	O	-5.3943	3.0556	0.3261
5	O	-5.1343	-3.3072	-0.0478
6	O	-4.643	1.5033	-2.6911
7	O	-1.0671	-0.4846	-1.4262
8	C	-4.1675	3.6725	-0.0023
9	H	-3.5526	3.0232	-0.6455
10	H	-3.6025	3.9379	0.9022
11	H	-4.4217	4.5823	-0.5507
12	O	-5.4535	-1.7745	2.9778
13	C	-10.9531	-2.2619	-0.399
14	C	-9.7736	-2.939	-0.0446
15	C	-3.9858	-4.0167	0.3634
16	H	-3.3906	-3.4189	1.07
17	H	-3.3648	-4.3066	-0.4962
18	H	-4.3461	-4.9146	0.87
19	C	-11.177	2.4177	-0.2013
20	C	-3.7207	-1.6068	-1.0511
21	H	-2.7834	-2.0964	-0.7872
22	C	-9.9662	3.1199	-0.0768
23	C	-1.9692	-1.3838	-4.2604
24	H	-2.0403	-2.1887	-3.5295
25	C	-8.5032	-2.419	-0.4095
26	C	-4.9586	-2.1507	-0.7191
27	C	-12.1885	-2.7754	-0.0474
28	H	-13.1029	-2.2539	-0.3251
29	C	-1.8672	-1.6689	-5.6135
30	H	-1.8797	-2.7077	-5.9434
31	C	-1.4662	1.214	5.5234
32	H	-1.0534	2.2051	5.7126
33	C	-5.3591	1.8957	1.0166
34	C	-3.6824	-0.3894	-1.725

35	C	-6.1421	-1.4588	-1.0736
36	C	-1.9825	-0.0492	-3.8609
37	C	-6.6806	0.0881	1.9897
38	H	-7.6588	-0.3432	2.1861
39	C	-4.1933	1.2461	1.3998
40	H	-3.2124	1.6529	1.1597
41	C	-1.7654	-0.6464	-6.566
42	C	-12.2802	-3.9841	0.6646
43	C	-2.5112	-1.3313	5.0596
44	H	-2.9122	-2.3261	4.8673
45	C	-1.6431	0.3312	6.596
46	C	-1.8153	0.8518	4.2305
47	H	-1.6697	1.541	3.3984
48	C	-8.8013	2.4732	0.4153
49	C	-1.7772	0.6824	-6.1317
50	H	-1.7049	1.4853	-6.8645
51	C	-6.6146	1.3071	1.3055
52	C	-9.918	4.4747	-0.4479
53	H	-8.9797	5.0178	-0.3528
54	C	-6.0688	-0.2305	-1.74
55	H	-6.996	0.2871	-1.9738
56	C	-4.2892	0.0197	2.0529
57	C	-4.8352	0.3211	-2.0676
58	C	-5.515	-0.5779	2.3593
59	C	-7.4079	-1.9888	-0.717
60	C	-12.2612	4.4103	-1.0467
61	C	-2.3447	-0.4196	4.0201
62	C	-12.3057	3.0525	-0.6855
63	H	-13.2419	2.5076	-0.797
64	C	-9.8652	-4.1447	0.6722
65	H	-8.9533	-4.6739	0.9432
66	C	-1.8862	0.99	-4.7817
67	H	-1.9162	2.0268	-4.4499
68	C	-2.164	-0.9423	6.3462
69	H	-2.2965	-1.6382	7.1738
70	C	-11.05	5.1118	-0.9222
71	H	-11.0134	6.1627	-1.2019
72	C	-5.78	2.3306	-2.9053
73	H	-5.3983	3.2602	-3.3322
74	H	-6.2876	2.5421	-1.9531
75	H	-6.4768	1.8635	-3.6126
76	C	-7.7982	1.9341	0.8417
77	C	-1.2784	0.7305	7.9918
78	H	-0.4258	0.1443	8.3611
79	H	-2.1096	0.5466	8.6841
80	H	-1.0134	1.7922	8.0547

81	C	-11.1003	-4.6594	1.0212
82	H	-11.1696	-5.5962	1.5704
83	C	-6.646	-2.542	3.0729
84	H	-6.3481	-3.5092	3.4826
85	H	-7.0976	-2.6836	2.0805
86	H	-7.3662	-2.0665	3.7508
87	C	-1.6224	-0.963	-8.0219
88	H	-0.5865	-0.8012	-8.3536
89	H	-2.2585	-0.3149	-8.637
90	H	-1.8808	-2.0057	-8.2379
91	S	2.1237	1.3432	2.2669
92	S	2.7075	-1.3453	-1.0728
93	O	1.7472	-0.165	-0.7228
94	O	5.7825	2.8135	-1.1126
95	O	5.173	-2.838	1.8589
96	O	4.6332	2.6273	2.3086
97	O	1.0858	0.1859	2.118
98	C	4.6423	3.6464	-1.0823
99	H	3.9896	3.4041	-0.2273
100	H	4.0719	3.566	-2.0187
101	H	5.0145	4.6675	-0.9716
102	O	5.1743	-2.6562	-1.3987
103	C	4.0324	-3.6662	1.7858
104	H	3.3975	-3.386	0.9298
105	H	3.4456	-3.6213	2.7144
106	H	4.404	-4.6831	1.6412
107	C	3.7498	-0.8952	2.1605
108	H	2.8236	-1.4667	2.1815
109	C	2.1326	0.9255	5.0063
110	H	2.3489	-0.122	4.7976
111	C	8.4634	-1.8419	1.39
112	C	4.9895	-1.511	2.0152
113	C	1.9962	1.374	6.3122
114	H	2.1134	0.6702	7.1358
115	C	1.5295	-1.2978	-4.9436
116	H	1.2081	-0.5706	-5.6909
117	C	5.5901	1.4825	-1.2373
118	C	3.6938	0.4922	2.2575
119	C	6.1598	-0.7177	1.9797
120	C	1.993	1.8442	3.9688
121	C	6.6518	-0.71	-1.3932
122	H	7.5672	-1.2961	-1.4174
123	C	4.3405	0.8742	-1.259
124	H	3.4205	1.4477	-1.1785
125	C	1.7233	2.7188	6.5914
126	C	2.3318	-3.1753	-3.041

127	H	2.6613	-3.8966	-2.2924
128	C	1.6323	-2.6497	-5.303
129	C	1.8413	-0.8731	-3.6621
130	H	1.7831	0.1809	-3.3919
131	C	9.0982	1.8521	-1.0026
132	C	1.5777	3.6146	5.5264
133	H	1.3641	4.6626	5.7339
134	C	6.7563	0.6829	-1.2941
135	C	6.0749	0.673	2.1091
136	H	6.9949	1.2505	2.0657
137	C	4.2678	-0.5122	-1.3183
138	C	4.8373	1.2947	2.2331
139	C	5.4032	-1.3251	-1.3854
140	C	7.4108	-1.3258	1.7112
141	C	2.2476	-1.8234	-2.7269
142	C	1.7085	3.1854	4.2126
143	H	1.6037	3.887	3.3864
144	C	2.0289	-3.5774	-4.3374
145	H	2.1069	-4.6296	-4.6073
146	C	5.7722	3.4743	2.2237
147	H	5.3912	4.4965	2.2663
148	H	6.3038	3.3151	1.2741
149	H	6.4509	3.3	3.0681
150	C	8.0273	1.2986	-1.1621
151	C	1.3178	-3.0859	-6.6997
152	H	0.2312	-3.1445	-6.8596
153	H	1.7359	-4.0749	-6.9175
154	H	1.7103	-2.3741	-7.4365
155	C	6.2817	-3.5278	-1.2064
156	H	5.869	-4.5388	-1.2033
157	H	6.7692	-3.3224	-0.243
158	H	7.0043	-3.4335	-2.027
159	C	1.5882	3.2038	8.0014
160	H	0.6249	3.7092	8.1546
161	H	2.3698	3.9367	8.2406
162	H	1.6627	2.3833	8.7235
163	Sc	-0.0473	-0.2455	0.3957
164	C	-13.5493	-4.5249	1.0012
165	C	-14.6374	-4.9972	1.2668
166	C	-15.9068	-5.5672	1.5496
167	C	-15.9954	-6.8575	2.0898
168	H	-15.076	-7.3983	2.306
169	H	-17.2817	-8.4413	2.7574
170	C	-17.2305	-7.4384	2.3389
171	C	-18.4019	-6.7396	2.049
172	H	-19.3718	-7.1947	2.2385

173	H	-19.244	-4.9047	1.2939
174	C	-18.3348	-5.4591	1.5183
175	C	-17.0974	-4.8518	1.2662
176	C	-16.8775	4.0816	-1.9743
177	C	-16.8994	2.9376	-1.5636
178	C	-16.9295	1.5981	-1.0888
179	C	-15.9855	1.1545	-0.1471
180	H	-15.2476	1.8579	0.2352
181	H	-15.2732	-0.492	1.0382
182	C	-16.0049	-0.1522	0.3072
183	C	-16.9774	-1.0532	-0.1584
184	H	-18.6835	-1.3019	-1.4539
185	C	-17.9274	-0.6076	-1.0926
186	C	-17.9023	0.6969	-1.5528
187	C	-13.4315	5.0549	-1.5262
188	C	-14.4499	5.5817	-1.9296
189	C	-15.6477	6.1739	-2.4083
190	C	-16.8505	5.4227	-2.4431
191	H	-18.9338	5.4402	-2.9654
192	C	-18.0149	6.0227	-2.9402
193	C	-17.9999	7.3369	-3.3861
194	H	-18.9144	7.787	-3.7667
195	H	-16.8076	9.1084	-3.6918
196	C	-16.8189	8.0775	-3.3446
197	C	-15.6536	7.5	-2.8611
198	H	-10.8841	-1.3335	-0.9622
199	H	-11.2171	1.3697	0.0881
200	C	-17.0087	-2.3913	0.3222
201	C	-17.0424	-3.5298	0.7465
202	H	-18.6373	1.0367	-2.2798
203	H	-14.726	8.0683	-2.8293
204	C	11.5557	2.0292	-1.1583
205	C	10.3097	2.563	-0.7877
206	C	10.6783	-1.7552	0.3341
207	C	9.6517	-2.4853	0.9555
208	C	12.7178	2.7479	-0.9367
209	H	13.6826	2.3397	-1.2356
210	C	12.6683	4.0181	-0.3358
211	C	9.7909	-3.8757	1.1078
212	H	8.9928	-4.4394	1.5878
213	C	11.9579	-3.7886	0.0313
214	C	11.8152	-2.3986	-0.1237
215	H	12.603	-1.8341	-0.619
216	C	10.2605	3.8352	-0.191
217	H	9.2948	4.2494	0.0935
218	C	10.9282	-4.5163	0.6541

219	H	11.0383	-5.5922	0.7732
220	C	11.4213	4.5511	0.033
221	H	11.3795	5.535	0.4958
222	C	13.8609	4.7565	-0.1129
223	C	14.8823	5.3906	0.0669
224	C	16.1007	6.0973	0.2502
225	C	16.1001	7.4752	0.5017
226	H	15.1463	7.9951	0.5701
227	H	17.2768	9.2369	0.8494
228	C	17.2936	8.1665	0.6557
229	C	18.5099	7.491	0.56
230	H	19.4464	8.0318	0.6791
231	H	19.4771	5.5906	0.244
232	C	18.5316	6.1249	0.3152
233	C	17.3385	5.4088	0.16
234	C	16.6219	-3.9293	-1.3626
235	C	16.7849	-2.7402	-1.1712
236	C	16.9369	-1.3484	-0.9351
237	C	15.9327	-0.642	-0.2508
238	H	15.0572	-1.1819	0.1062
239	H	15.2848	1.2659	0.5036
240	C	16.0606	0.7168	-0.0287
241	C	17.1965	1.409	-0.4838
242	H	19.0885	1.2334	-1.5034
243	C	18.206	0.7005	-1.1551
244	C	18.0776	-0.6592	-1.3785
245	C	13.1119	-4.474	-0.4361
246	C	14.0683	-5.1171	-0.8236
247	C	15.1574	-5.9044	-1.2857
248	C	16.4176	-5.3187	-1.5666
249	H	18.4241	-5.6738	-2.246
250	C	17.4595	-6.1312	-2.0342
251	C	17.2693	-7.4934	-2.2172
252	H	18.0903	-8.1088	-2.5786
253	H	15.8817	-9.1394	-2.0755
254	C	16.0318	-8.0711	-1.9346
255	C	14.9872	-7.2833	-1.4734
256	H	11.5999	1.0505	-1.6339
257	H	10.5621	-0.6788	0.2131
258	C	17.2995	2.8095	-0.2688
259	C	17.3486	4.0082	-0.0749
260	H	18.8589	-1.205	-1.9038
261	H	14.0169	-7.7249	-1.2544
262	C	0.1239	-3.5261	0.8861
263	O	0.1976	-2.3776	0.4312
264	C	-0.0495	-3.7689	2.3416

265	C	0.221	-4.6887	-0.0318
266	H	0.0482	-2.8437	2.9189
267	H	0.1632	-4.3708	-1.0771
268	H	0.6756	-4.5141	2.6935
269	H	-1.0405	-4.2138	2.5143
270	H	-0.557	-5.4284	0.1959
271	H	1.184	-5.1937	0.1384
272	C	0.0265	2.9378	-0.3553
273	O	-0.2896	1.9113	0.2619
274	C	-0.1293	4.2634	0.2913
275	C	0.5611	2.8772	-1.7387
276	H	-0.7233	4.19	1.2063
277	H	0.8725	1.8594	-1.9982
278	H	-0.5657	4.9909	-0.4035
279	H	0.8734	4.6411	0.5419
280	H	1.3821	3.5909	-1.8743
281	H	-0.2361	3.205	-2.423

Atomic coordinates of the DFT optimized structures used to calculate vibrational spectra

Atomic coordinates of compound (*S*,*S*)-1 (Structure detailed in Figure S20)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.499542	2.322061	0.761288
2	16	0	-2.433834	-1.435496	-1.034491
3	8	0	-1.480468	-1.106886	0.170279
4	8	0	-5.485989	-1.945547	3.142000
5	8	0	-5.885414	1.638646	-3.137131
6	8	0	-4.904437	1.902992	2.315304
7	8	0	-1.486214	1.875807	-0.339045
8	6	0	-4.336408	-1.948517	3.977355
9	1	0	-3.754504	-1.024372	3.862558
10	1	0	-3.691301	-2.810806	3.769253
11	1	0	-4.709108	-2.015198	4.999791
12	8	0	-4.936132	-1.858918	-2.371078
13	6	0	-11.377641	-0.024434	-1.760548
14	6	0	-10.327671	0.625458	-2.470702
15	6	0	-4.845079	1.880604	-4.075129
16	1	0	-4.042146	1.138312	-3.979674
17	1	0	-4.429703	2.889574	-3.960970
18	1	0	-5.303654	1.791748	-5.060139
19	6	0	-11.287740	-1.406014	2.048993
20	6	0	-4.329799	1.987681	-1.296081
21	1	0	-3.475886	2.141934	-1.942821
22	6	0	-11.208976	-0.917956	0.714698
23	6	0	-10.144901	-1.896037	2.744483
24	6	0	-1.822232	4.822207	-0.275321
25	1	0	-1.318270	4.277722	-1.065652
26	6	0	-9.065429	0.891647	-1.874097
27	6	0	-5.594788	1.720976	-1.813268
28	6	0	-12.609374	-0.227461	-2.413860
29	1	0	-13.408411	-0.720747	-1.871042
30	6	0	-1.835877	6.217767	-0.255794
31	1	0	-1.342239	6.763159	-1.055015
32	6	0	-1.855466	-5.453357	-1.581848
33	1	0	-2.106332	-6.386792	-1.085112
34	6	0	-5.303742	-1.937154	1.792950
35	6	0	-4.139880	2.021762	0.088440
36	6	0	-6.681030	1.487142	-0.923639
37	6	0	-2.454659	4.130990	0.753905
38	6	0	-6.383307	-1.998038	-0.398229
39	1	0	-7.298579	-2.037526	-0.973903
40	6	0	-4.062996	-1.823335	1.168435
41	1	0	-3.142472	-1.723451	1.728975
42	6	0	-2.471730	6.927053	0.772539
43	6	0	-12.803659	0.187332	-3.726784
44	1	0	-13.762329	0.018602	-4.207126
45	6	0	-1.239849	-3.055752	-2.867127
46	1	0	-1.004775	-2.119535	-3.365225
47	6	0	-1.142035	-5.487291	-2.792153
48	6	0	-2.262406	-4.248979	-1.013785
49	1	0	-2.824730	-4.241976	-0.086188
50	6	0	-8.867756	-1.936801	2.123726
51	6	0	-3.087337	6.197439	1.803220
52	1	0	-3.576991	6.727972	2.615177

53	6	0	-6.484271	-1.996578	1.005020
54	6	0	-10.287589	-2.354458	4.068365
55	1	0	-9.410125	-2.726709	4.586644
56	6	0	-11.228922	-0.479865	-0.420859
57	6	0	-6.465278	1.545640	0.463741
58	1	0	-7.307108	1.353722	1.115936
59	6	0	-3.995786	-1.789620	-0.225734
60	6	0	-5.198437	1.814325	0.986206
61	6	0	-5.142756	-1.890815	-1.027569
62	6	0	-7.963560	1.172000	-1.438076
63	6	0	-12.652048	-1.868527	4.013882
64	1	0	-13.622238	-1.859120	4.500562
65	6	0	-1.955891	-3.051478	-1.666133
66	6	0	-12.532737	-1.406800	2.707297
67	1	0	-13.402043	-1.035272	2.175438
68	6	0	-10.544913	1.033000	-3.802426
69	1	0	-9.737100	1.528662	-4.330561
70	6	0	-3.083357	4.805230	1.805301
71	1	0	-3.575564	4.254105	2.600769
72	6	0	-0.834836	-4.270197	-3.418265
73	1	0	-0.285102	-4.275469	-4.355395
74	6	0	-11.527247	-2.342298	4.697594
75	1	0	-11.619680	-2.704029	5.716730
76	6	0	-5.954330	1.661979	3.261475
77	1	0	-5.502471	1.807247	4.243018
78	1	0	-6.333960	0.638650	3.179532
79	1	0	-6.772467	2.378121	3.131027
80	6	0	-7.759604	-1.993409	1.624256
81	6	0	-0.751268	-6.801540	-3.420567
82	1	0	-0.559912	-7.568378	-2.664941
83	1	0	0.142035	-6.700788	-4.042639
84	1	0	-1.556677	-7.175186	-4.064403
85	6	0	-11.768370	0.818033	-4.425301
86	1	0	-11.918525	1.143435	-5.449764
87	6	0	-6.071862	-1.944202	-3.239358
88	1	0	-5.667513	-1.940019	-4.251628
89	1	0	-6.736228	-1.085280	-3.103774
90	1	0	-6.621353	-2.876995	-3.073401
91	6	0	-2.513129	8.435257	0.771289
92	1	0	-2.301485	8.842405	1.764768
93	1	0	-3.507022	8.795929	0.481477
94	1	0	-1.792225	8.857906	0.067011
95	6	0	11.284267	-1.422289	-1.976159
96	16	0	2.424958	-1.494235	1.135698
97	16	0	2.494000	2.285289	-0.769531
98	8	0	1.479321	1.887262	0.348123
99	8	0	5.868193	1.684013	3.151933
100	8	0	5.481445	-2.012942	-3.046318
101	8	0	4.953046	-1.843975	2.469017
102	8	0	1.493494	-1.112516	-0.066045
103	6	0	4.823476	1.938072	4.081751
104	1	0	4.023785	1.191016	3.996515
105	1	0	4.404303	2.943124	3.948374
106	1	0	5.278812	1.868740	5.069841
107	8	0	4.902235	1.838673	-2.307246
108	6	0	10.142566	-1.929166	-2.661338
109	6	0	4.330276	-2.044955	-3.877102

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110	1	0	3.736347	-1.126614	-3.776247
111	1	0	3.697275	-2.912163	-3.652027
112	1	0	4.700307	-2.124081	-4.899754
113	6	0	11.372651	0.020386	1.810802
114	6	0	4.063207	-1.875792	-1.069671
115	1	0	3.141294	-1.792803	-1.630448
116	6	0	11.225056	-0.456936	0.478656
117	6	0	10.320156	0.677127	2.510916
118	6	0	1.314772	-4.021094	0.718411
119	1	0	1.125099	-3.698571	-0.299507
120	6	0	8.866621	-1.966113	-2.037673
121	6	0	5.302535	-1.987149	-1.696219
122	6	0	12.528248	-1.427998	-2.636403
123	1	0	13.396594	-1.043702	-2.112086
124	6	0	0.946806	-5.293056	1.148476
125	1	0	0.474671	-5.972640	0.444822
126	6	0	1.889082	6.221288	0.119137
127	1	0	1.427042	6.800587	0.913412
128	6	0	5.581752	1.740867	1.825747
129	6	0	3.999916	-1.813992	0.322831
130	6	0	6.486079	-2.023264	-0.912065
131	6	0	1.912335	-3.151592	1.631659
132	6	0	6.459902	1.524903	-0.444818
133	1	0	7.304264	1.322590	-1.090574
134	6	0	4.317258	1.993142	1.299875
135	1	0	3.460339	2.155712	1.940544
136	6	0	1.170992	-5.712800	2.470136
137	6	0	12.647791	-1.910684	-3.935342
138	1	0	13.617156	-1.904785	-4.423718
139	6	0	3.055276	4.721956	-1.928339
140	1	0	3.516594	4.137386	-2.718280
141	6	0	2.494904	6.886246	-0.956403
142	6	0	1.866411	4.828020	0.191829
143	1	0	1.385587	4.318101	1.018818
144	6	0	9.056814	0.927821	1.910023
145	6	0	1.760115	-4.809130	3.365377
146	1	0	1.928609	-5.109420	4.395758
147	6	0	6.671658	1.494723	0.944142
148	6	0	10.536056	1.106976	3.835815
149	1	0	9.726352	1.607705	4.356237
150	6	0	11.205461	-0.913027	-0.649794
151	6	0	6.389151	-2.000675	0.490696
152	1	0	7.306586	-2.023702	1.063638
153	6	0	4.132220	2.000336	-0.085525
154	6	0	5.149351	-1.894238	1.122131
155	6	0	5.193733	1.778466	-0.976024
156	6	0	7.759754	-2.020855	-1.535204
157	6	0	12.798287	0.269630	3.772899
158	1	0	13.757776	0.112581	4.255568
159	6	0	2.458096	4.092933	-0.831786
160	6	0	12.605407	-0.166950	2.466845
161	1	0	13.406341	-0.665561	1.931741
162	6	0	10.285577	-2.408918	-3.977585
163	1	0	9.409182	-2.794325	-4.488002
164	6	0	2.128952	-3.527430	2.958164
165	1	0	2.585430	-2.836943	3.659671
166	6	0	3.069353	6.113485	-1.978980

167	1	0	3.534548	6.609052	-2.826601
168	6	0	11.760584	0.907138	4.461611
169	1	0	11.909701	1.249538	5.480672
170	6	0	6.099572	-1.894221	3.326147
171	1	0	5.707597	-1.869308	4.343140
172	1	0	6.751618	-1.030864	3.162575
173	1	0	6.658699	-2.824054	3.177005
174	6	0	7.954154	1.195033	1.467815
175	6	0	2.548883	8.393029	-1.011294
176	1	0	2.344818	8.764938	-2.019874
177	1	0	3.544718	8.755547	-0.730228
178	1	0	1.829301	8.847654	-0.325741
179	6	0	11.524147	-2.401186	-4.609065
180	1	0	11.616685	-2.779560	-5.622146
181	6	0	5.955153	1.581121	-3.245753
182	1	0	5.505227	1.704275	-4.231224
183	1	0	6.337538	0.560921	-3.141320
184	1	0	6.770603	2.302574	-3.128459
185	6	0	0.805165	-7.109239	2.908777
186	1	0	0.606583	-7.154859	3.982797
187	1	0	1.623904	-7.808108	2.698659
188	1	0	-0.078827	-7.478193	2.380889
189	30	0	0.005679	0.273496	0.045031
190	8	0	-0.016778	0.575125	-2.115737
191	8	0	0.013842	0.653034	2.173713
192	1	0	-0.621716	1.336708	-2.117358
193	1	0	0.826464	0.875256	-2.483792
194	1	0	-0.838070	0.900602	2.559183
195	1	0	0.578109	1.443835	2.175883

Atomic coordinates of compound (*S,S*)-1 (Structure detailed in Figure S21 red trace, octahedral complex with two acetone molecules)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	2.443738	1.861076	-0.955560
2	16	0	2.443970	-1.861269	0.955846
3	8	0	1.458232	-1.484599	-0.201314
4	8	0	5.665301	-1.499037	-3.123897
5	8	0	5.665906	1.499257	3.123548
6	8	0	4.954497	2.060605	-2.343088
7	8	0	1.458352	1.484114	0.201776
8	6	0	4.545681	-1.445111	-3.993561
9	1	0	3.908375	-0.580068	-3.766451
10	1	0	3.950313	-2.365770	-3.939198
11	1	0	4.952600	-1.342097	-5.000098
12	8	0	4.955015	-2.060255	2.342894
13	6	0	11.369949	0.629155	1.926520
14	6	0	10.259587	1.168098	2.637854
15	6	0	4.546441	1.444992	3.993401
16	1	0	3.909278	0.579847	3.766290
17	1	0	3.950880	2.365538	3.939253
18	1	0	4.953558	1.341940	4.999853
19	6	0	11.369508	-0.628265	-1.928071
20	6	0	4.179206	1.752756	1.207655
21	1	0	3.271666	1.688224	1.792954
22	6	0	11.266833	-0.199318	-0.575611
23	6	0	10.259010	-1.167262	-2.639150
24	6	0	2.749989	4.638675	-0.542989
25	1	0	3.386366	4.409753	0.304956

26	6	0	8.990068	1.333428	2.020421
27	6	0	5.442248	1.658061	1.790180
28	6	0	12.607431	0.514846	2.589621
29	1	0	13.451981	0.106100	2.045355
30	6	0	2.500288	5.963450	-0.894372
31	1	0	2.945256	6.761329	-0.306107
32	6	0	2.501597	-5.963655	0.895355
33	1	0	2.946851	-6.761518	0.307283
34	6	0	5.441917	-1.657828	-1.790482
35	6	0	4.064835	1.886296	-0.177897
36	6	0	6.600104	1.684138	0.968094
37	6	0	2.190971	3.611989	-1.308823
38	6	0	6.457403	-1.834145	0.422348
39	1	0	7.354647	-1.834983	1.027067
40	6	0	4.178999	-1.752716	-1.207717
41	1	0	3.271338	-1.688377	-1.792849
42	6	0	1.697865	6.287984	-2.000495
43	6	0	12.750161	0.910564	3.915165
44	1	0	13.714124	0.812446	4.404436
45	6	0	1.378545	-3.909301	2.408080
46	1	0	0.939995	-3.106626	2.993131
47	6	0	1.699082	-6.288196	2.001408
48	6	0	2.751008	-4.638879	0.543770
49	1	0	3.387456	-4.409956	-0.304120
50	6	0	8.989644	-1.332695	-2.021429
51	6	0	1.133806	5.239127	-2.742899
52	1	0	0.506973	5.468467	-3.600208
53	6	0	6.599934	-1.683678	-0.968613
54	6	0	10.424458	-1.556536	-3.982847
55	1	0	9.571403	-1.967063	-4.512916
56	6	0	11.266969	0.200172	0.574095
57	6	0	6.457286	1.834652	-0.422835
58	1	0	7.354417	1.835674	-1.027722
59	6	0	4.064909	-1.886213	0.177863
60	6	0	5.194622	1.931663	-1.009424
61	6	0	5.194865	-1.931344	1.009177
62	6	0	7.884699	1.510266	1.542689
63	6	0	12.749261	-0.909546	-3.917054
64	1	0	13.713101	-0.811359	-4.406554
65	6	0	2.191602	-3.612206	1.309333
66	6	0	12.606824	-0.513867	-2.591469
67	1	0	13.451479	-0.105081	-2.047395
68	6	0	10.425333	1.557413	3.981501
69	1	0	9.572382	1.967899	4.511767
70	6	0	1.378014	3.909082	-2.407645
71	1	0	0.939779	3.106403	-2.992929
72	6	0	1.134624	-5.239353	2.743529
73	1	0	0.507710	-5.468715	3.600771
74	6	0	11.655344	-1.430660	-4.616385
75	1	0	11.765363	-1.740825	-5.650671
76	6	0	6.073979	2.078821	-3.235739
77	1	0	5.652921	2.215783	-4.231948
78	1	0	6.624714	1.133576	-3.193296
79	1	0	6.743030	2.915847	-3.009448
80	6	0	7.884391	-1.509640	-1.543467
81	6	0	1.480098	-7.725284	2.404278
82	1	0	1.562127	-8.400784	1.548644
83	1	0	0.498734	-7.869146	2.864609
84	1	0	2.232343	-8.038512	3.138317
85	6	0	11.656380	1.431627	4.614745
86	1	0	11.766627	1.741823	5.648997
87	6	0	6.074688	-2.078477	3.235316
88	1	0	5.653843	-2.215560	4.231597

89	1	0	6.625345	-1.133188	3.192842
90	1	0	6.743747	-2.915434	3.008803
91	6	0	1.478509	7.725074	-2.403156
92	1	0	0.496008	7.869259	-2.860978
93	1	0	2.228942	8.037749	-3.139282
94	1	0	1.563067	8.400751	-1.547922
95	6	0	-11.358837	-0.813183	1.855395
96	16	0	-2.475676	-1.811644	-1.177254
97	16	0	-2.475748	1.810820	1.178146
98	8	0	-1.489461	1.495055	0.014856
99	8	0	-5.644716	2.083628	-2.942045
100	8	0	-5.646054	-2.083600	2.941897
101	8	0	-5.024419	-1.638080	-2.551766
102	8	0	-1.489744	-1.495504	-0.013765
103	6	0	-4.517412	2.294658	-3.779581
104	1	0	-3.816512	1.451134	-3.726384
105	1	0	-3.991995	3.221588	-3.518134
106	1	0	-4.909264	2.377281	-4.793878
107	8	0	-5.024930	1.637667	2.551785
108	6	0	-10.264156	-1.437951	2.519670
109	6	0	-4.519052	-2.294742	3.779815
110	1	0	-3.818012	-1.451325	3.726784
111	1	0	-3.993691	-3.221770	3.518606
112	1	0	-4.911246	-2.377235	4.793991
113	6	0	-11.358121	0.814334	-1.857330
114	6	0	-4.190875	-2.021877	0.987718
115	1	0	-3.273467	-2.107678	1.556792
116	6	0	-11.240671	0.255904	-0.553504
117	6	0	-10.263117	1.438891	-2.521273
118	6	0	-1.309050	-4.303467	-0.752455
119	1	0	-0.803699	-3.828813	0.080910
120	6	0	-8.990536	-1.558155	1.900911
121	6	0	-5.442497	-1.992723	1.599595
122	6	0	-12.601489	-0.746878	2.515604
123	1	0	-13.434191	-0.272768	2.007271
124	6	0	-1.081970	-5.643499	-1.071672
125	1	0	-0.391103	-6.219661	-0.462834
126	6	0	-1.082314	5.642791	1.073763
127	1	0	-0.391657	6.219269	0.464973
128	6	0	-5.441617	1.992661	-1.599678
129	6	0	-4.099200	-1.886224	-0.398230
130	6	0	-6.607899	-1.816801	0.806284
131	6	0	-2.190106	-3.568007	-1.540285
132	6	0	-6.486602	1.709530	0.589738
133	1	0	-7.390234	1.564305	1.166803
134	6	0	-4.190181	2.021524	-0.987397
135	1	0	-3.272571	2.107157	-1.556171
136	6	0	-1.719658	-6.254782	-2.159615
137	6	0	-12.764549	-1.271273	3.793267
138	1	0	-13.732240	-1.207404	4.280860
139	6	0	-2.832009	4.138408	2.645277
140	1	0	-3.519378	3.553765	3.248227
141	6	0	-1.719647	6.253559	2.162286
142	6	0	-1.309449	4.302956	0.754018
143	1	0	-0.804346	3.828670	-0.079709
144	6	0	-8.989654	1.558828	-1.902137
145	6	0	-2.593418	-5.479936	-2.939548
146	1	0	-3.093443	-5.932394	-3.791687
147	6	0	-6.607309	1.816952	-0.806754
148	6	0	-10.449291	1.959903	-3.816856
149	1	0	-9.608217	2.435731	-4.310213
150	6	0	-11.240886	-0.254777	0.551606
151	6	0	-6.486718	-1.709476	-0.590172

152	1	0	-7.390134	-1.564100	-1.167538
153	6	0	-4.098986	1.885781	0.398569
154	6	0	-5.235799	-1.740779	-1.207055
155	6	0	-5.235877	1.740533	1.207021
156	6	0	-7.883336	-1.699368	1.415245
157	6	0	-12.763165	1.272725	-3.795617
158	1	0	-13.730724	1.209051	-4.283497
159	6	0	-2.190166	3.567038	1.541901
160	6	0	-12.600590	0.748282	-2.517912
161	1	0	-13.433537	0.274331	-2.009833
162	6	0	-10.450818	-1.958909	3.815204
163	1	0	-9.609986	-2.434898	4.308816
164	6	0	-2.832423	-4.139966	-2.643151
165	1	0	-3.520134	-3.555645	-3.246029
166	6	0	-2.592944	5.478307	2.942222
167	1	0	-3.092559	5.930294	3.794842
168	6	0	-11.684764	1.879181	-4.448660
169	1	0	-11.810454	2.290660	-5.445132
170	6	0	-6.158363	-1.430322	-3.403133
171	1	0	-5.759769	-1.390541	-4.417219
172	1	0	-6.660696	-0.486869	-3.169484
173	1	0	-6.865316	-2.263280	-3.325184
174	6	0	-7.882573	1.699806	-1.416130
175	6	0	-1.492608	7.710658	2.482394
176	1	0	-1.435799	7.880325	3.561702
177	1	0	-2.317341	8.325561	2.102625
178	1	0	-0.570101	8.083048	2.029472
179	6	0	-11.686462	-1.877933	4.446639
180	1	0	-11.812532	-2.289373	5.443079
181	6	0	-6.159207	1.430323	3.402809
182	1	0	-5.760943	1.390437	4.417021
183	1	0	-6.661785	0.487031	3.169037
184	1	0	-6.865853	2.263519	3.324607
185	6	0	-1.492428	-7.711851	-2.479735
186	1	0	-1.423252	-7.879542	-3.558684
187	1	0	-2.323126	-8.325472	-2.111135
188	1	0	-0.576197	-8.087318	-2.016789
189	30	0	-0.023942	-0.000268	0.000376
190	6	0	0.097038	0.334341	3.272406
191	8	0	-0.055845	-0.289544	2.221166
192	6	0	-0.116553	-0.362392	4.593328
193	6	0	0.491713	1.785581	3.308245
194	1	0	-0.609824	-1.323881	4.446173
195	1	0	0.845184	2.119419	2.332090
196	1	0	-0.700579	0.263387	5.275644
197	1	0	0.855880	-0.526736	5.074361
198	1	0	1.250010	1.955545	4.079876
199	1	0	-0.381212	2.383122	3.599807
200	6	0	0.096705	-0.335045	-3.271682
201	8	0	-0.056128	0.288811	-2.220421
202	6	0	0.491236	-1.786326	-3.307570
203	6	0	-0.116919	0.361718	-4.592585
204	1	0	0.844844	-2.120178	-2.331470
205	1	0	-0.609802	1.323395	-4.445363
206	1	0	1.249368	-1.956396	-4.079337
207	1	0	-0.381814	-2.383778	-3.598944
208	1	0	-0.701375	-0.263885	-5.274702
209	1	0	0.855443	0.525643	-5.073897

Atomic coordinates of compound (*S,S*)-1 (Structure detailed in Figure S21 dark yellow trace, octahedral complex with two water molecules)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.406037	-2.181625	-0.490539
2	16	0	-2.490134	2.051961	0.394109
3	8	0	-1.571544	1.281441	-0.588941
4	8	0	-5.656269	0.459727	-3.410037
5	8	0	-5.190046	-0.158104	3.400720
6	8	0	-5.072957	-2.703782	-1.521809
7	8	0	-1.336385	-1.609902	0.468207
8	6	0	-4.511059	0.011342	-4.132444
9	1	0	-3.961441	-0.755348	-3.578323
10	1	0	-3.834333	0.839363	-4.371099
11	1	0	-4.896199	-0.415288	-5.059743
12	8	0	-4.998432	2.978935	1.482536
13	6	0	-11.018301	0.555091	2.308313
14	6	0	-9.855082	0.305213	3.092918
15	6	0	-3.966107	0.158081	4.072920
16	1	0	-3.345778	0.847120	3.491998
17	1	0	-3.390788	-0.745717	4.300204
18	1	0	-4.262985	0.637672	5.006363
19	6	0	-11.370124	0.131090	-1.711509
20	6	0	-3.926765	-1.206698	1.599826
21	1	0	-2.954863	-1.009580	2.039283
22	6	0	-11.148266	0.283891	-0.313440
23	6	0	-10.336062	0.344418	-2.669349
24	6	0	-2.836522	-4.662332	0.790676
25	1	0	-3.316917	-4.116675	1.595816
26	6	0	-8.642168	-0.158609	2.514815
27	6	0	-5.119895	-0.799816	2.208261
28	6	0	-12.192616	0.991389	2.954379
29	1	0	-13.074860	1.177290	2.350642
30	6	0	-2.721859	-6.048584	0.852653
31	1	0	-3.117978	-6.577926	1.715718
32	6	0	-1.738631	5.736620	-1.199917
33	1	0	-1.698574	6.196451	-2.184108
34	6	0	-5.453556	1.087344	-2.219740
35	6	0	-3.966225	-1.841180	0.360984
36	6	0	-6.351470	-1.031899	1.543197
37	6	0	-2.335655	-3.983174	-0.323077
38	6	0	-6.490348	2.112301	-0.256721
39	1	0	-7.395359	2.361979	0.281414
40	6	0	-4.194244	1.333773	-1.665924
41	1	0	-3.276177	1.002724	-2.137916
42	6	0	-2.106627	-6.773663	-0.180233
43	6	0	-12.227353	1.189748	4.329831
44	1	0	-13.143977	1.529018	4.802848
45	6	0	-1.812707	4.541004	1.326768
46	1	0	-1.805717	4.055516	2.297847
47	6	0	-1.457047	6.511566	-0.061889
48	6	0	-2.065069	4.389387	-1.088623
49	1	0	-2.272229	3.795550	-1.972850
50	6	0	-9.032098	0.742339	-2.269793
51	6	0	-1.589409	-6.066467	-1.273791
52	1	0	-1.095009	-6.606495	-2.077027
53	6	0	-6.615432	1.452670	-1.495212

54	6	0	-10.622542	0.158580	-4.036024
55	1	0	-9.827761	0.322431	-4.756321
56	6	0	-11.036576	0.385452	0.894689
57	6	0	-6.362546	-1.683742	0.294032
58	1	0	-7.316459	-1.823610	-0.197689
59	6	0	-4.098933	1.962422	-0.427997
60	6	0	-5.174409	-2.088366	-0.308484
61	6	0	-5.234458	2.373125	0.285986
62	6	0	-7.574124	-0.566058	2.096501
63	6	0	-12.910555	-0.417853	-3.520121
64	1	0	-13.904637	-0.710013	-3.844944
65	6	0	-2.111562	3.805639	0.179942
66	6	0	-12.650085	-0.244373	-2.165342
67	1	0	-13.433140	-0.402804	-1.431044
68	6	0	-9.913449	0.517452	4.485250
69	1	0	-9.021485	0.325083	5.072380
70	6	0	-1.698909	-4.677648	-1.354840
71	1	0	-1.277854	-4.141892	-2.199035
72	6	0	-1.492397	5.893703	1.193578
73	1	0	-1.255362	6.472580	2.082369
74	6	0	-11.892394	-0.218190	-4.458552
75	1	0	-12.090623	-0.353180	-5.517621
76	6	0	-6.262872	-2.893416	-2.283519
77	1	0	-5.949177	-3.395645	-3.199448
78	1	0	-6.731659	-1.934954	-2.531929
79	1	0	-6.977971	-3.531144	-1.749896
80	6	0	-7.907310	1.086462	-1.958584
81	6	0	-1.140610	7.982272	-0.194524
82	1	0	-0.548131	8.186023	-1.092174
83	1	0	-0.584940	8.352192	0.671667
84	1	0	-2.059442	8.576937	-0.273083
85	6	0	-11.081974	0.954466	5.098017
86	1	0	-11.102431	1.108566	6.172703
87	6	0	-6.104297	3.227878	2.347103
88	1	0	-5.678566	3.668342	3.249249
89	1	0	-6.623537	2.297695	2.600669
90	1	0	-6.807949	3.938456	1.896567
91	6	0	-2.030666	-8.281052	-0.125431
92	1	0	-1.946591	-8.642228	0.904090
93	1	0	-1.175512	-8.660466	-0.692096
94	1	0	-2.932883	-8.734584	-0.554695
95	6	0	11.241663	1.347034	1.818746
96	16	0	2.401802	1.388421	-1.436354
97	16	0	2.448607	-1.511619	1.462299
98	8	0	1.558808	-1.387136	0.203357
99	8	0	5.662486	-2.324896	-2.537217
100	8	0	5.472807	2.460841	2.644229
101	8	0	4.946451	1.364037	-2.757939
102	8	0	1.378763	1.518956	-0.277432
103	6	0	4.515021	-2.527744	-3.370102
104	1	0	3.869607	-1.644814	-3.398290
105	1	0	3.925851	-3.389095	-3.036335
106	1	0	4.911533	-2.726039	-4.366750
107	8	0	4.994463	-1.302529	2.872433
108	6	0	10.110815	2.027861	2.356109
109	6	0	4.314352	2.584832	3.472047
110	1	0	3.724637	1.664637	3.482362
111	1	0	3.667926	3.403203	3.140671
112	1	0	4.692724	2.799766	4.472640
113	6	0	11.342161	-0.810410	-1.615350
114	6	0	4.041011	2.084337	0.701032
115	1	0	3.110182	2.150296	1.257363
116	6	0	11.204054	-0.070031	-0.407270

117	6	0	10.268747	-1.564751	-2.171840
118	6	0	2.073039	4.122605	-1.939648
119	1	0	2.183594	4.271118	-0.870282
120	6	0	8.849792	2.017484	1.701286
121	6	0	5.291201	2.213887	1.320961
122	6	0	12.468055	1.414677	2.509849
123	1	0	13.324893	0.895551	2.092888
124	6	0	1.839758	5.200369	-2.788355
125	1	0	1.780440	6.203466	-2.373285
126	6	0	1.168650	-5.362084	1.755800
127	1	0	0.639414	-6.070669	1.124557
128	6	0	5.457294	-2.088581	-1.217023
129	6	0	3.984929	1.803805	-0.662555
130	6	0	6.473319	2.035544	0.558991
131	6	0	2.149353	2.838334	-2.482688
132	6	0	6.481359	-1.573805	0.944399
133	1	0	7.379170	-1.359956	1.509508
134	6	0	4.198279	-2.046801	-0.612485
135	1	0	3.284601	-2.178185	-1.180699
136	6	0	1.679159	5.013917	-4.171520
137	6	0	12.585001	2.120239	3.702010
138	1	0	13.540442	2.155003	4.216851
139	6	0	2.478729	-3.511648	3.386644
140	1	0	2.972909	-2.782663	4.019799
141	6	0	1.543524	-5.735678	3.055194
142	6	0	1.446403	-4.090176	1.259638
143	1	0	1.137998	-3.788191	0.263884
144	6	0	8.999482	-1.641015	-1.537494
145	6	0	1.739779	3.711651	-4.682809
146	1	0	1.598071	3.548080	-5.748120
147	6	0	6.611746	-1.826161	-0.434761
148	6	0	10.477102	-2.256809	-3.381741
149	1	0	9.652085	-2.826141	-3.797077
150	6	0	11.173421	0.598802	0.609501
151	6	0	6.385542	1.770196	-0.821033
152	1	0	7.304547	1.617587	-1.371743
153	6	0	4.096276	-1.767724	0.747306
154	6	0	5.145311	1.648428	-1.439681
155	6	0	5.225762	-1.546219	1.548230
156	6	0	7.746528	2.055167	1.188893
157	6	0	12.764678	-1.488961	-3.476806
158	1	0	13.728595	-1.458755	-3.975907
159	6	0	2.111694	-3.182564	2.082344
160	6	0	12.581387	-0.794650	-2.286378
161	1	0	13.394586	-0.219890	-1.855285
162	6	0	10.252885	2.733099	3.568070
163	1	0	9.385014	3.246431	3.968831
164	6	0	1.969383	2.616475	-3.847792
165	1	0	1.993692	1.603414	-4.238979
166	6	0	2.196594	-4.792963	3.860521
167	1	0	2.477625	-5.059184	4.876324
168	6	0	11.707293	-2.220707	-4.028004
169	1	0	11.844116	-2.764022	-4.958219
170	6	0	6.081259	1.073629	-3.569208
171	1	0	5.685853	0.872935	-4.565533
172	1	0	6.615983	0.190741	-3.202933
173	1	0	6.763926	1.930873	-3.617188
174	6	0	7.893455	-1.754672	-1.042765
175	6	0	1.258248	-7.127684	3.567497
176	1	0	0.293985	-7.496352	3.203745
177	1	0	1.243383	-7.158463	4.660787
178	1	0	2.024167	-7.837324	3.230084
179	6	0	11.471958	2.779825	4.234423

180	1	0	11.556771	3.331806	5.165759
181	6	0	6.095391	-0.902042	3.686276
182	1	0	5.680515	-0.734517	4.681035
183	1	0	6.545160	0.025656	3.317228
184	1	0	6.855679	-1.690629	3.741045
185	6	0	1.465712	6.196747	-5.086253
186	1	0	0.864390	6.974141	-4.604371
187	1	0	0.962919	5.902165	-6.011845
188	1	0	2.422362	6.655902	-5.365716
189	30	0	-0.023359	-0.022968	-0.023260
190	8	0	1.322035	2.101585	3.084398
191	16	0	0.053627	1.360679	3.172822
192	8	0	-1.151468	2.143186	3.513929
193	8	0	-0.174717	0.356616	2.077180
194	6	0	0.273337	0.230068	4.633324
195	9	0	0.407488	0.944614	5.758329
196	9	0	1.372488	-0.531752	4.487324
197	9	0	-0.786165	-0.584255	4.772278
198	8	0	-0.080537	-0.502158	-2.137516
199	16	0	0.527213	-1.409649	-3.168505
200	8	0	1.611858	-0.789285	-3.953905
201	8	0	0.747161	-2.799264	-2.724509
202	6	0	-0.876012	-1.540285	-4.386698
203	9	0	-1.321115	-0.325388	-4.748227
204	9	0	-1.915940	-2.216665	-3.850363
205	9	0	-0.484031	-2.192971	-5.486996

Atomic coordinates of compound (*S,S*)-1 (Structure detailed in Figure S21 green trace, corresponding to X-Ray structure of octahedral complex with three water molecules and four triflate anions)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.207163	-8.106926	-1.961852
2	6	0	-2.298483	-6.598650	-1.934509
3	6	0	-1.704977	-5.872761	-0.889744
4	6	0	-1.772253	-4.482660	-0.846297
5	6	0	-2.452902	-3.812718	-1.864620
6	6	0	-3.036500	-4.502881	-2.924223
7	6	0	-2.960510	-5.896845	-2.947878
8	6	0	-3.943800	-1.949724	-0.607022
9	6	0	-3.621604	-1.775636	0.732032
10	6	0	-4.644055	-1.710902	1.688294
11	6	0	-5.994525	-1.793290	1.260822
12	6	0	-6.292812	-1.970911	-0.106469
13	6	0	-5.272456	-2.057162	-1.047055
14	6	0	-6.770955	-2.095174	-2.908637
15	6	0	-3.081338	-1.561689	3.501250
16	6	0	-7.050891	-1.644714	2.196345
17	6	0	-7.974846	-1.484890	2.973478
18	6	0	-9.016085	-1.329207	3.923233
19	6	0	-8.787446	-1.661894	5.274770
20	6	0	-9.792464	-1.538381	6.226938
21	6	0	-11.061212	-1.079260	5.853988
22	6	0	-11.309864	-0.737799	4.529430
23	6	0	-10.305075	-0.845281	3.547547
24	6	0	-10.589642	-0.459140	2.208376
25	6	0	-10.864577	-0.101676	1.077662
26	6	0	-11.244863	0.276926	-0.239471
27	6	0	-12.583681	0.106643	-0.646290

28	6	0	-12.995845	0.439072	-1.931588
29	6	0	-12.070143	0.953827	-2.846591
30	6	0	-10.746131	1.139130	-2.466792
31	6	0	-10.303454	0.815458	-1.166734
32	6	0	-8.945751	1.041228	-0.819568
33	6	0	-7.772034	1.281565	-0.599052
34	6	0	-6.403883	1.552130	-0.331230
35	6	0	-5.970422	1.764410	0.995548
36	6	0	-4.627341	2.014177	1.271265
37	6	0	-3.722815	2.039550	0.200160
38	6	0	-4.118328	1.823632	-1.111152
39	6	0	-5.464400	1.582951	-1.393850
40	6	0	-4.999489	1.379371	-3.725776
41	6	0	-4.803127	1.844471	3.668387
42	6	0	-2.095594	4.164337	0.426686
43	6	0	-1.837103	4.798742	-0.786270
44	6	0	-1.973999	6.184436	-0.859779
45	6	0	-2.369473	6.937383	0.254596
46	6	0	-2.619364	6.268091	1.459186
47	6	0	-2.480024	4.883015	1.558273
48	6	0	-2.504975	8.439842	0.154217
49	6	0	1.521677	7.957014	1.707954
50	6	0	1.788191	6.566418	1.181275
51	6	0	2.414721	6.367864	-0.053077
52	6	0	2.636625	5.080254	-0.545747
53	6	0	2.236340	3.986038	0.217233
54	6	0	1.601673	4.151988	1.451182
55	6	0	1.385921	5.443616	1.922346
56	6	0	3.910547	1.880008	0.659421
57	6	0	3.651768	1.112234	1.789012
58	6	0	4.719639	0.668576	2.582471
59	6	0	6.046242	0.995998	2.197186
60	6	0	6.276783	1.798316	1.060755
61	6	0	5.213376	2.249130	0.288309
62	6	0	6.620232	3.213858	-1.389079
63	6	0	3.273508	-0.553697	4.063764
64	6	0	7.160025	0.460504	2.894983
65	6	0	8.153855	-0.012326	3.416738
66	6	0	9.277887	-0.565411	4.081422
67	6	0	9.168134	-0.953202	5.433276
68	6	0	10.252260	-1.484367	6.121814
69	6	0	11.484162	-1.641630	5.476259
70	6	0	11.616294	-1.272846	4.142410
71	6	0	10.529908	-0.740206	3.419357
72	6	0	10.713094	-0.400939	2.048795
73	6	0	10.941210	-0.150295	0.879084
74	6	0	11.303349	0.179987	-0.457523
75	6	0	12.628135	0.582698	-0.723093
76	6	0	13.033941	0.935448	-2.004917
77	6	0	12.115480	0.892145	-3.060218
78	6	0	10.805895	0.490647	-2.826213
79	6	0	10.369799	0.122732	-1.535435
80	6	0	9.027074	-0.294928	-1.348274
81	6	0	7.864607	-0.650940	-1.266550
82	6	0	6.515624	-1.056961	-1.092836
83	6	0	5.512427	-0.659317	-2.012105
84	6	0	4.178850	-1.001640	-1.760665
85	6	0	3.862702	-1.737340	-0.630011
86	6	0	4.839991	-2.157780	0.286598
87	6	0	6.165818	-1.813757	0.048513
88	6	0	5.261259	-3.248600	2.389546
89	6	0	4.901137	0.485959	-4.015343
90	6	0	2.154669	-3.822046	-0.858707

91	6	0	2.102929	-4.072545	-2.230540
92	6	0	2.145014	-5.391967	-2.672033
93	6	0	2.245372	-6.457492	-1.764054
94	6	0	2.286584	-6.170075	-0.395603
95	6	0	2.235389	-4.854441	0.072717
96	6	0	2.303859	-7.882795	-2.264309
97	8	0	-1.497694	0.601985	-3.046585
98	8	0	-1.362652	-1.507518	-1.057663
99	8	0	-1.277773	1.948386	-0.794080
100	8	0	1.380941	1.439877	0.019410
101	8	0	1.367968	-1.322724	-1.372164
102	8	0	-4.439268	-1.529910	3.010594
103	8	0	-5.455587	-2.241136	-2.392765
104	8	0	-4.097836	2.262133	2.498964
105	8	0	-5.940602	1.344817	-2.646234
106	8	0	4.372709	-2.869105	1.346236
107	8	0	4.589457	-0.100950	3.684696
108	8	0	1.469717	0.833417	-2.921463
109	8	0	5.326458	3.027315	-0.831713
110	8	0	5.911448	0.076571	-3.082876
111	8	0	-0.469831	-0.273643	1.233876
112	16	0	-2.590366	-1.999147	-1.832352
113	16	0	-1.955709	2.346307	0.531788
114	16	0	2.542063	2.327528	-0.454813
115	16	0	2.112382	-2.099852	-0.270679
116	30	0	-0.038502	0.267750	-1.238714
117	6	0	-0.502498	-5.323605	3.045357
118	8	0	-0.154394	-3.014874	1.879077
119	8	0	1.754674	-3.977819	3.183881
120	8	0	-0.262909	-3.072334	4.377238
121	9	0	-0.014424	-6.046373	2.010265
122	9	0	-1.831838	-5.207767	2.867066
123	9	0	-0.296450	-6.037220	4.165315
124	16	0	0.311093	-3.650781	3.151692
125	6	0	0.084392	-3.339497	-5.277146
126	8	0	0.822423	-1.578236	-7.082354
127	8	0	1.598634	-1.273340	-4.717244
128	8	0	-0.800919	-0.877505	-5.301972
129	9	0	1.172289	-4.119141	-5.463016
130	9	0	-0.892519	-3.801916	-6.076117
131	9	0	-0.315906	-3.494640	-4.002706
132	16	0	0.472280	-1.559926	-5.655788
133	6	0	-0.187739	3.414152	4.911411
134	8	0	0.679150	1.076712	5.717825
135	8	0	0.375848	1.463278	3.268380
136	8	0	-1.637262	1.236748	4.744216
137	9	0	1.061887	3.915314	4.841084
138	9	0	-0.691921	3.739972	6.115932
139	9	0	-0.927409	4.057354	3.978180
140	16	0	-0.202165	1.571988	4.646309
141	6	0	0.159407	5.416676	-3.995265
142	8	0	1.005390	3.013806	-4.572106
143	8	0	-0.626508	4.110793	-6.133590
144	8	0	-1.379632	3.292172	-3.883392
145	9	0	1.160853	6.012973	-4.664510
146	9	0	0.543400	5.285853	-2.711006
147	9	0	-0.903146	6.251666	-4.019079
148	16	0	-0.263415	3.769880	-4.751964
149	1	0	-1.164236	-8.440094	-2.022695
150	1	0	-2.742898	-8.526089	-2.819120
151	1	0	-2.630077	-8.548782	-1.051727
152	1	0	-1.181065	-6.394821	-0.095360
153	1	0	-1.298820	-3.930379	-0.039313

154	1	0	-3.539123	-3.963094	-3.720128
155	1	0	-3.411718	-6.442661	-3.773386
156	1	0	-2.579237	-1.646210	1.000738
157	1	0	-7.333651	-2.006858	-0.400734
158	1	0	-6.679506	-2.200610	-3.991363
159	1	0	-7.181599	-1.108005	-2.669349
160	1	0	-7.442026	-2.877477	-2.529241
161	1	0	-3.153211	-1.401834	4.575363
162	1	0	-2.480483	-0.760319	3.066792
163	1	0	-2.622559	-2.530937	3.297959
164	1	0	-7.802441	-2.021086	5.554040
165	1	0	-9.588359	-1.801886	7.260939
166	1	0	-11.849881	-0.983503	6.594959
167	1	0	-12.286720	-0.370672	4.230033
168	1	0	-13.290595	-0.301575	0.069324
169	1	0	-14.032689	0.294466	-2.221899
170	1	0	-12.382536	1.213399	-3.854267
171	1	0	-10.022367	1.544213	-3.166505
172	1	0	-6.700981	1.711135	1.793348
173	1	0	-3.352688	1.803714	-1.877155
174	1	0	-5.577876	1.160724	-4.624576
175	1	0	-4.211157	0.630674	-3.599873
176	1	0	-4.535210	2.367691	-3.819972
177	1	0	-4.069777	1.901219	4.473124
178	1	0	-5.150711	0.811804	3.565323
179	1	0	-5.654049	2.508458	3.872884
180	1	0	-1.537647	4.217190	-1.651990
181	1	0	-1.768172	6.680097	-1.803149
182	1	0	-2.925570	6.834689	2.335864
183	1	0	-2.676543	4.372635	2.492230
184	1	0	-3.082298	8.730241	-0.730707
185	1	0	-1.524241	8.924497	0.067897
186	1	0	-3.003660	8.857283	1.034617
187	1	0	1.940479	8.723796	1.049016
188	1	0	1.953809	8.096511	2.705966
189	1	0	0.444302	8.140200	1.796732
190	1	0	2.717394	7.226605	-0.647548
191	1	0	3.102102	4.932145	-1.514308
192	1	0	1.276448	3.289509	2.027077
193	1	0	0.890629	5.576299	2.878396
194	1	0	2.622778	0.854882	2.018115
195	1	0	7.301795	2.009938	0.784994
196	1	0	6.470200	3.800730	-2.296933
197	1	0	7.085346	2.256046	-1.646426
198	1	0	7.274990	3.771611	-0.706259
199	1	0	3.419501	-1.117221	4.984947
200	1	0	2.859418	-1.219263	3.300407
201	1	0	2.595616	0.280466	4.256324
202	1	0	8.210508	-0.822888	5.926507
203	1	0	10.138737	-1.774188	7.162663
204	1	0	12.335305	-2.054477	6.010403
205	1	0	12.564283	-1.399042	3.628670
206	1	0	13.329429	0.619716	0.104728
207	1	0	14.059800	1.246212	-2.181632
208	1	0	12.422400	1.168492	-4.065116
209	1	0	10.088159	0.447496	-3.638905
210	1	0	3.366585	-0.674359	-2.398310
211	1	0	6.948035	-2.082020	0.747445
212	1	0	4.633873	-3.764965	3.116586
213	1	0	5.722264	-2.370896	2.855389
214	1	0	6.041180	-3.926826	2.018006
215	1	0	5.428085	1.050479	-4.785839
216	1	0	4.147174	1.120464	-3.538984

217	1	0	4.398806	-0.375826	-4.468323
218	1	0	2.011903	-3.249957	-2.931410
219	1	0	2.081454	-5.590589	-3.737498
220	1	0	2.339674	-6.983088	0.324686
221	1	0	2.250940	-4.640972	1.136213
222	1	0	2.237853	-8.599197	-1.439652
223	1	0	3.240343	-8.080535	-2.801437
224	1	0	1.486283	-8.094288	-2.963291
225	1	0	-1.312449	0.072864	-3.850647
226	1	0	-1.494285	1.537507	-3.349378
227	1	0	1.287408	1.630405	-3.466527
228	1	0	1.497104	0.089602	-3.565066
229	1	0	-0.171837	0.313429	1.961940
230	1	0	-0.333146	-1.197527	1.528582

Atomic coordinates of compound (*S,S*)-2 (Structure detailed in Figure S23 green trace, corresponding to octahedral complex with two water molecules.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.249819	-2.908394	-0.230277
2	16	0	2.984621	-3.894847	-1.823555
3	16	0	1.991723	-3.124712	2.435608
4	8	0	1.491777	-3.397743	-1.860984
5	8	0	3.197672	-0.549900	1.810946
6	8	0	1.613620	-3.757818	1.052334
7	8	0	7.034651	-4.492811	2.555958
8	8	0	0.862423	-0.871883	0.278600
9	8	0	-0.723578	-4.777762	-0.882820
10	6	0	3.254417	-4.587448	-3.459976
11	6	0	3.526477	-5.954697	-3.529513
12	6	0	3.704582	-6.553829	-4.777186
13	6	0	3.614297	-5.805286	-5.957543
14	6	0	3.835005	-6.444943	-7.305238
15	6	0	3.335024	-4.429762	-5.857684
16	6	0	3.156129	-3.815686	-4.623342
17	6	0	3.956801	-2.382047	-1.896008
18	6	0	5.347744	-2.481641	-1.734342
19	6	0	6.097357	-1.305493	-1.691477
20	6	0	5.477880	-0.044819	-1.798750
21	6	0	6.238032	1.147906	-1.715869
22	6	0	6.871820	2.186145	-1.645434
23	6	0	7.569543	3.420551	-1.574750
24	6	0	6.855691	4.637907	-1.632164
25	6	0	7.521620	5.850913	-1.568552
26	6	0	8.928387	5.896588	-1.445890
27	6	0	9.609246	7.139583	-1.388935
28	6	0	10.201796	8.202369	-1.350599
29	6	0	10.886983	9.446266	-1.329490
30	6	0	10.184402	10.641753	-1.573014
31	6	0	12.290875	9.501998	-1.082772
32	6	0	13.031669	8.319739	-0.813743
33	6	0	13.673344	7.314510	-0.572404
34	6	0	14.403991	6.128161	-0.290524
35	6	0	13.769022	5.023893	0.317887
36	6	0	14.475572	3.861609	0.587046
37	6	0	15.843423	3.756158	0.255989
38	6	0	16.564519	2.560881	0.520937

39	6	0	17.179797	1.534509	0.742658
40	6	0	17.937311	0.361409	1.000386
41	6	0	17.305073	-0.870935	1.341204
42	6	0	18.101244	-2.004160	1.598414
43	6	0	19.487322	-1.935644	1.519994
44	6	0	20.108205	-0.728320	1.180982
45	6	0	19.342654	0.404132	0.924878
46	6	0	15.891301	-0.975870	1.417969
47	6	0	14.682149	-1.103499	1.486430
48	6	0	13.276612	-1.263563	1.572213
49	6	0	12.720499	-2.491922	1.997200
50	6	0	11.348472	-2.654354	2.085925
51	6	0	10.475639	-1.593129	1.755653
52	6	0	9.073408	-1.777223	1.856686
53	6	0	7.875376	-1.978740	1.962538
54	6	0	6.494337	-2.248010	2.095787
55	6	0	5.535864	-1.235527	1.908775
56	6	0	4.172961	-1.502336	2.022363
57	6	0	3.595379	0.832932	1.776742
58	6	0	3.754614	-2.804774	2.351276
59	6	0	1.933968	-4.502157	3.595237
60	6	0	2.085707	-4.235904	4.959725
61	6	0	2.020545	-5.292164	5.862834
62	6	0	1.793547	-6.609860	5.428295
63	6	0	1.630680	-6.838495	4.055860
64	6	0	1.695891	-5.793265	3.131540
65	6	0	1.715279	-7.740184	6.424871
66	6	0	4.696552	-3.830201	2.526485
67	6	0	6.056863	-3.568572	2.406425
68	6	0	6.670182	-5.819237	2.924052
69	6	0	11.027809	-0.364947	1.330314
70	6	0	12.401180	-0.205103	1.238040
71	6	0	16.479748	4.863530	-0.344409
72	6	0	12.935170	10.752862	-1.101924
73	6	0	9.641761	4.677797	-1.390086
74	6	0	8.975324	3.463738	-1.452994
75	6	0	4.068198	0.026863	-1.975848
76	8	0	3.542076	1.277439	-2.062857
77	6	0	2.158778	1.408951	-2.374078
78	6	0	3.317009	-1.147630	-2.022525
79	8	0	5.846479	-3.742363	-1.633678
80	6	0	7.260921	-3.912129	-1.505726
81	6	0	15.774147	6.027293	-0.611296
82	6	0	12.220877	11.920975	-1.348262
83	6	0	10.842556	11.866579	-1.581833
84	16	0	-2.513683	-3.160966	1.336468
85	16	0	-1.628543	-0.772216	-1.921932
86	8	0	-1.111104	-2.449019	1.323567
87	8	0	-3.512434	1.395324	-1.529075
88	8	0	-1.167361	-2.245696	-1.674352
89	8	0	-6.052536	-3.357316	-2.839420
90	6	0	-2.596307	-4.099851	2.865901
91	6	0	-2.526515	-5.489653	2.742629
92	6	0	-2.571964	-6.279191	3.891033
93	6	0	-2.686127	-5.700446	5.162077
94	6	0	-2.780489	-6.556584	6.400198
95	6	0	-2.742205	-4.298950	5.257573
96	6	0	-2.700705	-3.495673	4.123156
97	6	0	-3.684549	-1.835507	1.644090
98	6	0	-5.048201	-2.117390	1.464291
99	6	0	-5.967077	-1.077970	1.613226
100	6	0	-5.543592	0.227907	1.924546
101	6	0	-6.483305	1.281649	2.038212

102	6	0	-7.293937	2.186710	2.132716
103	6	0	-8.219542	3.255987	2.255910
104	6	0	-7.768216	4.552498	2.587266
105	6	0	-8.664736	5.601168	2.712775
106	6	0	-10.048296	5.396392	2.511957
107	6	0	-10.965963	6.468976	2.649162
108	6	0	-11.762102	7.381108	2.776984
109	6	0	-12.679512	8.450607	2.954720
110	6	0	-12.232757	9.678534	3.479411
111	6	0	-14.058900	8.294157	2.627429
112	6	0	-14.549025	7.079436	2.076307
113	6	0	-14.988612	6.053175	1.592311
114	6	0	-15.490110	4.849928	1.024733
115	6	0	-14.659204	4.028367	0.232972
116	6	0	-15.145652	2.852945	-0.319080
117	6	0	-16.480023	2.449862	-0.098174
118	6	0	-16.975632	1.239254	-0.653581
119	6	0	-17.398855	0.199229	-1.123189
120	6	0	-17.935772	-0.998181	-1.666922
121	6	0	-17.090567	-2.016404	-2.199387
122	6	0	-17.672487	-3.181609	-2.735248
123	6	0	-19.052343	-3.350122	-2.747516
124	6	0	-19.882004	-2.353884	-2.221318
125	6	0	-19.329912	-1.194046	-1.688231
126	6	0	-15.677608	-1.875831	-2.190020
127	6	0	-14.463542	-1.784489	-2.189299
128	6	0	-13.050569	-1.665415	-2.185068
129	6	0	-12.238455	-2.670039	-2.757687
130	6	0	-10.857993	-2.551379	-2.755833
131	6	0	-10.234516	-1.420125	-2.185032
132	6	0	-8.820196	-1.300584	-2.188437
133	6	0	-7.605053	-1.208886	-2.200471
134	6	0	-6.193880	-1.092596	-2.202999
135	6	0	-5.578977	0.127192	-1.867765
136	6	0	-4.188848	0.247889	-1.825220
137	6	0	-4.266748	2.559440	-1.170907
138	6	0	-3.412479	-0.882798	-2.121877
139	6	0	-1.083894	-0.423787	-3.618096
140	6	0	-1.417197	0.806182	-4.194452
141	6	0	-0.963423	1.090762	-5.479366
142	6	0	-0.178113	0.172472	-6.197238
143	6	0	0.149950	-1.041886	-5.580818
144	6	0	-0.293109	-1.351080	-4.291658
145	6	0	0.280492	0.488312	-7.599522
146	6	0	-3.997628	-2.099698	-2.484619
147	6	0	-5.383796	-2.217434	-2.527860
148	6	0	-5.301590	-4.498545	-3.229566
149	6	0	-11.043783	-0.414841	-1.612185
150	6	0	-12.423876	-0.537424	-1.609063
151	6	0	-17.312265	3.275533	0.687591
152	6	0	-14.936294	9.371584	2.851180
153	6	0	-10.498597	4.098300	2.180733
154	6	0	-9.601889	3.048791	2.055587
155	6	0	-4.156506	0.486503	2.103316
156	8	0	-3.824935	1.775326	2.385219
157	6	0	-2.459130	2.088368	2.609211
158	6	0	-3.237078	-0.551204	1.962330
159	8	0	-5.355426	-3.405332	1.157538
160	6	0	-6.725878	-3.747313	0.925172
161	6	0	-16.827329	4.452996	1.236985
162	6	0	-14.473004	10.574513	3.374127
163	6	0	-13.118250	10.730201	3.686739
164	1	0	4.821326	-6.179090	-7.703669

165	1	0	3.785008	-7.534753	-7.246889
166	1	0	3.091948	-6.106369	-8.033782
167	1	0	3.919625	-7.617023	-4.832688
168	1	0	3.267483	-3.834637	-6.764605
169	1	0	2.955090	-2.751075	-4.560826
170	1	0	3.606462	-6.546042	-2.621877
171	1	0	7.634721	-3.459387	-0.581299
172	1	0	7.426749	-4.989029	-1.477617
173	1	0	7.785969	-3.486561	-2.367970
174	1	0	1.976285	2.480390	-2.463302
175	1	0	1.913852	0.919306	-3.323955
176	1	0	1.527041	0.994140	-1.579013
177	1	0	2.241311	-1.132467	-2.139827
178	1	0	7.170769	-1.337446	-1.556293
179	1	0	9.534246	2.533949	-1.418290
180	1	0	10.723087	4.704257	-1.305561
181	1	0	6.966524	6.781760	-1.615758
182	1	0	5.775406	4.611800	-1.731531
183	1	0	9.116814	10.589671	-1.759665
184	1	0	10.284813	12.777976	-1.772979
185	1	0	12.737779	12.875549	-1.356615
186	1	0	14.003173	10.790740	-0.915556
187	1	0	12.719866	5.101264	0.585144
188	1	0	13.984736	3.022788	1.070045
189	1	0	17.531980	4.794394	-0.599329
190	1	0	16.272510	6.871834	-1.075329
191	1	0	19.820295	1.342783	0.665108
192	1	0	21.190446	-0.670902	1.118326
193	1	0	20.084286	-2.819467	1.721483
194	1	0	17.610677	-2.936343	1.858371
195	1	0	12.820740	0.737618	0.903807
196	1	0	10.365013	0.456352	1.076815
197	1	0	10.929698	-3.599383	2.415870
198	1	0	13.384934	-3.308935	2.257074
199	1	0	5.888805	-0.245359	1.652680
200	1	0	4.348040	-4.824858	2.770439
201	1	0	6.145953	-5.836304	3.887080
202	1	0	6.042626	-6.290083	2.157131
203	1	0	7.606036	-6.370708	3.012940
204	1	0	4.173630	1.086215	2.669672
205	1	0	4.169946	1.059197	0.873975
206	1	0	2.667169	1.405208	1.767868
207	1	0	2.263335	-3.224448	5.314449
208	1	0	1.562482	-5.966853	2.069439
209	1	0	1.451332	-7.849642	3.701041
210	1	0	2.146591	-5.092527	6.923453
211	1	0	2.583240	-7.741822	7.092168
212	1	0	0.825886	-7.644667	7.058392
213	1	0	1.668440	-8.712255	5.928258
214	1	0	-2.243030	-6.106401	7.240120
215	1	0	-3.825407	-6.672230	6.712294
216	1	0	-2.378588	-7.558528	6.228774
217	1	0	-2.830035	-3.834285	6.235915
218	1	0	-2.766504	-2.416328	4.212049
219	1	0	-2.439787	-5.948418	1.761969
220	1	0	-2.526303	-7.360445	3.797121
221	1	0	-2.050305	1.522012	3.455856
222	1	0	-1.851420	1.897463	1.714273
223	1	0	-2.429627	3.152811	2.843685
224	1	0	-7.334773	-3.551352	1.814380
225	1	0	-7.130126	-3.202666	0.065605
226	1	0	-6.729746	-4.816755	0.715014
227	1	0	-2.173530	-0.388566	2.074614

228	1	0	-7.025893	-1.250827	1.471398
229	1	0	-6.707932	4.718253	2.748205
230	1	0	-8.311022	6.593704	2.970682
231	1	0	-11.560383	3.931400	2.032917
232	1	0	-9.959349	2.054143	1.808757
233	1	0	-11.181613	9.788026	3.725128
234	1	0	-12.755979	11.669049	4.093631
235	1	0	-15.167433	11.392944	3.536704
236	1	0	-15.984973	9.248168	2.602521
237	1	0	-13.634540	4.336051	0.049834
238	1	0	-14.505859	2.236429	-0.942188
239	1	0	-17.475553	5.079375	1.840674
240	1	0	-18.340839	2.977255	0.860914
241	1	0	-19.969491	-0.417715	-1.282011
242	1	0	-20.959969	-2.482050	-2.228715
243	1	0	-19.482320	-4.255079	-3.165097
244	1	0	-17.021158	-3.949635	-3.139135
245	1	0	-12.710632	-3.538878	-3.203603
246	1	0	-10.242681	-3.326766	-3.200345
247	1	0	-13.040565	0.233173	-1.159356
248	1	0	-10.573128	0.458925	-1.172779
249	1	0	-3.352514	-2.940524	-2.703395
250	1	0	-6.215575	0.968203	-1.626320
251	1	0	-6.032887	-5.270402	-3.470139
252	1	0	-4.689157	-4.291749	-4.115974
253	1	0	-4.657341	-4.853425	-2.414080
254	1	0	-4.853249	2.390525	-0.262579
255	1	0	-3.529122	3.340994	-0.988043
256	1	0	-4.924889	2.867767	-1.990416
257	1	0	-0.018807	-2.284063	-3.811610
258	1	0	-1.225000	2.041535	-5.935850
259	1	0	0.758535	-1.765018	-6.117379
260	1	0	-2.027832	1.522947	-3.653981
261	1	0	1.061657	-0.199648	-7.932383
262	1	0	-0.552411	0.411705	-8.308240
263	1	0	0.671060	1.508071	-7.672108
264	1	0	1.737418	-0.791013	0.714936
265	1	0	0.200315	-0.739415	0.975713
266	1	0	-0.028783	-4.985672	-1.529826
267	1	0	-1.418013	-4.346360	-1.407510

Atomic coordinates of compound (*S,S*)-2 (Structure detailed in Figure S23 discontinuous blue line, corresponding to X-Ray structure of octahedral complex with two water molecules and two triflate anions).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.027598	-1.329721	0.018058
2	16	0	-2.610683	-1.927127	1.633331
3	16	0	-2.116458	-0.493588	-2.298283
4	8	0	-1.370608	-1.007702	1.586944
5	8	0	-4.148482	1.269521	-3.225652
6	8	0	-1.556085	-1.599522	-1.370771
7	8	0	-6.302388	-3.479888	-1.381882
8	8	0	0.248040	0.756709	-0.144219
9	8	0	-0.146640	-3.408531	0.360285
10	6	0	-2.563727	-2.790528	3.224124
11	6	0	-1.952123	-4.047804	3.197432
12	6	0	-1.831285	-4.775353	4.379945
13	6	0	-2.321307	-4.268661	5.590627

14	6	0	-2.168698	-5.055166	6.871638
15	6	0	-2.926935	-3.003559	5.592670
16	6	0	-3.041221	-2.256273	4.421799
17	6	0	-3.973224	-0.758473	1.886983
18	6	0	-5.298198	-1.228372	1.939480
19	6	0	-6.330771	-0.298982	1.982768
20	6	0	-6.057057	1.086283	1.958793
21	6	0	-7.126708	2.016321	1.977000
22	6	0	-8.055559	2.804579	1.984609
23	6	0	-9.101624	3.760236	1.975798
24	6	0	-8.807954	5.141645	1.904257
25	6	0	-9.824177	6.083475	1.885677
26	6	0	-11.178797	5.687357	1.935081
27	6	0	-12.220117	6.653115	1.904042
28	6	0	-13.117314	7.476386	1.871352
29	6	0	-14.142536	8.457028	1.850225
30	6	0	-13.836358	9.803911	2.130975
31	6	0	-15.495250	8.110203	1.553208
32	6	0	-15.855690	6.772584	1.239261
33	6	0	-16.179531	5.634062	0.955046
34	6	0	-16.543728	4.301201	0.623861
35	6	0	-15.556215	3.320068	0.386608
36	6	0	-15.912343	2.017768	0.069050
37	6	0	-17.270595	1.643892	-0.025768
38	6	0	-17.638170	0.308408	-0.342167
39	6	0	-17.946440	-0.839722	-0.604262
40	6	0	-18.335997	-2.176751	-0.883582
41	6	0	-17.370036	-3.173319	-1.216765
42	6	0	-17.812515	-4.490221	-1.455409
43	6	0	-19.160255	-4.822603	-1.378937
44	6	0	-20.107336	-3.842441	-1.061287
45	6	0	-19.696360	-2.537130	-0.816702
46	6	0	-15.988418	-2.863347	-1.315445
47	6	0	-14.796528	-2.635067	-1.421085
48	6	0	-13.405000	-2.375530	-1.544635
49	6	0	-12.466238	-3.425321	-1.439000
50	6	0	-11.108273	-3.178321	-1.559468
51	6	0	-10.626381	-1.870040	-1.797158
52	6	0	-9.235236	-1.631007	-1.922845
53	6	0	-8.031781	-1.469686	-2.030093
54	6	0	-6.632454	-1.274845	-2.153449
55	6	0	-6.129423	-0.041212	-2.623469
56	6	0	-4.757516	0.159641	-2.741770
57	6	0	-4.884257	2.479893	-3.363020
58	6	0	-3.892095	-0.873870	-2.342092
59	6	0	-1.654435	-0.981221	-3.980496
60	6	0	-1.411217	0.023289	-4.916506
61	6	0	-1.028134	-0.356231	-6.206150
62	6	0	-0.873045	-1.703392	-6.553343
63	6	0	-1.113135	-2.683947	-5.577032
64	6	0	-1.504146	-2.335291	-4.288225
65	6	0	-0.445820	-2.104686	-7.946502
66	6	0	-4.357345	-2.101338	-1.890069
67	6	0	-5.738017	-2.321618	-1.805428
68	6	0	-5.429705	-4.574617	-1.057134
69	6	0	-11.567776	-0.821056	-1.905463
70	6	0	-12.926487	-1.068192	-1.780136
71	6	0	-18.257330	2.625933	0.207678
72	6	0	-16.478797	9.118505	1.562150
73	6	0	-11.473848	4.308636	2.012103
74	6	0	-10.457702	3.365829	2.032559
75	6	0	-4.714174	1.543445	1.894276
76	8	0	-4.530945	2.876442	1.874720

77	6	0	-3.202876	3.385764	1.643432
78	6	0	-3.677109	0.598913	1.854402
79	8	0	-5.455684	-2.585273	1.950746
80	6	0	-6.777773	-3.107337	1.948152
81	6	0	-17.901325	3.927681	0.525236
82	6	0	-16.151190	10.439375	1.846544
83	6	0	-14.824084	10.782296	2.129132
84	16	0	2.694875	-2.398970	-1.336278
85	16	0	2.113285	-0.298513	2.318196
86	8	0	1.421113	-1.544977	-1.535398
87	8	0	4.102647	1.590480	3.085124
88	8	0	1.596816	-1.486462	1.476119
89	8	0	6.360612	-3.318497	1.908707
90	6	0	2.784252	-3.465937	-2.784173
91	6	0	2.615308	-4.832547	-2.547335
92	6	0	2.528310	-5.695182	-3.638038
93	6	0	2.600902	-5.214331	-4.951358
94	6	0	2.434518	-6.163310	-6.114325
95	6	0	2.778183	-3.838028	-5.156920
96	6	0	2.857934	-2.956308	-4.081427
97	6	0	4.027659	-1.210752	-1.666556
98	6	0	5.368269	-1.636172	-1.644692
99	6	0	6.369035	-0.682093	-1.783458
100	6	0	6.048322	0.686752	-1.923590
101	6	0	7.087011	1.644678	-2.034842
102	6	0	7.992019	2.456168	-2.118836
103	6	0	9.010365	3.437309	-2.202369
104	6	0	8.677965	4.808380	-2.301549
105	6	0	9.667595	5.775539	-2.373447
106	6	0	11.033401	5.417040	-2.346565
107	6	0	12.046892	6.410341	-2.408429
108	6	0	12.919876	7.258735	-2.455025
109	6	0	13.914576	8.267532	-2.530378
110	6	0	13.575802	9.559458	-2.981174
111	6	0	15.268697	8.004967	-2.161828
112	6	0	15.661636	6.728802	-1.677325
113	6	0	16.014756	5.646193	-1.246970
114	6	0	16.414906	4.379059	-0.743975
115	6	0	15.456170	3.394858	-0.417961
116	6	0	15.848258	2.156727	0.068916
117	6	0	17.215073	1.852835	0.251008
118	6	0	17.619756	0.582385	0.742059
119	6	0	17.959987	-0.511200	1.154687
120	6	0	18.385053	-1.787531	1.610530
121	6	0	17.442649	-2.767915	2.044271
122	6	0	17.919940	-4.027822	2.458313
123	6	0	19.279318	-4.319347	2.456803
124	6	0	20.202987	-3.354015	2.040316
125	6	0	19.757559	-2.105128	1.622487
126	6	0	16.049835	-2.495455	2.069600
127	6	0	14.849673	-2.292311	2.114674
128	6	0	13.449338	-2.056672	2.166762
129	6	0	12.537250	-3.134707	2.160874
130	6	0	11.170974	-2.909004	2.209803
131	6	0	10.654314	-1.594161	2.272802
132	6	0	9.255126	-1.374266	2.323988
133	6	0	8.046597	-1.223102	2.367723
134	6	0	6.641741	-1.033418	2.415221
135	6	0	6.112445	0.241252	2.711278
136	6	0	4.735169	0.438091	2.757562
137	6	0	4.825154	2.816361	3.102775
138	6	0	3.892895	-0.645332	2.454243
139	6	0	1.624987	-0.657907	4.026386

140	6	0	1.432818	0.417651	4.892885
141	6	0	1.049805	0.145425	6.208875
142	6	0	0.844332	-1.166592	6.650211
143	6	0	1.030417	-2.220088	5.740786
144	6	0	1.415838	-1.980537	4.424802
145	6	0	0.395513	-1.450861	8.065020
146	6	0	4.384911	-1.912640	2.167378
147	6	0	5.769403	-2.126014	2.164080
148	6	0	5.520151	-4.475491	1.776612
149	6	0	11.569017	-0.516515	2.282591
150	6	0	12.935985	-0.742823	2.228778
151	6	0	18.172902	2.838073	-0.072014
152	6	0	16.221256	9.036897	-2.271604
153	6	0	11.367350	4.048183	-2.253036
154	6	0	10.377942	3.079796	-2.183295
155	6	0	4.690178	1.100551	-1.925023
156	8	0	4.460054	2.420289	-2.056823
157	6	0	3.109810	2.902622	-1.915457
158	6	0	3.685343	0.129947	-1.788854
159	8	0	5.569760	-2.976898	-1.484461
160	6	0	6.906079	-3.454464	-1.422528
161	6	0	17.780959	4.075648	-0.558719
162	6	0	15.861889	10.301637	-2.723325
163	6	0	14.533067	10.563076	-3.076432
164	9	0	-0.594828	-6.090864	-4.519011
165	8	0	-2.699019	-4.972756	-2.789853
166	8	0	-0.534861	-5.306195	-1.584523
167	8	0	-2.416390	-6.940690	-1.274088
168	9	0	-0.144915	-7.758144	-3.195812
169	9	0	-2.092644	-7.623493	-4.150217
170	16	0	-1.772537	-5.928233	-2.127509
171	6	0	-1.114088	-6.904205	-3.571502
172	9	0	0.302491	-7.257741	3.266938
173	8	0	3.082472	-6.347380	3.073986
174	8	0	1.483968	-4.620989	2.236895
175	8	0	2.751066	-6.032212	0.611099
176	9	0	-0.202326	-6.753848	1.211198
177	9	0	1.211866	-8.357229	1.626231
178	16	0	2.195528	-5.912824	1.977331
179	6	0	0.797307	-7.140450	2.011346
180	9	0	-0.777803	5.961928	-2.690232
181	8	0	-1.688137	3.375216	-4.003342
182	8	0	-2.083250	3.516021	-1.533815
183	8	0	-0.127556	2.227747	-2.428084
184	9	0	0.631460	4.905412	-1.410024
185	9	0	0.860368	4.830267	-3.569547
186	16	0	-1.120457	3.328280	-2.636256
187	6	0	-0.041860	4.842603	-2.566919
188	9	0	0.784327	6.183398	2.316773
189	8	0	1.584542	3.569676	3.655796
190	8	0	2.051581	3.721244	1.199986
191	8	0	0.043624	2.466065	2.023524
192	9	0	-0.655667	5.167885	1.039148
193	9	0	-0.885634	5.102852	3.199073
194	16	0	1.053948	3.540806	2.272326
195	6	0	0.017356	5.084833	2.196138
196	1	0	0.061503	1.283259	-0.956412
197	1	0	-0.323670	-4.045138	-0.370945
198	1	0	-1.553493	-4.446755	2.270459
199	1	0	-1.337986	-5.742003	4.349263
200	1	0	-1.185869	-4.878657	7.326816
201	1	0	-2.250057	-6.131476	6.691297
202	1	0	-2.926232	-4.772755	7.609825

203	1	0	-3.311212	-2.594901	6.524727
204	1	0	-3.503646	-1.275010	4.440175
205	1	0	-7.365733	-0.614806	2.012970
206	1	0	-7.769692	5.453072	1.860147
207	1	0	-9.584653	7.140468	1.826232
208	1	0	-12.806363	10.062764	2.353485
209	1	0	-14.509602	3.599112	0.451396
210	1	0	-15.146039	1.269405	-0.104962
211	1	0	-17.073681	-5.244323	-1.706220
212	1	0	-19.474153	-5.844894	-1.569153
213	1	0	-21.161398	-4.097468	-1.002434
214	1	0	-20.421669	-1.770366	-0.563722
215	1	0	-12.821743	-4.435026	-1.258824
216	1	0	-10.393628	-3.990516	-1.476948
217	1	0	-6.831395	0.739486	-2.889383
218	1	0	-4.142210	3.226965	-3.641837
219	1	0	-5.358859	2.758576	-2.414839
220	1	0	-5.649775	2.387976	-4.145669
221	1	0	-1.507810	1.072492	-4.651524
222	1	0	-0.833081	0.415695	-6.946861
223	1	0	-0.990029	-3.737256	-5.815026
224	1	0	-1.684434	-3.104007	-3.543149
225	1	0	-0.278512	-1.230063	-8.582284
226	1	0	-1.203154	-2.732739	-8.431429
227	1	0	0.483192	-2.687047	-7.924363
228	1	0	-3.635676	-2.861473	-1.612817
229	1	0	-6.090606	-5.414696	-0.837371
230	1	0	-4.829679	-4.340098	-0.171302
231	1	0	-4.762550	-4.825938	-1.885440
232	1	0	-11.211562	0.187467	-2.088441
233	1	0	-13.639186	-0.254410	-1.873188
234	1	0	-19.304231	2.348830	0.136191
235	1	0	-17.503821	8.842375	1.336032
236	1	0	-12.511523	3.993590	2.064089
237	1	0	-10.695599	2.308631	2.090441
238	1	0	-3.297263	4.469350	1.700305
239	1	0	-2.838724	3.108029	0.650414
240	1	0	-2.502328	3.045175	2.409839
241	1	0	-2.635753	0.893169	1.783931
242	1	0	-6.666951	-4.191895	1.979069
243	1	0	-7.315184	-2.825565	1.036046
244	1	0	-7.337391	-2.775887	2.832613
245	1	0	-18.668075	4.674489	0.704806
246	1	0	-16.925619	11.200813	1.845745
247	1	0	-14.561026	11.812782	2.349763
248	1	0	2.534400	-5.218265	-1.533895
249	1	0	2.353873	-6.752020	-3.460078
250	1	0	2.602089	-5.662716	-7.072855
251	1	0	1.419044	-6.574862	-6.116826
252	1	0	3.127974	-7.009496	-6.046763
253	1	0	2.832939	-3.450125	-6.171515
254	1	0	2.962820	-1.888825	-4.247235
255	1	0	7.414451	-0.962678	-1.764975
256	1	0	7.630921	5.091927	-2.316664
257	1	0	9.398082	6.824543	-2.445120
258	1	0	12.544870	9.754845	-3.257575
259	1	0	14.403013	3.620966	-0.549129
260	1	0	15.104052	1.404753	0.310313
261	1	0	17.198835	-4.770029	2.784815
262	1	0	19.620388	-5.297863	2.782330
263	1	0	21.265922	-3.577026	2.039418
264	1	0	20.464830	-1.351246	1.291691
265	1	0	12.919732	-4.149510	2.113942

266	1	0	10.476858	-3.742873	2.203380
267	1	0	6.797858	1.057304	2.904040
268	1	0	4.068925	3.582323	3.267156
269	1	0	5.329564	2.986647	2.144426
270	1	0	5.564202	2.825646	3.915648
271	1	0	1.565772	1.441627	4.551801
272	1	0	0.894533	0.974136	6.895727
273	1	0	0.864804	-3.245576	6.061739
274	1	0	1.531383	-2.800492	3.720474
275	1	0	0.985711	-2.255037	8.519236
276	1	0	-0.654273	-1.769936	8.088725
277	1	0	0.485918	-0.564570	8.700340
278	1	0	3.679020	-2.700839	1.927501
279	1	0	6.202163	-5.317111	1.648974
280	1	0	4.867426	-4.404569	0.902797
281	1	0	4.914160	-4.640420	2.671426
282	1	0	11.185571	0.497423	2.331265
283	1	0	13.627958	0.093688	2.243895
284	1	0	19.226068	2.614586	0.065154
285	1	0	17.247646	8.824535	-1.989628
286	1	0	12.414168	3.760199	-2.245064
287	1	0	10.645638	2.030679	-2.110392
288	1	0	3.169184	3.978444	-2.072771
289	1	0	2.723010	2.711021	-0.910977
290	1	0	2.445426	2.465775	-2.665882
291	1	0	2.634987	0.395170	-1.752579
292	1	0	6.827287	-4.537659	-1.322145
293	1	0	7.433461	-3.048096	-0.552288
294	1	0	7.456957	-3.214929	-2.341600
295	1	0	18.525740	4.825470	-0.805584
296	1	0	16.612670	11.082846	-2.798024
297	1	0	14.244974	11.549649	-3.427839
298	1	0	0.144188	1.363459	0.624959
299	1	0	0.509051	-3.816437	0.971960

Structure of compound (*S,S*)-1: two representative conformations with no counter-ion and Ag complexes with one , two or three Ag+ [4]

Conf1 (Red line, Figure S28)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.083214	2.023544	-0.904771
2	16	0	-1.983463	-4.252582	-2.000540
3	8	0	-1.327482	-5.503309	-1.441311
4	8	0	2.650143	-2.501789	-0.451172
5	8	0	-0.570467	-1.021667	2.483926
6	8	0	-0.383136	3.236945	-1.067805
7	8	0	-4.077326	0.886221	-0.721677
8	6	0	2.722405	-3.598835	0.450852
9	1	0	2.671097	-4.559354	-0.076435
10	1	0	1.922242	-3.549569	1.198608
11	1	0	3.688468	-3.508978	0.947924
12	8	0	-1.988414	-1.598894	-3.351463
13	6	0	5.376629	-0.331158	2.378514
14	6	0	4.148306	-0.614490	3.045923
15	6	0	-1.783967	-1.742760	2.672968
16	1	0	-2.139521	-2.183105	1.736564
17	1	0	-2.568139	-1.102166	3.095001

18	1	0	-1.548647	-2.536691	3.382619
19	6	0	5.501087	1.634293	-1.172992
20	6	0	-1.706794	0.481357	0.933937
21	1	0	-2.673776	0.000600	1.025958
22	6	0	5.425680	0.922818	0.056651
23	6	0	4.519679	1.468105	-2.194149
24	6	0	-4.848561	3.163511	0.892748
25	1	0	-5.318243	2.186015	0.850732
26	6	0	2.909995	-0.190775	2.494901
27	6	0	-0.576650	0.021731	1.614486
28	6	0	6.585344	-0.742776	2.970428
29	1	0	7.515568	-0.521996	2.457455
30	6	0	-5.378846	4.202515	1.658682
31	1	0	-6.281169	4.030642	2.240155
32	6	0	-4.382101	-4.284078	1.279745
33	1	0	-4.592228	-4.991868	2.078197
34	6	0	1.498906	-2.317963	-1.143665
35	6	0	-1.602776	1.560990	0.062529
36	6	0	0.672148	0.651692	1.390087
37	6	0	-3.693998	3.388420	0.150451
38	6	0	0.257068	-0.886227	-2.682873
39	1	0	0.222621	0.018373	-3.276022
40	6	0	0.425172	-3.212705	-1.145013
41	1	0	0.455600	-4.158874	-0.615646
42	6	0	-4.773791	5.464842	1.685986
43	6	0	6.593980	-1.425537	4.181965
44	1	0	7.537973	-1.736115	4.619138
45	6	0	-3.832623	-2.475819	-0.777391
46	1	0	-3.618752	-1.756349	-1.559227
47	6	0	-5.081991	-3.071561	1.230876
48	6	0	-3.421333	-4.602084	0.317939
49	1	0	-2.872913	-5.538369	0.345696
50	6	0	3.439885	0.553216	-2.052370
51	6	0	-3.618766	5.665504	0.914491
52	1	0	-3.140229	6.641790	0.914507
53	6	0	1.422334	-1.143249	-1.933213
54	6	0	4.637516	2.223851	-3.377829
55	1	0	3.890405	2.088505	-4.153126
56	6	0	5.393409	0.352339	1.130729
57	6	0	0.753481	1.738352	0.499157
58	1	0	1.725322	2.183457	0.334056
59	6	0	-0.718176	-2.933242	-1.883798
60	6	0	-0.376954	2.197402	-0.172980
61	6	0	-0.819648	-1.770704	-2.660851
62	6	0	1.854295	0.178367	2.017703
63	6	0	6.658124	3.266698	-2.566482
64	1	0	7.484662	3.956344	-2.707543
65	6	0	-3.153250	-3.693988	-0.704004
66	6	0	6.562020	2.535154	-1.388270
67	1	0	7.305648	2.652584	-0.606999
68	6	0	4.182254	-1.310524	4.269194
69	1	0	3.243172	-1.522377	4.769497
70	6	0	-3.076231	4.640573	0.142735
71	1	0	-2.180955	4.805443	-0.446994
72	6	0	-4.783769	-2.171688	0.195890
73	1	0	-5.280772	-1.207529	0.146208
74	6	0	5.689907	3.112704	-3.563766
75	1	0	5.759965	3.680257	-4.486734
76	6	0	0.871155	3.795439	-1.447122
77	1	0	0.647917	4.535254	-2.216954
78	1	0	1.541676	3.030047	-1.853720
79	1	0	1.361196	4.291731	-0.600676
80	6	0	2.512220	-0.232339	-1.986468

81	6	0	-6.149806	-2.748237	2.249386
82	1	0	-7.147929	-2.991425	1.864375
83	1	0	-6.154209	-1.683158	2.501190
84	1	0	-6.010054	-3.317059	3.173311
85	6	0	5.388933	-1.712444	4.831241
86	1	0	5.391765	-2.246324	5.776676
87	6	0	-2.102354	-0.478203	-4.219127
88	1	0	-3.086136	-0.558677	-4.681995
89	1	0	-1.329520	-0.496877	-4.997510
90	1	0	-2.040968	0.466946	-3.666504
91	6	0	-5.336446	6.580955	2.533432
92	1	0	-6.374591	6.385145	2.815247
93	1	0	-5.303429	7.539942	2.006646
94	1	0	-4.761430	6.701690	3.459773

Conf2 (Orange dashed line, Figure S28)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.105766	-2.499311	1.886819
2	16	0	4.105768	-2.499358	-1.886842
3	8	0	5.389957	-1.684612	-1.939638
4	8	0	2.407041	2.399006	-1.695517
5	8	0	-2.406950	2.399015	1.695550
6	8	0	-1.186670	-3.004388	1.894151
7	8	0	-5.389915	-1.684507	1.939705
8	6	0	3.761516	2.819184	-1.570632
9	1	0	4.359104	2.516155	-2.438444
10	1	0	4.222664	2.422457	-0.659184
11	1	0	3.727245	3.906844	-1.510914
12	8	0	1.186677	-3.004367	-1.894373
13	6	0	1.702843	4.845822	1.099909
14	6	0	1.991696	3.656318	1.835110
15	6	0	-3.761397	2.819210	1.570401
16	1	0	-4.359109	2.516368	2.438194
17	1	0	-4.222436	2.422313	0.658972
18	1	0	-3.727085	3.906857	1.510469
19	6	0	-1.702727	4.845853	-1.099977
20	6	0	-3.131051	0.076484	1.734472
21	1	0	-4.188995	0.309702	1.708803
22	6	0	-0.509476	4.935512	-0.331314
23	6	0	-1.991589	3.656377	-1.835218
24	6	0	-4.634229	-2.535376	-0.852719
25	1	0	-5.138212	-1.590859	-0.675431
26	6	0	1.059619	2.582517	1.856747
27	6	0	-2.148574	1.070068	1.748159
28	6	0	2.625771	5.906195	1.127545
29	1	0	2.397161	6.808306	0.569540
30	6	0	-4.625832	-3.113154	-2.118832
31	1	0	-5.113979	-2.598450	-2.942523
32	6	0	4.625646	-3.113396	2.118804
33	1	0	5.113803	-2.598764	2.942535
34	6	0	2.148649	1.070065	-1.748216
35	6	0	-2.766456	-1.264087	1.780488
36	6	0	-0.782626	0.696755	1.837875
37	6	0	-4.006404	-3.196619	0.203542
38	6	0	0.439872	-0.668110	-1.893843
39	1	0	-0.609686	-0.927193	-1.947119

40	6	0	3.131107	0.076462	-1.734487
41	1	0	4.189052	0.309656	-1.708707
42	6	0	-4.011791	-4.355389	-2.347428
43	6	0	3.813710	5.803181	1.845551
44	1	0	4.514266	6.632601	1.850934
45	6	0	3.398769	-4.435425	-0.009662
46	1	0	2.929088	-4.949468	-0.842051
47	6	0	4.011497	-4.355591	2.347329
48	6	0	4.634135	-2.535566	0.852716
49	1	0	5.138200	-1.591082	0.675486
50	6	0	-1.059516	2.582572	-1.856897
51	6	0	-3.400051	-5.003392	-1.266649
52	1	0	-2.932740	-5.972951	-1.419885
53	6	0	0.782699	0.696780	-1.838020
54	6	0	-3.201148	3.574114	-2.548468
55	1	0	-3.415932	2.667288	-3.104193
56	6	0	0.509615	4.935499	0.331212
57	6	0	-0.439824	-0.668146	1.893648
58	1	0	0.609732	-0.927249	1.946866
59	6	0	2.766487	-1.264101	-1.780566
60	6	0	-1.423613	-1.655574	1.862219
61	6	0	1.423641	-1.655558	-1.862390
62	6	0	0.224766	1.698341	1.860790
63	6	0	-3.813601	5.803241	-1.845564
64	1	0	-4.514157	6.632661	-1.850909
65	6	0	4.006292	-3.196714	-0.203595
66	6	0	-2.625656	5.906229	-1.127566
67	1	0	-2.397038	6.808321	-0.569533
68	6	0	3.201249	3.574027	2.548366
69	1	0	3.416029	2.667181	3.104059
70	6	0	-3.398992	-4.435372	0.009540
71	1	0	-2.929334	-4.949492	0.841894
72	6	0	3.399735	-5.003498	1.266505
73	1	0	2.932333	-5.973021	1.419685
74	6	0	-4.103969	4.633117	-2.553119
75	1	0	-5.031612	4.547918	-3.110646
76	6	0	0.159894	-3.444188	2.036618
77	1	0	0.115328	-4.532415	2.090919
78	1	0	0.613193	-3.054915	2.955801
79	1	0	0.773041	-3.151941	1.177347
80	6	0	-0.224669	1.698391	-1.860954
81	6	0	4.049231	-4.989921	3.717301
82	1	0	3.315515	-5.795449	3.808493
83	1	0	3.848514	-4.255887	4.504185
84	1	0	5.036793	-5.419785	3.923770
85	6	0	4.104071	4.633031	2.553064
86	1	0	5.031710	4.547808	3.110593
87	6	0	-0.159886	-3.444142	-2.036924
88	1	0	-0.115333	-4.532368	-2.091261
89	1	0	-0.613135	-3.054830	-2.956116
90	1	0	-0.773071	-3.151917	-1.177672
91	6	0	-4.049610	-4.989651	-3.717429
92	1	0	-5.037282	-5.419212	-3.923996
93	1	0	-3.316121	-5.795389	-3.808599
94	1	0	-3.848614	-4.255642	-4.504267

(S,S)-1_Ag (Green line, Figure S28)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.619801	-1.997840	1.068218
2	16	0	3.619700	1.997936	-1.068285
3	8	0	3.301556	1.770900	-2.539401
4	8	0	-1.542734	2.107970	-1.378933
5	8	0	-1.542625	-2.107916	1.378956
6	8	0	2.957931	-1.881329	-1.846887
7	8	0	3.301683	-1.770785	2.539336
8	6	0	-1.410419	2.371255	-2.778192
9	1	0	-0.846644	1.578250	-3.281481
10	1	0	-0.920148	3.335204	-2.949022
11	1	0	-2.426605	2.402960	-3.170768
12	8	0	2.957885	1.881257	1.846813
13	6	0	-5.580367	-1.306951	-1.568323
14	6	0	-4.434536	-1.935495	-2.139476
15	6	0	-1.410290	-2.371197	2.778215
16	1	0	-0.846529	-1.578177	3.281497
17	1	0	-0.919994	-3.335133	2.949041
18	1	0	-2.426472	-2.402925	3.170801
19	6	0	-5.580406	1.306810	1.568357
20	6	0	0.881717	-2.175064	1.126278
21	1	0	1.092384	-2.243772	2.188575
22	6	0	-5.473222	0.398859	0.468496
23	6	0	-4.434592	1.935385	2.139510
24	6	0	4.023999	-4.549433	2.053821
25	1	0	3.643939	-4.123238	2.976882
26	6	0	-3.115595	-1.725439	-1.609749
27	6	0	-0.411875	-2.096942	0.615658
28	6	0	-6.852257	-1.582287	-2.103657
29	1	0	-7.721576	-1.104472	-1.665047
30	6	0	4.449981	-5.875467	1.979449
31	1	0	4.386082	-6.506310	2.862306
32	6	0	4.449769	5.875606	-1.979449
33	1	0	4.385865	6.506457	-2.862299
34	6	0	-0.411971	2.096974	-0.615656
35	6	0	1.969522	-2.103000	0.269052
36	6	0	-0.597859	-1.928740	-0.779239
37	6	0	4.108157	-3.748941	0.917695
38	6	0	0.519936	1.854062	1.636739
39	1	0	0.353938	1.710656	2.696976
40	6	0	0.881613	2.175127	-1.126295
41	1	0	1.092261	2.243882	-2.188592
42	6	0	4.967089	-6.406786	0.789708
43	6	0	-6.995771	-2.447074	-3.183631
44	1	0	-7.983956	-2.644264	-3.586153
45	6	0	4.630607	4.241328	0.279547
46	1	0	4.697867	3.604642	1.155312
47	6	0	4.966842	6.406922	-0.789699
48	6	0	4.023831	4.549553	-2.053847
49	1	0	3.643797	4.123362	-2.976921
50	6	0	-3.115648	1.725369	1.609778
51	6	0	5.047412	-5.570114	-0.334267
52	1	0	5.449535	-5.963288	-1.264408
53	6	0	-0.597927	1.928720	0.779238
54	6	0	-4.604636	2.804002	3.231407
55	1	0	-3.731253	3.280709	3.663102
56	6	0	-5.473210	-0.398994	-0.468463

57	6	0	0.519989	-1.854111	-1.636762
58	1	0	0.353974	-1.710756	-2.697003
59	6	0	1.969432	2.103041	-0.269090
60	6	0	1.814367	-1.944810	-1.119324
61	6	0	1.814305	1.944791	1.119283
62	6	0	-1.930135	-1.797071	-1.272174
63	6	0	-6.995839	2.446885	3.183673
64	1	0	-7.984029	2.644045	3.586198
65	6	0	4.108003	3.749049	-0.917738
66	6	0	-6.852303	1.582107	2.103695
67	1	0	-7.721609	1.104269	1.665085
68	6	0	-4.604558	-2.804121	-3.231370
69	1	0	-3.731162	-3.280805	-3.663064
70	6	0	4.630781	-4.241222	-0.279574
71	1	0	4.698019	-3.604554	-1.155353
72	6	0	5.047189	5.570229	0.334267
73	1	0	5.449299	5.963400	1.264415
74	6	0	-5.871541	3.055444	3.749446
75	1	0	-5.981991	3.729026	4.593046
76	6	0	2.884909	-1.489856	-3.222688
77	1	0	3.912767	-1.503167	-3.583732
78	1	0	2.492955	-0.472677	-3.312585
79	1	0	2.287974	-2.202652	-3.803345
80	6	0	-1.930194	1.797023	1.272193
81	6	0	5.460006	7.832357	-0.726589
82	1	0	6.539162	7.881767	-0.916851
83	1	0	5.284549	8.274067	0.258733
84	1	0	4.968233	8.460232	-1.474700
85	6	0	-5.871456	-3.055602	-3.749405
86	1	0	-5.981889	-3.729191	-4.593001
87	6	0	2.884877	1.489914	3.222648
88	1	0	3.912733	1.503308	3.583695
89	1	0	2.492970	0.472725	3.312636
90	1	0	2.287905	2.202737	3.803235
91	6	0	5.460316	-7.832202	0.726670
92	1	0	6.539282	-7.881658	0.918000
93	1	0	5.285837	-8.273637	-0.258945
94	1	0	4.967814	-8.460289	1.474127
95	47	0	-3.064790	-0.000052	0.000013

(S,S)-1_Ag2 (Pale green line, Figure S28)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.497992	3.103880	0.305864
2	16	0	3.498907	-3.103168	-0.306106
3	8	0	3.968607	-1.990693	0.701894
4	8	0	-1.010980	-1.093935	1.419383
5	8	0	-1.011559	1.093540	-1.419226
6	8	0	1.693951	4.309420	2.191630
7	8	0	3.967904	1.991637	-0.702314
8	6	0	-0.357607	-0.628835	2.604520
9	1	0	0.434270	0.088924	2.363707
10	1	0	0.056158	-1.466060	3.175976
11	1	0	-1.129261	-0.134091	3.193323
12	8	0	1.694972	-4.309173	-2.191726
13	6	0	-6.125183	1.848936	0.832515
14	6	0	-5.012455	2.682164	1.122238
15	6	0	-0.358145	0.628441	-2.604339

16	1	0	0.433841	-0.089182	-2.363485
17	1	0	0.055481	1.465679	-3.175877
18	1	0	-1.129741	0.133540	-3.193088
19	6	0	-6.124610	-1.850281	-0.832531
20	6	0	1.069844	2.095418	-0.628303
21	1	0	1.679098	1.648069	-1.404354
22	6	0	-5.956742	-0.562366	-0.248209
23	6	0	-5.011660	-2.683274	-1.122047
24	6	0	3.430022	4.751149	-1.943128
25	1	0	3.024962	3.907274	-2.491167
26	6	0	-3.666785	2.288677	0.827494
27	6	0	-0.307013	1.865043	-0.548705
28	6	0	-7.423060	2.304196	1.129584
29	1	0	-8.270760	1.665850	0.906646
30	6	0	3.682045	5.957197	-2.585228
31	1	0	3.454492	6.054520	-3.643003
32	6	0	3.685111	-5.955558	2.585743
33	1	0	3.458712	-6.052398	3.643809
34	6	0	-0.306330	-1.865272	0.548800
35	6	0	1.691495	2.909687	0.315275
36	6	0	-1.042523	2.447628	0.510185
37	6	0	3.735015	4.638503	-0.582270
38	6	0	-0.393924	-3.271005	-1.454223
39	1	0	-0.982587	-3.709928	-2.249639
40	6	0	1.070584	-2.095346	0.628289
41	1	0	1.679798	-1.647902	1.404315
42	6	0	4.229978	7.054233	-1.894075
43	6	0	-7.616922	3.555397	1.705558
44	1	0	-8.623407	3.892160	1.930805
45	6	0	4.291190	-5.702340	-0.131287
46	1	0	4.537694	-5.596646	-1.183216
47	6	0	4.231761	-7.053079	1.894371
48	6	0	3.432916	-4.749611	1.943496
49	1	0	3.028923	-3.905318	2.491680
50	6	0	-3.666085	-2.289450	-0.827262
51	6	0	4.524708	6.907245	-0.531618
52	1	0	4.954370	7.740438	0.016340
53	6	0	-1.041783	-2.447980	-0.510062
54	6	0	-5.228972	-3.944709	-1.706231
55	1	0	-4.377970	-4.580584	-1.924305
56	6	0	-5.956942	0.561091	0.248154
57	6	0	-0.394777	3.270817	1.454278
58	1	0	-0.983476	3.709630	2.249727
59	6	0	1.692348	-2.909433	-0.315369
60	6	0	0.974465	3.523074	1.357817
61	6	0	0.975379	-3.522972	-1.357861
62	6	0	-2.451104	2.260334	0.627053
63	6	0	-7.615860	-3.557156	-1.705603
64	1	0	-8.622240	-3.894163	-1.930952
65	6	0	3.736435	-4.637601	0.582270
66	6	0	-7.422350	-2.305860	-1.129723
67	1	0	-8.270218	-1.667680	-0.906946
68	6	0	-5.230120	3.943485	1.706528
69	1	0	-4.379291	4.579532	1.924769
70	6	0	4.291044	5.702748	0.131029
71	1	0	4.538665	5.596579	1.182650
72	6	0	4.525034	-6.906702	0.531522
73	1	0	4.953705	-7.740285	-0.016625
74	6	0	-6.519472	-4.376237	-1.994787
75	1	0	-6.671440	-5.352169	-2.443817
76	6	0	1.034063	4.951196	3.287822
77	1	0	1.807569	5.512495	3.810213
78	1	0	0.595183	4.214093	3.969321

79	1	0	0.260984	5.639793	2.930356
80	6	0	-2.450401	-2.260973	-0.626853
81	6	0	4.522795	-8.343250	2.616965
82	1	0	5.464894	-8.267364	3.173115
83	1	0	4.616988	-9.181616	1.922896
84	1	0	3.738471	-8.580916	3.341366
85	6	0	-6.520757	4.374690	1.994972
86	1	0	-6.672998	5.350538	2.444092
87	6	0	1.035176	-4.950900	-3.288003
88	1	0	1.808778	-5.511944	-3.810525
89	1	0	0.596109	-4.213774	-3.969355
90	1	0	0.262260	-5.639725	-2.930624
91	6	0	4.520642	8.344540	-2.616573
92	1	0	5.460503	8.267494	-3.176329
93	1	0	4.618838	9.182124	-1.922128
94	1	0	3.734038	8.584211	-3.337856
95	47	0	-3.464232	-0.000359	0.000051
96	47	0	4.132365	0.000505	-0.000226

(S,S)-1_Ag3 (Dashed pale green line, Figure S28)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	3.050807	-2.160446	0.517923
2	16	0	3.049715	2.161024	-0.517938
3	8	0	3.189738	1.339452	-1.837141
4	8	0	-1.929460	1.648944	-1.934023
5	8	0	-1.928409	-1.649212	1.934156
6	8	0	1.787024	-2.729144	-2.038997
7	8	0	3.190808	-1.338994	1.837186
8	6	0	-1.561408	1.582267	-3.319891
9	1	0	-0.890047	0.737195	-3.508808
10	1	0	-1.090381	2.516049	-3.642057
11	1	0	-2.492837	1.437342	-3.864946
12	8	0	1.785913	2.729662	2.038979
13	6	0	-6.531747	-1.844768	-0.864954
14	6	0	-5.397612	-2.652029	-1.163385
15	6	0	-1.560329	-1.582636	3.320017
16	1	0	-0.889153	-0.737434	3.509025
17	1	0	-1.089077	-2.516350	3.642052
18	1	0	-2.491771	-1.437992	3.865124
19	6	0	-6.532665	1.843212	0.864650
20	6	0	0.387170	-1.993736	1.269762
21	1	0	0.789493	-1.790323	2.254963
22	6	0	-6.391515	0.559255	0.256156
23	6	0	-5.398904	2.650916	1.163290
24	6	0	2.851718	-4.741803	1.546106
25	1	0	1.858572	-4.494850	1.904946
26	6	0	-4.066595	-2.237420	-0.825253
27	6	0	-0.986971	-1.943154	1.014318
28	6	0	-7.815383	-2.319744	-1.185137
29	1	0	-8.680327	-1.705997	-0.959342
30	6	0	3.396575	-5.993376	1.800676
31	1	0	2.816487	-6.718615	2.363496
32	6	0	3.395059	5.993810	-1.801277
33	1	0	2.814962	6.718851	-2.364348
34	6	0	-0.988048	1.943166	-1.014245
35	6	0	1.271199	-2.287896	0.230605
36	6	0	-1.459465	-2.182628	-0.305541

37	6	0	3.609680	-3.816572	0.812226
38	6	0	-0.549302	2.475917	1.336190
39	1	0	-0.932381	2.651237	2.333997
40	6	0	0.386077	1.993937	-1.269741
41	1	0	0.788399	1.790478	-2.254931
42	6	0	4.682907	-6.343859	1.344644
43	6	0	-7.975090	-3.563247	-1.791630
44	1	0	-8.972079	-3.915796	-2.034368
45	6	0	4.891757	4.134863	-0.343595
46	1	0	5.478702	3.412635	0.217422
47	6	0	4.681252	6.344595	-1.345046
48	6	0	2.850365	4.742202	-1.546591
49	1	0	1.857334	4.495012	-1.905592
50	6	0	-4.067698	2.236860	0.825275
51	6	0	5.415042	-5.395078	0.610185
52	1	0	6.405542	-5.648584	0.245373
53	6	0	-1.460548	2.182683	0.305602
54	6	0	-5.581964	3.900817	1.781052
55	1	0	-4.717106	4.514788	2.007467
56	6	0	-6.391225	-0.560720	-0.256491
57	6	0	-0.548209	-2.475655	-1.336176
58	1	0	-0.931296	-2.650969	-2.333980
59	6	0	1.270092	2.288301	-0.230637
60	6	0	0.820858	-2.526444	-1.078575
61	6	0	0.819738	2.526855	1.078533
62	6	0	-2.861724	-2.130576	-0.578907
63	6	0	-7.976843	3.561036	1.791227
64	1	0	-8.974011	3.913164	2.033845
65	6	0	3.608342	3.817216	-0.812402
66	6	0	-7.816543	2.317639	1.184675
67	1	0	-8.681203	1.703553	0.958716
68	6	0	-5.580076	-3.902050	-1.781085
69	1	0	-4.714935	-4.515681	-2.007340
70	6	0	4.893247	-4.133922	0.343606
71	1	0	5.480177	-3.411497	-0.217175
72	6	0	5.413397	5.396073	-0.610291
73	1	0	6.403787	5.649804	-0.245340
74	6	0	-6.862450	4.350720	2.090845
75	1	0	-6.991675	5.317904	2.564972
76	6	0	1.408876	-3.375995	-3.280423
77	1	0	2.343342	-3.605703	-3.790423
78	1	0	0.803336	-2.708185	-3.899311
79	1	0	0.866705	-4.299792	-3.065496
80	6	0	-2.862786	2.130430	0.579016
81	6	0	5.262759	7.695755	-1.657872
82	1	0	5.724116	7.685054	-2.653341
83	1	0	6.036768	7.978959	-0.941252
84	1	0	4.493170	8.471972	-1.667132
85	6	0	-6.860332	-4.352499	-2.091030
86	1	0	-6.989094	-5.319768	-2.565108
87	6	0	1.407813	3.377055	3.280163
88	1	0	2.342299	3.606968	3.790033
89	1	0	0.802281	2.709512	3.899343
90	1	0	0.865647	4.300760	3.064839
91	6	0	5.264702	-7.694918	1.657360
92	1	0	5.728798	-7.683282	2.651549
93	1	0	6.036738	-7.979126	0.938990
94	1	0	4.494907	-8.470868	1.669496
95	47	0	-3.997738	-0.000406	-0.000072
96	47	0	3.451842	-0.850642	-1.776681
97	47	0	3.450224	0.851380	1.777339

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