Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

1D-helical platinum(II) complexes bearing metal-induced chirality, aggregation-induced red phosphorescence and circularly polarized luminescence

Jintong Song, Man Wang, Xuemei Xu, Lang Qu, Xiangge Zhou, and Haifeng Xiang*

College of Chemistry, Sichuan University

29 Wangjiang Road, Chengdu 610064, PR China

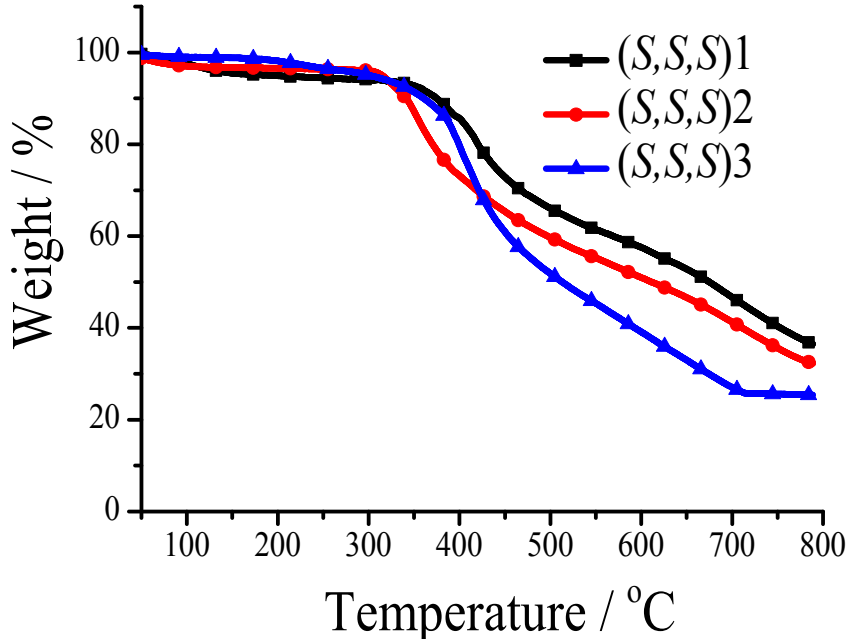


Fig. S1. Thermogravimetric analysis of the complexes.

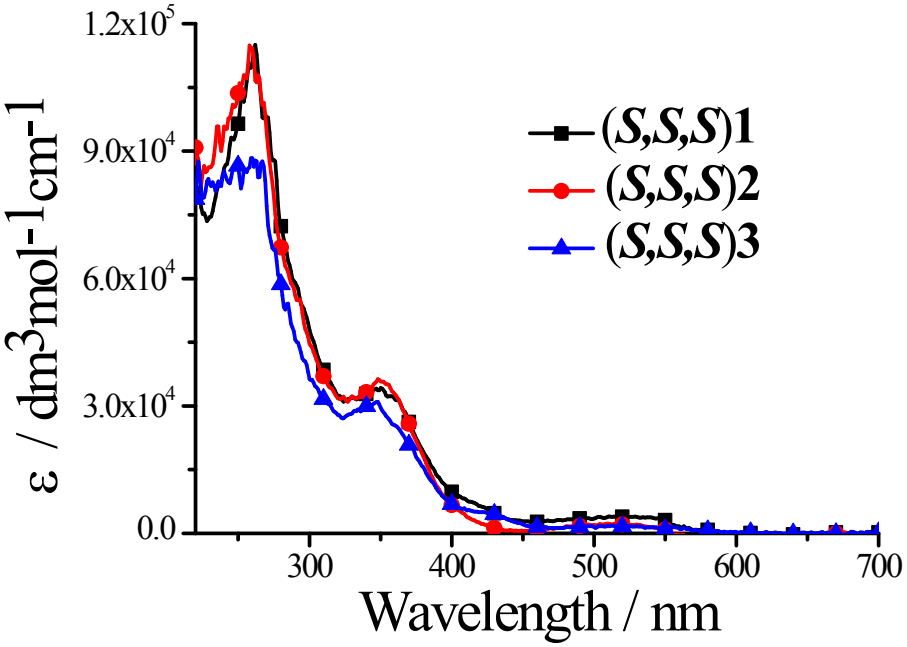


Fig. S2. Absorption spectra of the **(*S*,*S*,*S*)** complexes in MeCN (1.0×10^{-5} mol dm^{-3}).

.

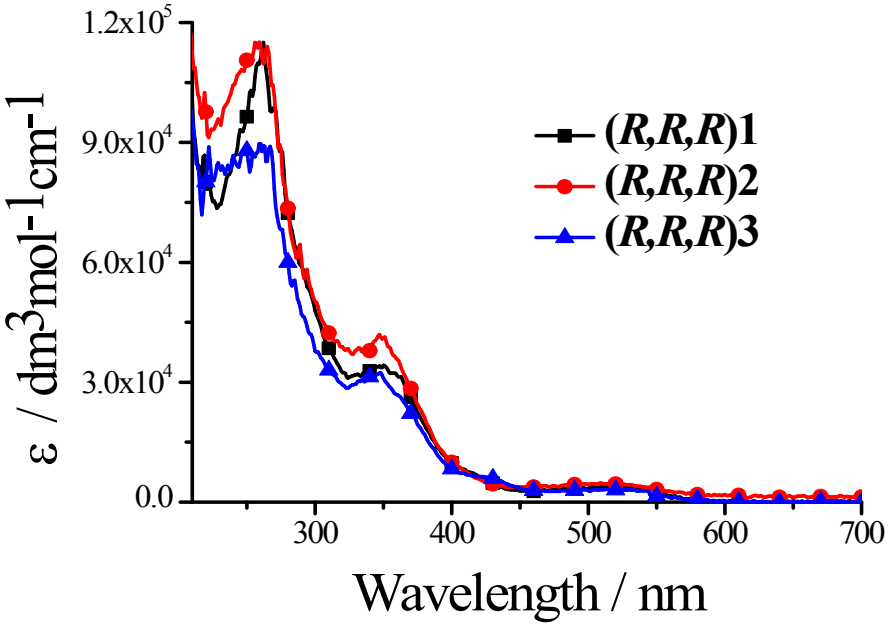


Fig. S3. Absorption spectra of the **(*R*,*R*,*R*)** complexes in MeCN. (1.0×10^{-5} mol dm^{-3}).

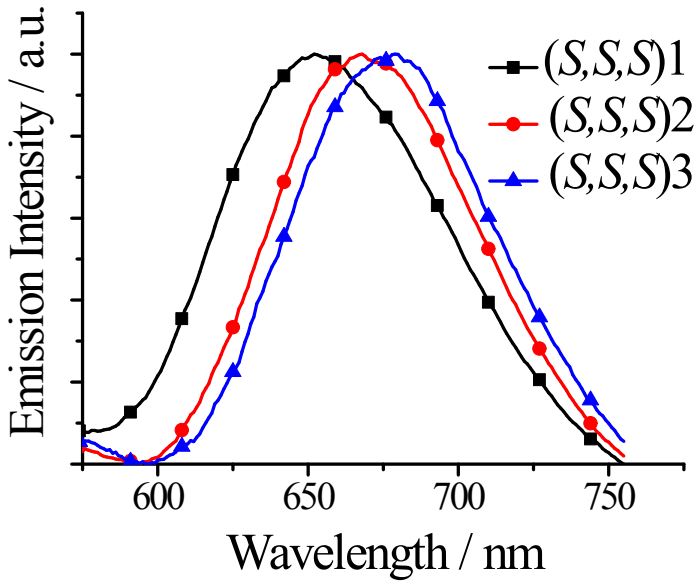


Fig. S4. Normalized emission spectra of **(*S*,*S*,*S*)1–3** in powder at 298 K.

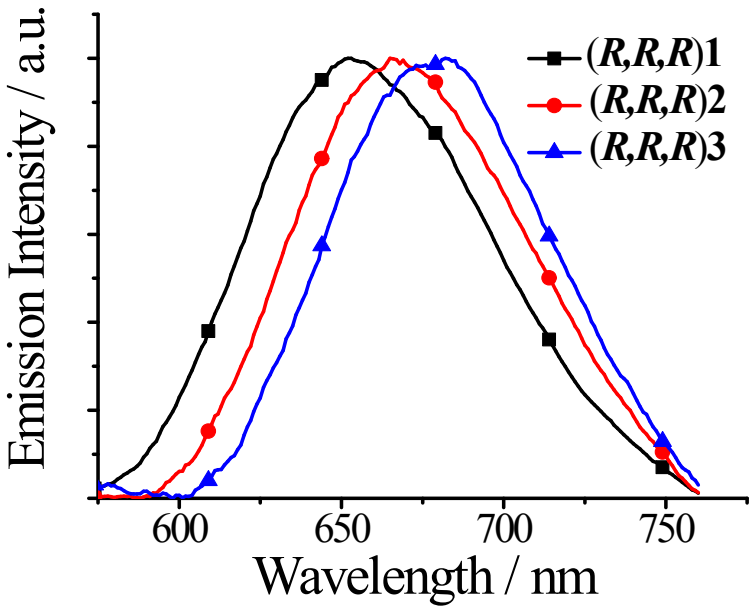


Fig. S5. Normalized emission spectra of **(*R*,*R*,*R*) 1–3** in powder at 298 K.

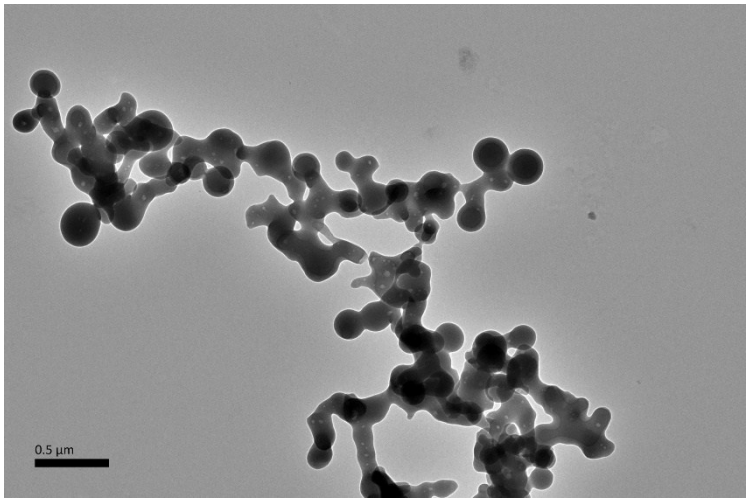


Fig. S6. Transmission electron microscopy of **(*S*,*S*,*S*)1** (H2O volume 70% in MeCN) on the carbon-coated copper grids after the solvent evaporation.

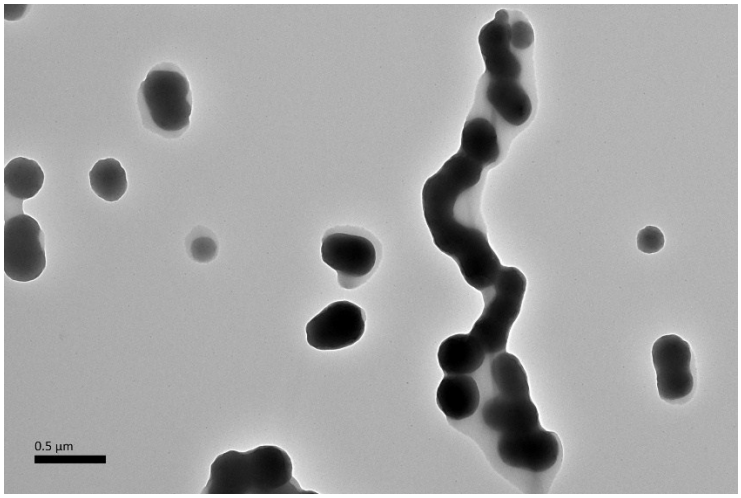


Fig. S7. Transmission electron microscopy of **(*Rac*)1** (H_2O volume 70% in MeCN) on the carbon-coated copper grids after the solvent evaporation.

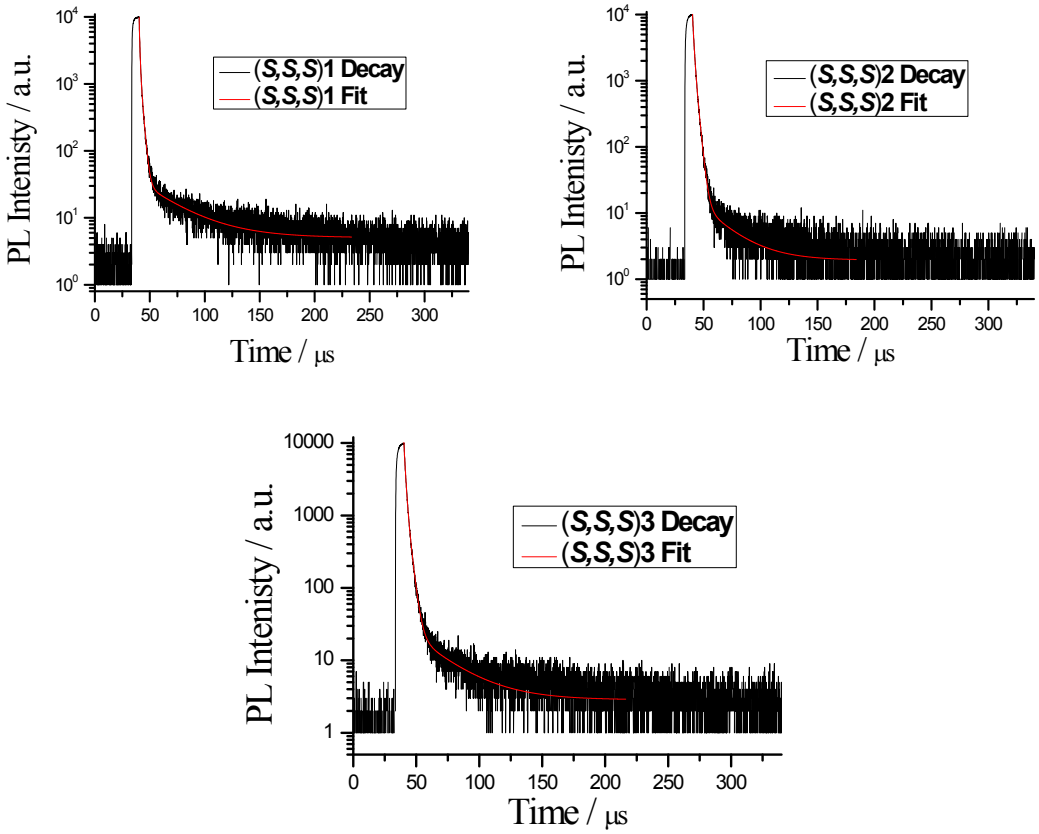


Fig. S8. Emission time decay spectra (excited at 371 nm) of **(*S,S,S*)**1-3 powder samples in Horiba Jobin Yvon Fluorolog-3 fluorescence spectrometer..

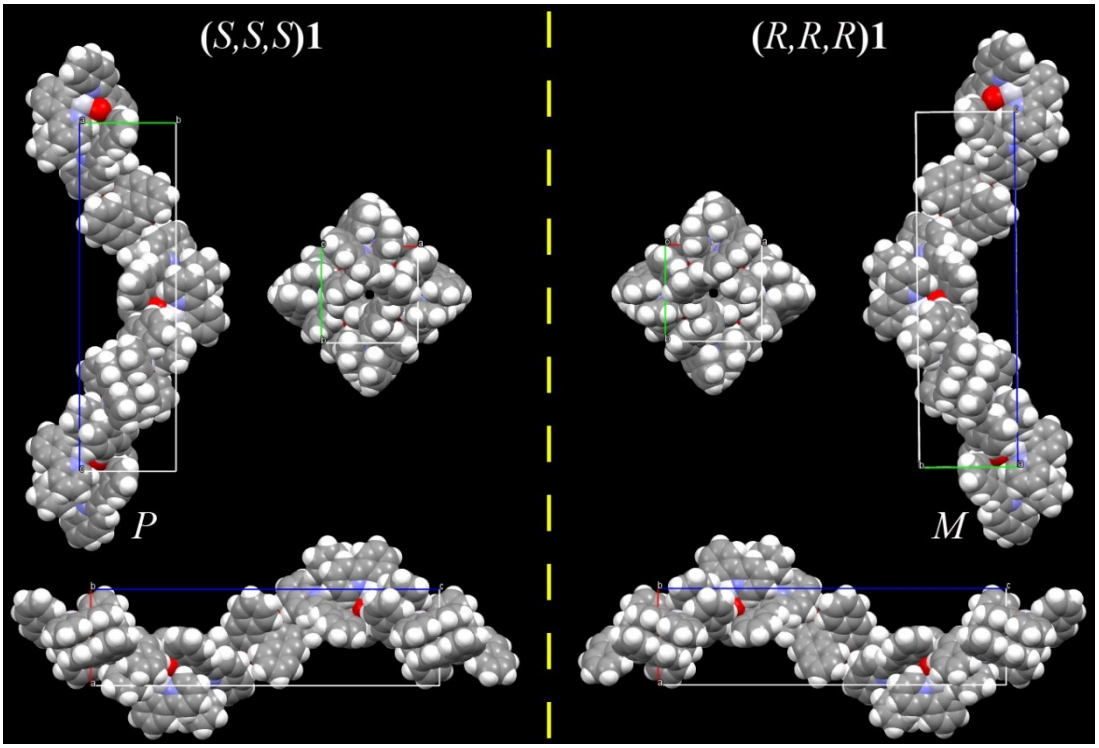


Fig. S9. X-ray single-crystal structures and packings of **(*S*,*S*,*S*)1** (left) and **(*R*,*R*,*R*)1** (right) molecules in one crystal cell with view down crystallographic, a, b, and c axis (solvent molecules are omitted).

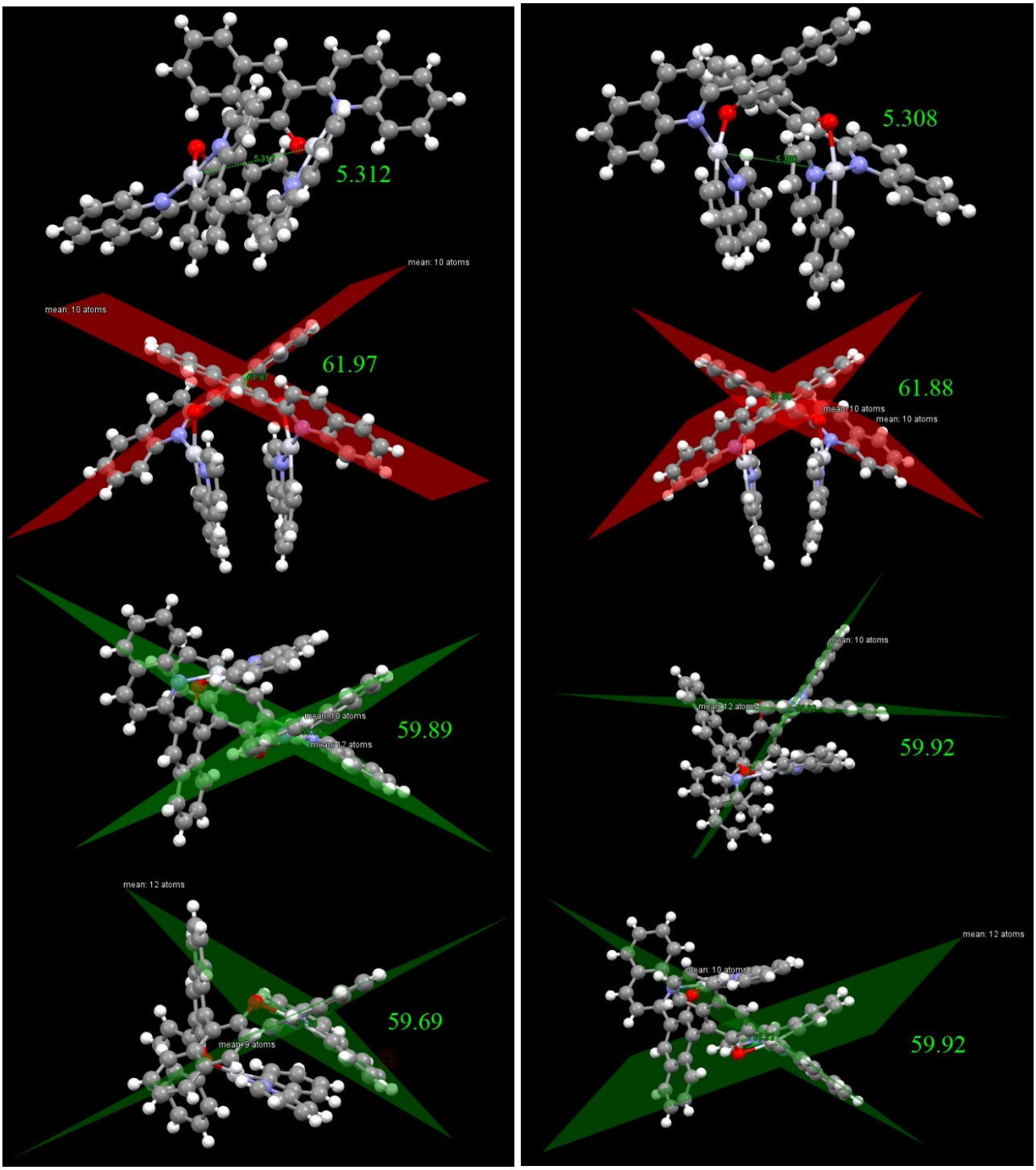


Fig. S10. X-ray single-crystal structures of one **(*S*,*S*,*S*)1** (left) and **(*R*,*R*,*R*)1** (right) molecule (solvent molecules are omitted).

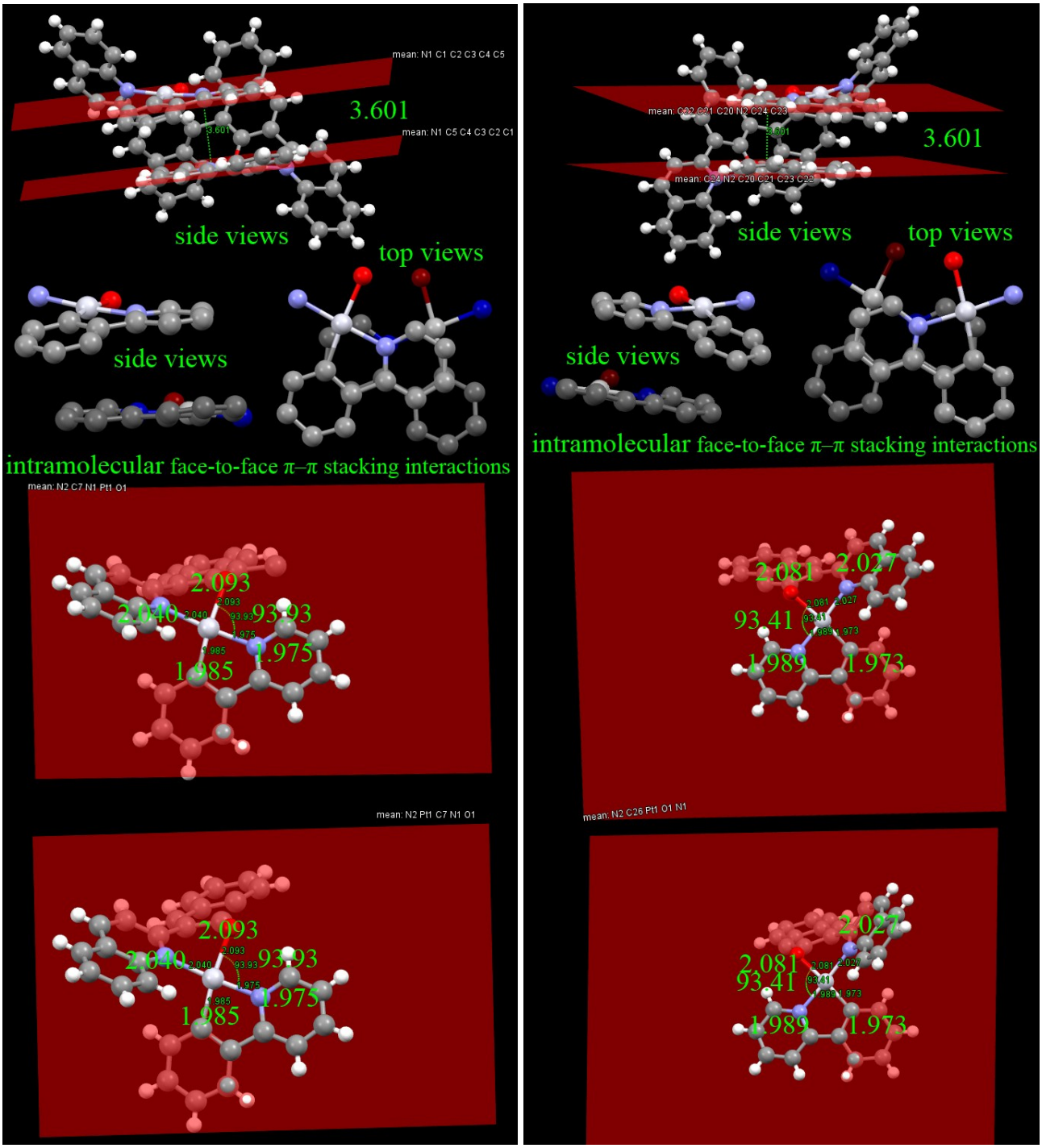


Fig. S11. X-ray single-crystal structures of one **(*S*,*S*,*S*)1** (left) and **(*R*,*R*,*R*)1** (right) molecule (some atoms and solvent molecules are omitted).

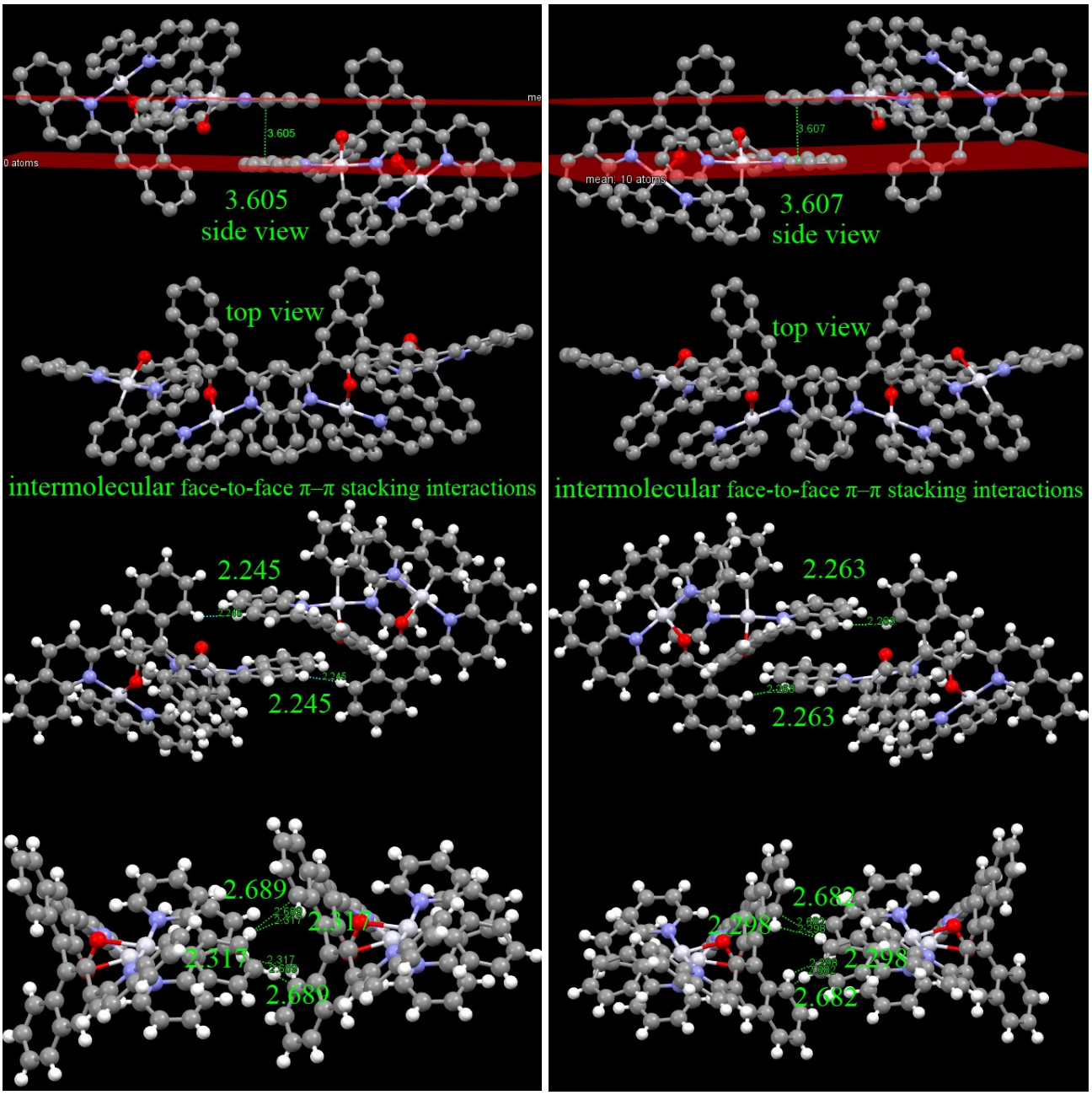


Fig. S12. Intermolecular interactions of two neighboring **(*S*,*S*,*S*)1** (left) and **(*R*,*R*,*R*)1** (right) molecules (some H atoms and solvent molecules are omitted).

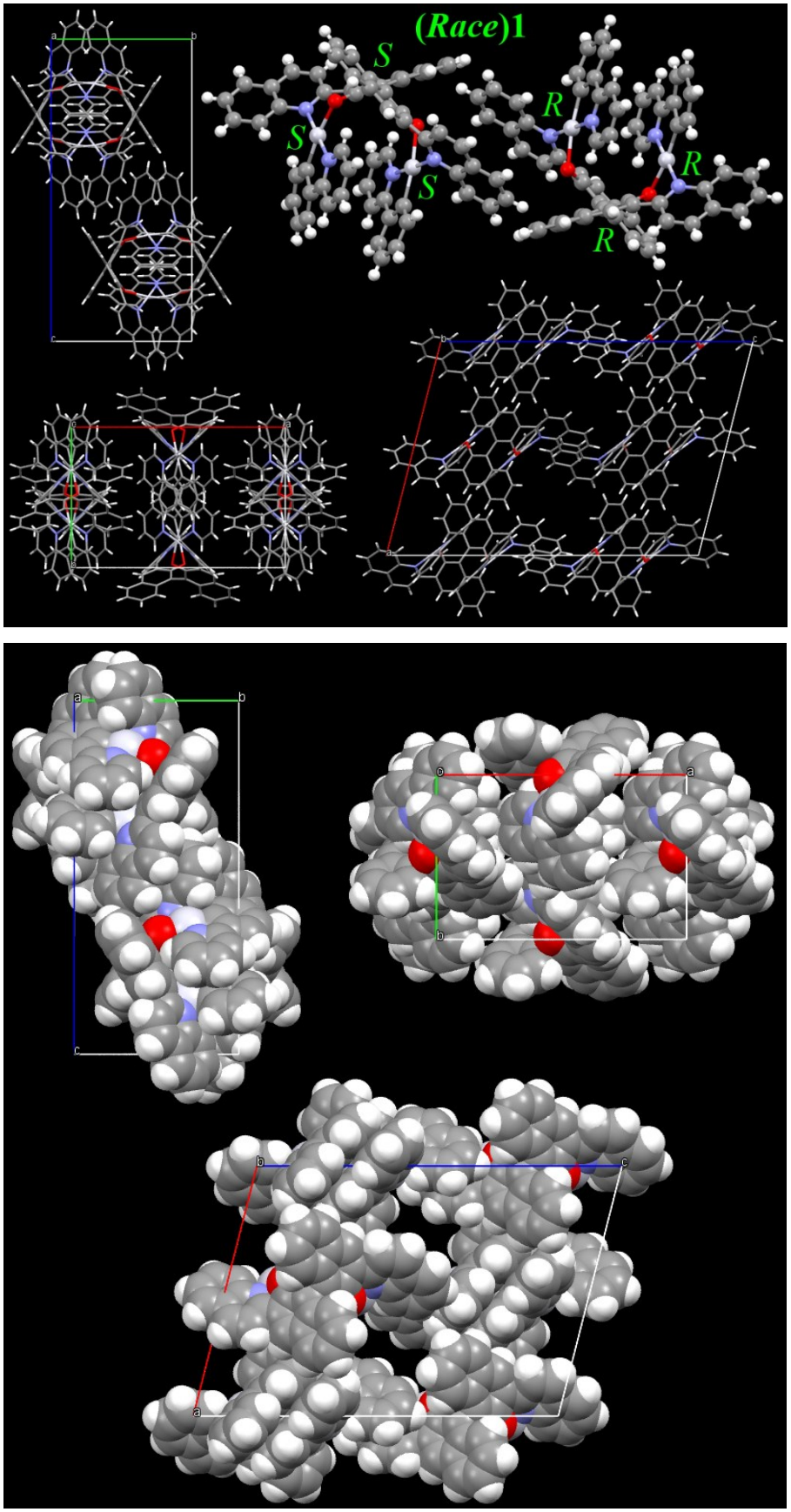


Fig. S13. X-ray single-crystal structures and packings of **(*Rac*)1** molecules (solvent molecules are omitted).

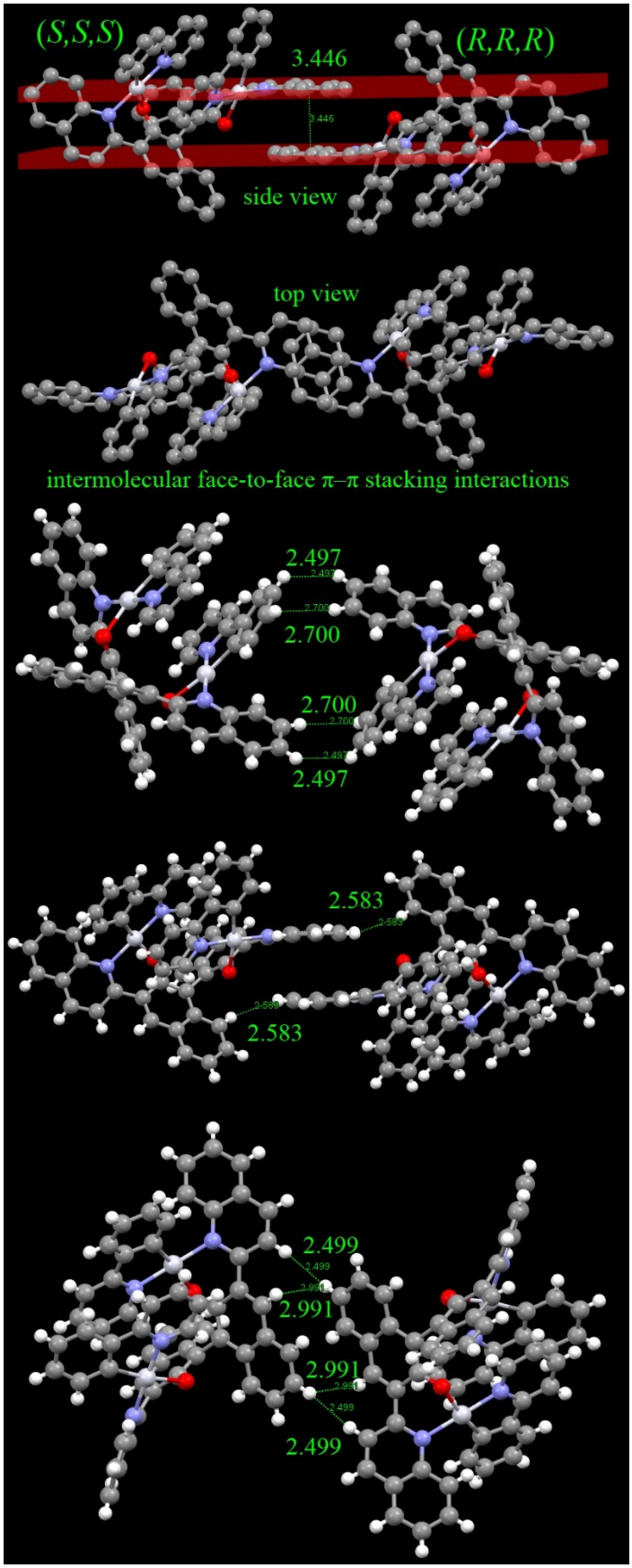


Fig. S14. Intermolecular interactions of two neighboring **(*Rac*)1** molecules (some H atoms and solvent molecules are omitted).

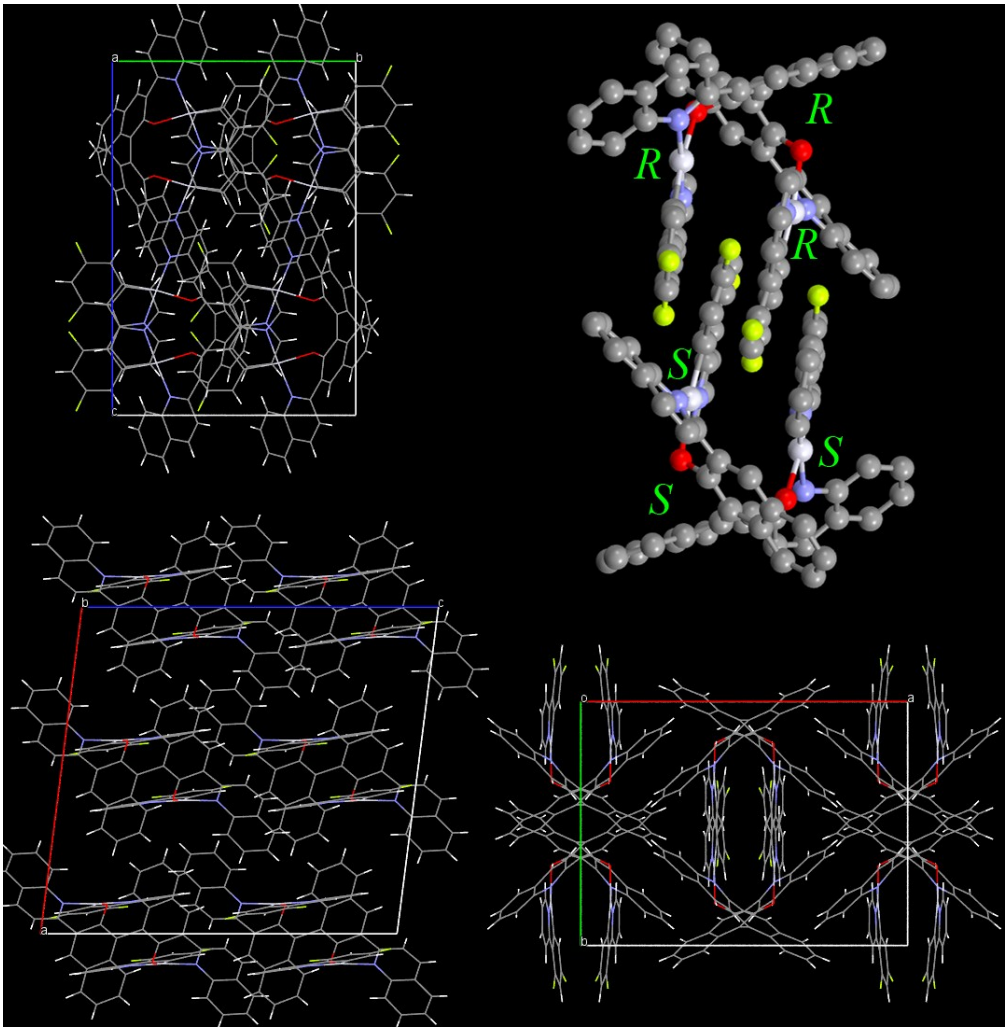


Fig. S15. X-ray single-crystal structures and packings of **(*Rac*)2** molecules in one crystal cell with view down crystallographic, a, b, and c axis. (some H atoms and solvent molecules are omitted).

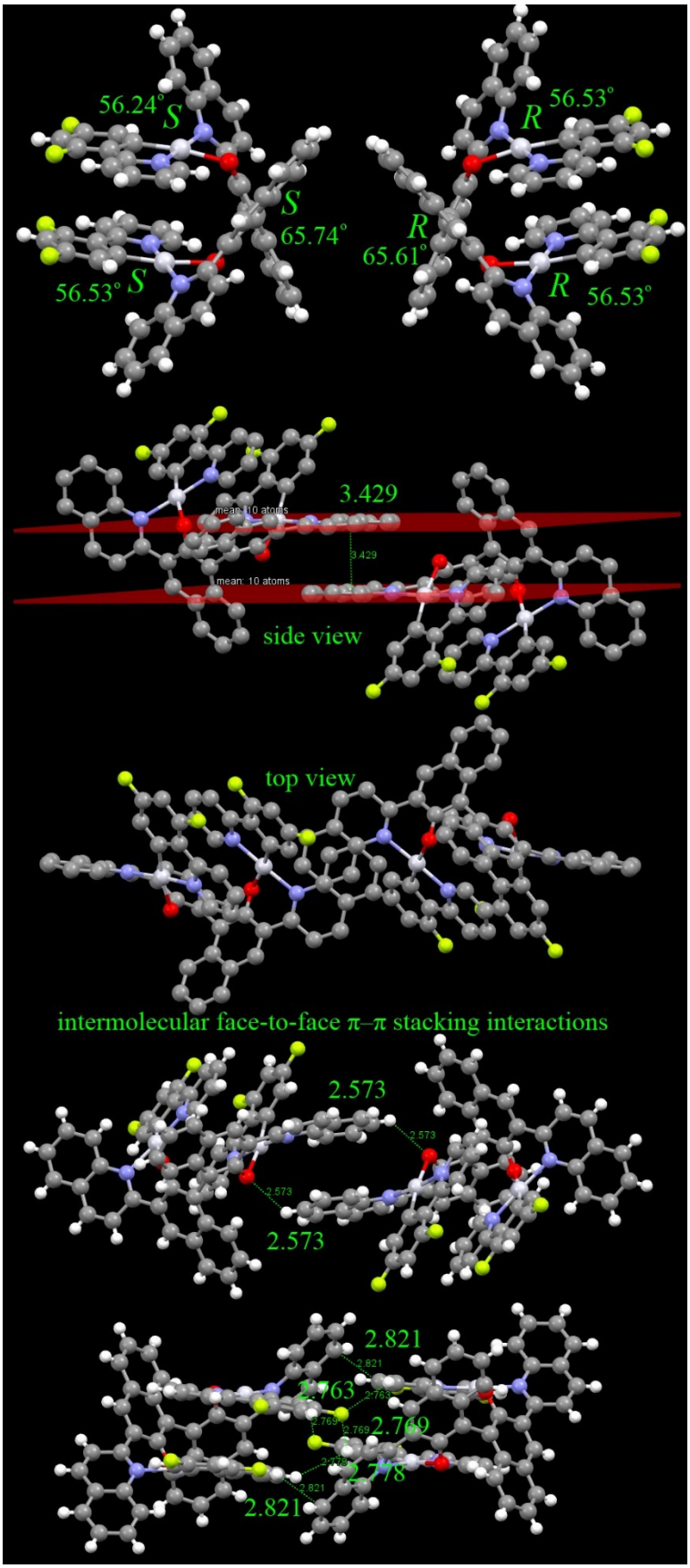


Fig. S16. Intermolecular interactions of two neighboring **(*Rac*)2** molecules. (some H atoms and solvent molecules are omitted).

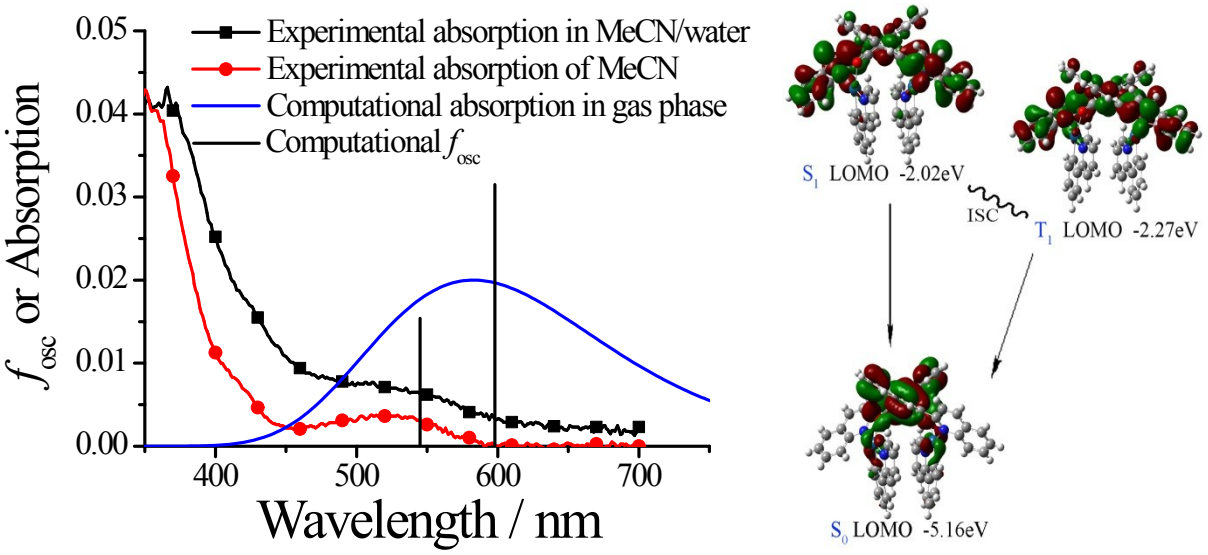


Fig. S17. Left: Computational (in gas phase) absorption of **(*S*,*S*,*S*)1** and experimental absorption (in MeCN and MeCN/water, water% = 70%, 1.0×10^{-5} mol dm^{-3}) of the two closest aggregated **(*S*,*S*,*S*)1** molecules. Right: the data S_1 energy of the main singlet excitations **(*S*,*S*,*S*)1**. The data T_1 energy of the main triplet excitations **(*S*,*S*,*S*)1**.

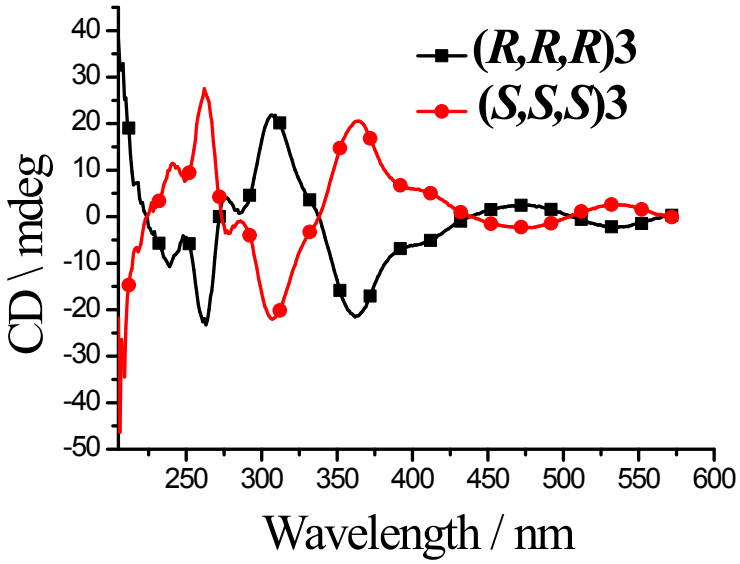


Fig. S18. CD spectra of the **(*R*,*R*,*R*)3** and **(*S*,*S*,*S*)3** in MeCN (5.0×10^{-5} mol dm^{-3}).

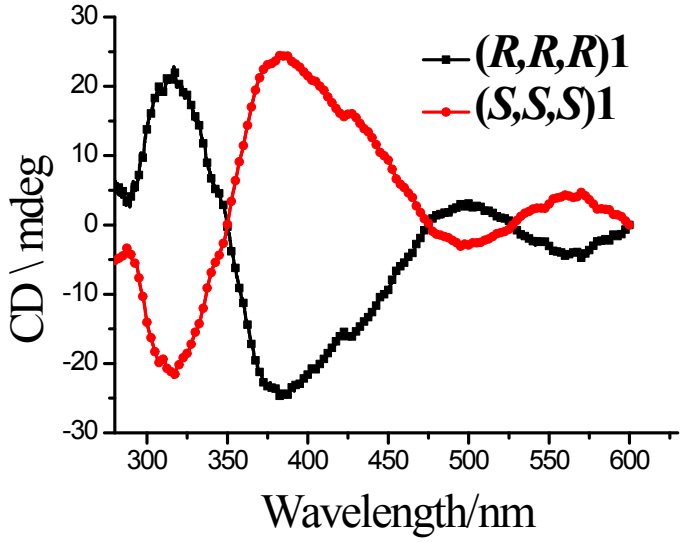


Fig. S19. Solid-state CD spectra of the ***(R,R,R)*1** and ***(S,S,S)*1** in potassium bromide ($m_{(S,S,S)1}$:m_{KBr} = 5/10000, $m_{(R,R,R)1}$:m_{KBr} = 5/10000, m stand for weight)

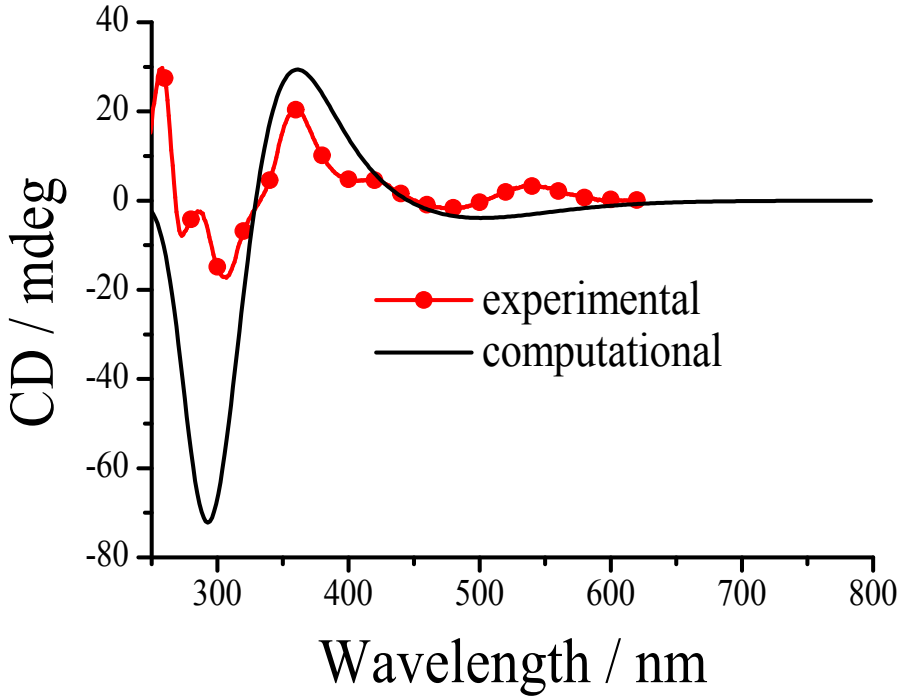


Fig. S20. CD spectra of ***(S,S,S)*1** (5.0×10^{-5} mol dm^{-3} in MeCN) in experiment and computation.

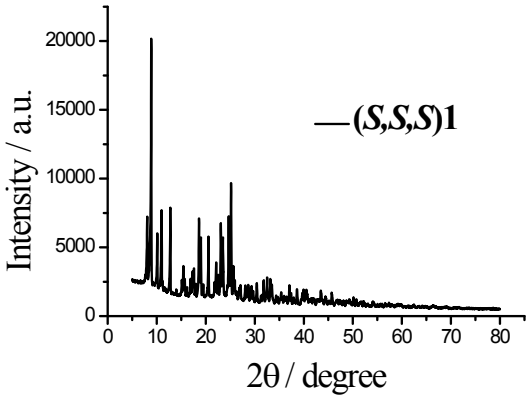


Fig. S21. X-ray powder diffraction of **(*S*,*S*,*S*)1** powder.

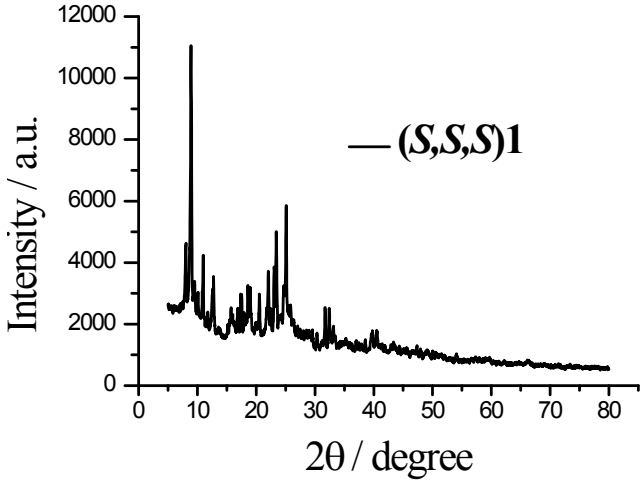


Fig. S22. X-ray powder diffraction of **(*S*,*S*,*S*)1** casting film.

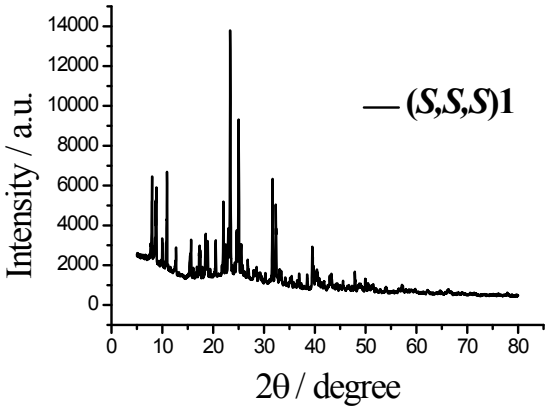
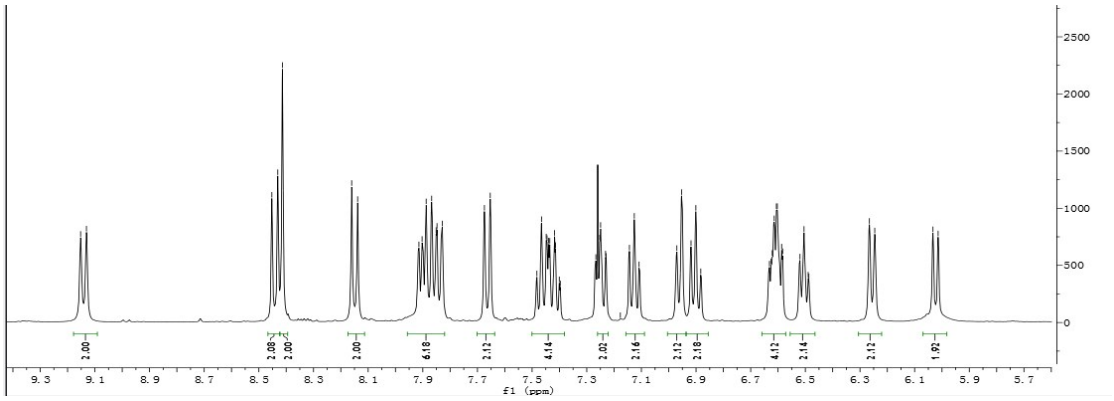
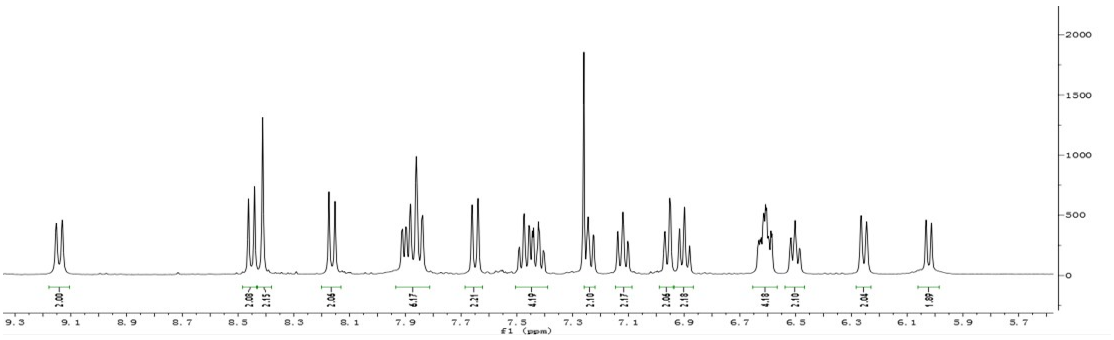


Fig. S23. X-ray powder diffraction of **(*S*,*S*,*S*)1** single crystalline sample.

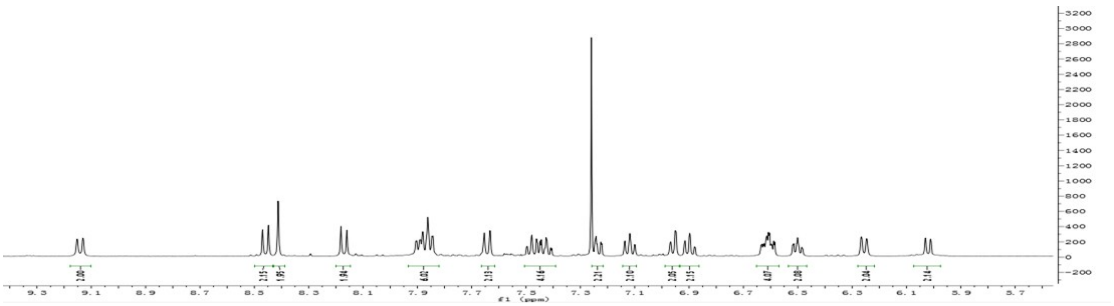
(a)



(b)



(c)



(d)

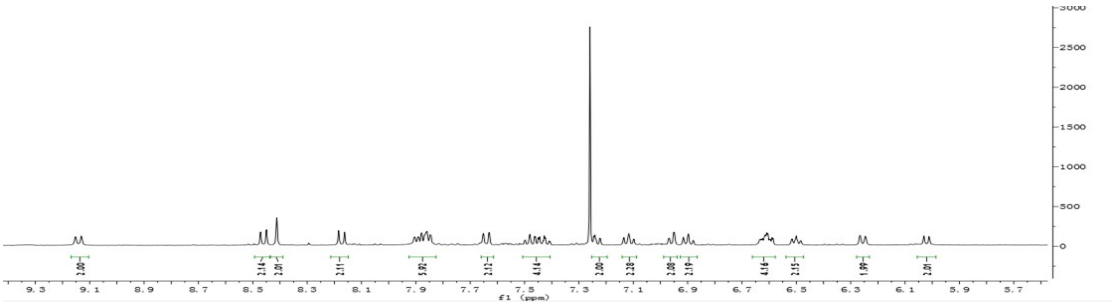


Fig. S24. Concentration-dependent 1H NMR spectra of **(*S,S,S*)1** at 298 K in $CDCl_3$-d.The concentrations of **(*S,S,S*)1** is (a) 21.6, (b) 8.27, (c) 3.31, and (d) 0.83 mmol dm^{-3}.

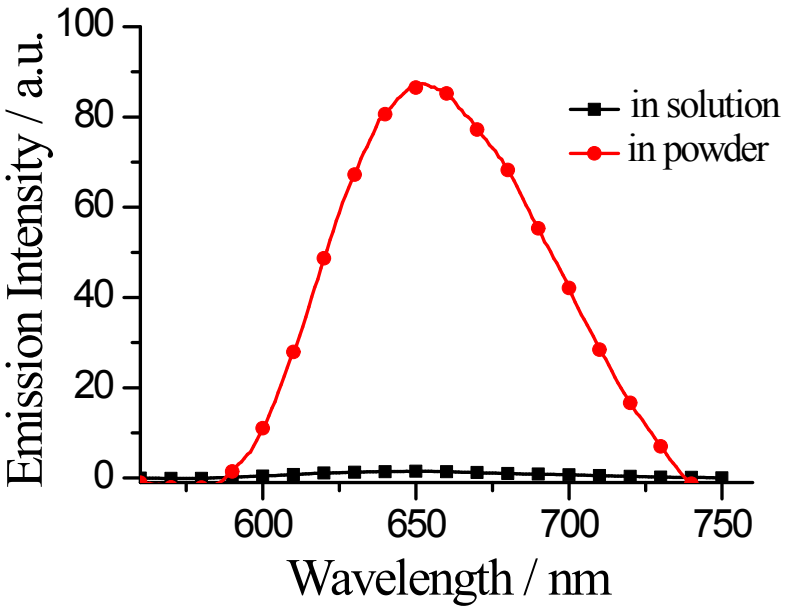


Fig. S25. Emission spectra of **(*S*,*S*,*S*)1** in powder and **(*S*,*S*,*S*)1** in solution (21.6 mmol dm^{-3} in CH_2Cl_2 at 298 K.)

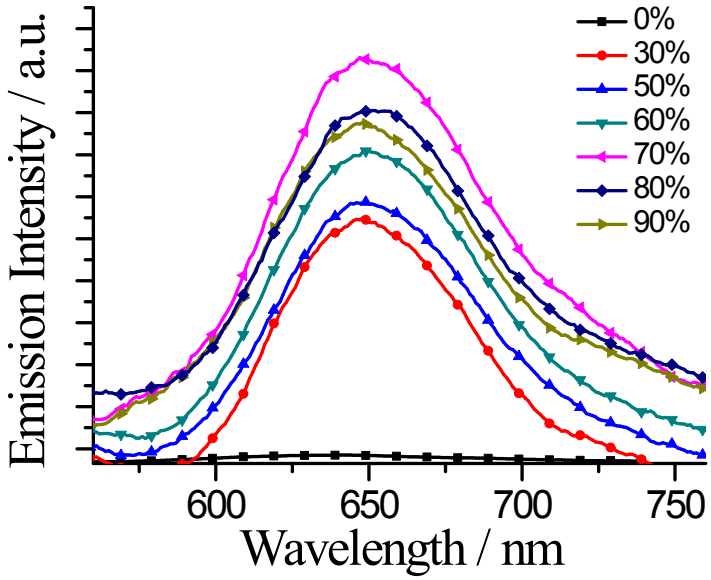


Fig. S26. Emission spectra of **(*S*,*S*,*S*)1** in 298K. (H_2O volume% in MeCN, 1.0×10^{-5} mol dm^{-3})

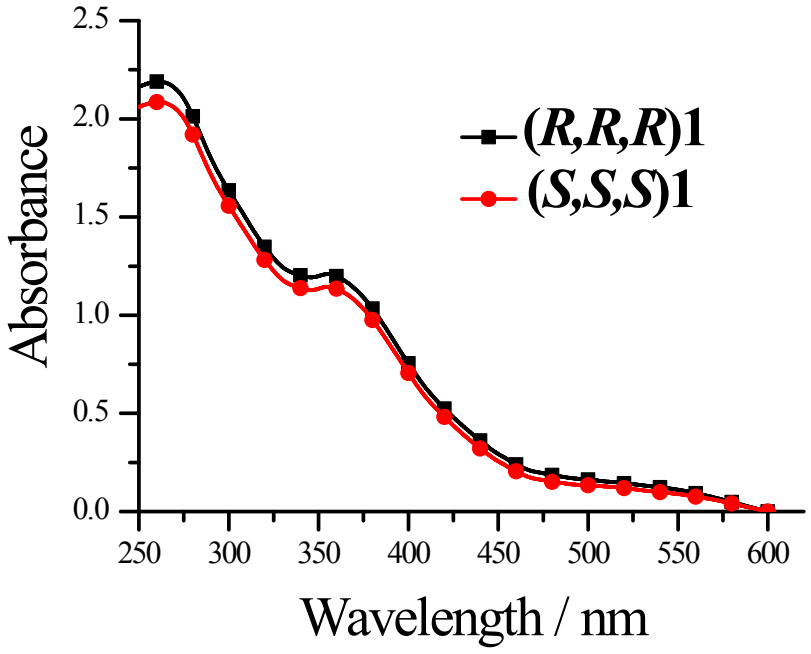


Fig. S27. Solid-state absorption spectra of the **(*R*,*R*,*R*)1** and **(*S*,*S*,*S*)1** in potassium bromide ($m_{(S,S,S)1}$:m_{KBr} = 5/10000, $m_{(R,R,R)1}$:m_{KBr} = 5/10000, m stand for weight)

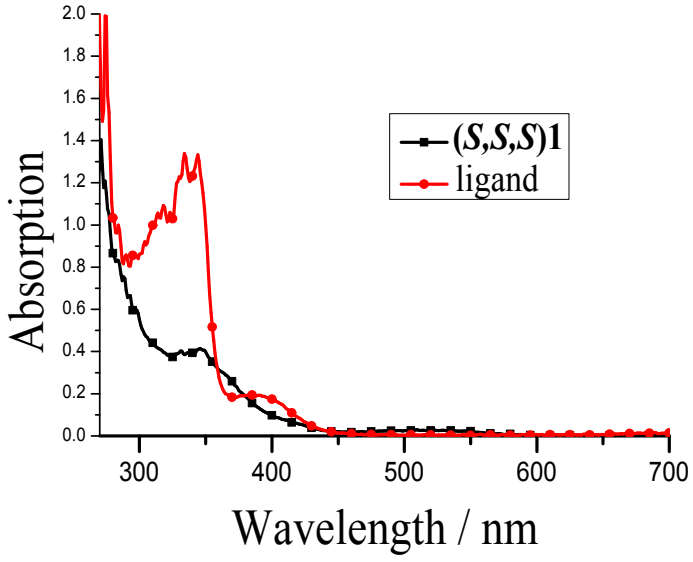


Fig. S28. Absorption spectra of the ligand ((*S*)-2,2'-bis(methoxymethyl)-1,1'-binaphthol) and

(*S*,*S*,*S*)1 in MeCN. The concentrations of ligand and **(*S*,*S*,*S*)1** in MeCN are 1.0×10^{-5} mol dm^{-3} respectively.

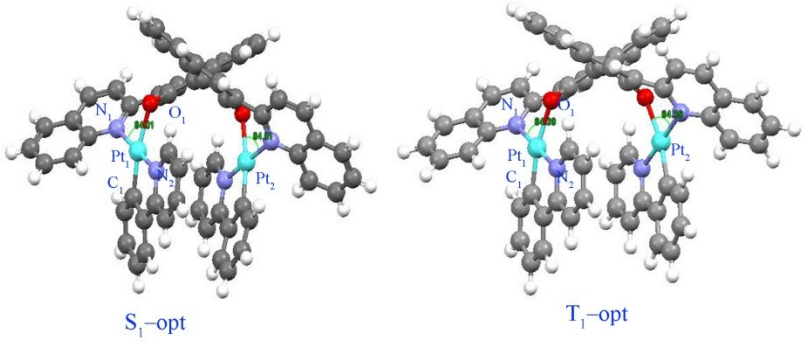


Fig. 29. S1-opt:Bond angles N_1–Pt_1–O_1 84.01°; O_1–Pt_1–N_2 93.93°; O_1–Pt_1–C_1 81.30°; C_1–Pt_1–N_1 101.38°. Bond distances N_1–Pt_1 2.040 Å; O_1–Pt_1 2.093 Å; N_2–Pt_1 1.975 Å; C_1–Pt_1 1.985 Å. T1-opt: Bond angles N_1–Pt_1–O_1 84.39°; O_1–Pt_1–N_2 92.95°; O_1–Pt_1–C_1 80.81°; C_1–Pt_1–N_1 102.03°. Bond distances N_1–Pt_1 2.045 Å; O_1–Pt_1 2.124 Å; N_2–Pt_1 2.023 Å; C_1–Pt_1 1.994 Å.

We calculated seventy the data of the main singlet excitations. We listed five excitations.

Excited State 1: Singlet-B 2.4043 eV 515.68 nm f=0.0311 <S**2>=0.000

222 ->241	0.01242
223 ->240	0.01837
233 ->241	0.01500
234 ->241	-0.03344
235 ->240	-0.03869
236 ->241	-0.01522
237 ->240	-0.03563
238 ->241	-0.28634
238 ->243	0.01816
238 ->245	-0.01744

238 ->251 0.01157

239 ->240 0.63824

239 ->242 0.01999

239 ->244 0.04118

239 ->250 -0.02254

239 ->252 0.01072

This state for optimization and/or second-order correction.

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.4440 eV 507.31 nm f=0.0063 <S**2>=0.000

222 ->240 0.01642

223 ->241 0.02199

233 ->240 0.01385

234 ->240 -0.03057

235 ->241 -0.03269

236 ->240 -0.01766

237 ->241 -0.04204

238 ->240 -0.33076

238 ->242 -0.01332

238 ->248 0.01360

238 ->250 0.01137

238 ->256 -0.01395

239 ->241 0.61736

239 ->245 0.02723

239 ->246 -0.01121

239 ->249 -0.01172

239 ->251 -0.01913

239 ->253 0.01198

Excited State 3: Singlet-A 2.7317 eV 453.87 nm f=0.0031
<S**2>=0.000

222 ->240	-0.01134
235 ->241	0.02075
236 ->240	0.01691
237 ->241	0.06308
238 ->240	0.61286
238 ->244	0.04532
238 ->250	-0.01950
238 ->252	0.01450
239 ->241	0.33662
239 ->243	0.03616
239 ->245	0.02615
239 ->249	0.01494

Excited State 4: Singlet-B 2.7528 eV 450.39 nm f=0.0026
<S**2>=0.000

222 ->241	-0.01422
235 ->240	0.02520
236 ->241	0.03012
236 ->243	0.01585
237 ->240	0.07699
238 ->241	0.63381
238 ->243	0.01712
238 ->245	0.03776
238 ->251	-0.01747
238 ->253	0.01500
239 ->240	0.29176
239 ->244	0.03759

Excited State 5: Singlet-B 3.0545 eV 405.91 nm f=0.0404 <S**2>=0.000

220 ->243	-0.01539
222 ->243	-0.01482
223 ->242	0.02698
224 ->242	0.01071
225 ->243	-0.01086
227 ->243	-0.02027
228 ->242	-0.01413
231 ->243	-0.01455
232 ->240	-0.01434
232 ->242	0.02608
234 ->243	0.01793
235 ->240	-0.01327
235 ->242	-0.02177
236 ->241	0.10496
236 ->243	0.06526
237 ->240	0.11485
237 ->242	-0.09812
238 ->243	0.19893
238 ->249	0.01555
238 ->253	-0.01228
239 ->240	-0.02164
239 ->242	0.64205
239 ->244	0.01135
239 ->247	0.04022
239 ->252	0.01837

Datablock: (*S,S,S*)1 single crystal

Bond precision: C-C = 0.0206 A Wavelength=0.71073
Cell: a=11.3862(3) b=11.3862(3) c=41.1226(14)
alpha=90 beta=90 gamma=90
Temperature: 293 K
Calculated Reported
Volume 5331.4(3) 5331.4(3)
Space group P 41 2 2 P 41 2 2
Hall group P 4w 2c P 4w 2c
Moiety formula
C60 H38 N4 O2 Pt2, C H4 O,
H2 O
C60 H38 N4 O2 Pt2, 0.5(C2
H12 O4)
Sum formula C61 H44 N4 O4 Pt2 C61 H44 N4 O4 Pt2
Mr 1287.16 1287.18
Dx,g cm-3 1.604 1.604
Z 4 4
Mu (mm-1) 5.292 5.292
F000 2504.0 2504.0
F000' 2491.71
h,k,lmax 14,14,51 14,12,51
Nref 5459[3241] 5222
Tmin,Tmax 0.171,0.266 0.429,1.000
Tmin' 0.144
Correction method= # Reported T Limits: Tmin=0.429 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 1.61/0.96 Theta(max)= 26.371
R(reflections)= 0.0423(4830) wR2(reflections)= 0.1201(5222)
S = 1.130 Npar= 336

Datablock: (*R,R,R*)1 single crystal

Bond precision: C-C = 0.0153 A Wavelength=0.71073

Cell: a=11.3937(3) b=11.3937(3) c=41.0779(14)

alpha=90 beta=90 gamma=90

Temperature: 293 K

Calculated Reported

Volume 5332.6(3) 5332.6(3)

Space group P 43 2 2 P 43 2 2

Hall group P 4cw 2c P 4cw 2c

Moiety formula

C60 H38 N4 O2 Pt2, 2(C2

H5), 2(H O)

C60 H38 N4 O2 Pt2, 2(C2 H6

O)

Sum formula C64 H50 N4 O4 Pt2 C64 H50 N4 O4 Pt2

Mr 1329.24 1329.26

Dx,g cm-3 1.656 1.656

Z 4 4

Mu (mm-1) 5.294 5.294

F000 2600.0 2600.0

F000' 2587.70

h,k,lmax 14,14,51 14,14,51

Nref 5463[3244] 5397

Tmin,Tmax 0.401,0.452 0.487,1.000

Tmin' 0.116

Correction method= # Reported T Limits: Tmin=0.487 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.99 Theta(max)= 26.369

R(reflections)= 0.0349(5020) wR2(reflections)= 0.0862(5397)

S = 1.101 Npar= 335

Datablock: (*Rac*)1 single crystal

Bond precision: C-C = 0.0094 A Wavelength=0.71073

Cell: a=18.5883(8) b=11.8497(3) c=26.2885(9)

alpha=90 beta=104.291(4) gamma=90

Temperature: 293 K

Calculated Reported

Volume 5611.3(4) 5611.3(4)

Space group I 2/c I 1 2/c 1

Hall group -I 2yc -I 2yc

Moiety formula

C60 H38 N4 O2 Pt2, 2(C7

H8)

C60 H38 N4 O2 Pt2, 2(C7

H8)

Sum formula C74 H54 N4 O2 Pt2 C74 H54 N4 O2 Pt2

Mr 1421.37 1421.39

Dx,g cm-3 1.683 1.683

Z 4 4

Mu (mm-1) 5.035 5.035

F000 2792.0 2792.0

F000' 2779.66

h,k,lmax 23,14,32 23,14,32

Nref 5746 5737

Tmin,Tmax 0.311,0.668 0.393,1.000

Tmin' 0.212

Correction method= # Reported T Limits: Tmin=0.393 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.372

R(reflections)= 0.0371(4247) wR2(reflections)= 0.0864(5737)

S = 1.051 Npar= 359

Datablock: (*Rac*)2 single crystal

Bond precision: C-C = 0.0126 A Wavelength=0.71073

Cell: a=18.4923(19) b=13.6885(15) c=20.0091(16)

alpha=90 beta=97.229(9) gamma=90

Temperature: 293 K

Calculated Reported

Volume 5024.7(9) 5024.7(9)

Space group C 2/c C 1 2/c 1

Hall group -C 2yc -C 2yc

Moiety formula

C60 H34 F4 N4 O2 Pt2 [+

solvent]

C60 H34 F4 N4 O2 Pt2

Sum formula

C60 H34 F4 N4 O2 Pt2 [+

solvent]

C60 H34 F4 N4 O2 Pt2

Mr 1309.07 1309.09

Dx,g cm-3 1.730 1.730

Z 4 4

Mu (mm-1) 5.625 5.625

F000 2520.0 2520.0

F000’ 2507.88

h,k,lmax 23,17,24 23,17,24

Nref 5143 5134

Tmin,Tmax 0.152,0.245 0.265,1.000

Tmin’ 0.128

Correction method= # Reported T Limits: Tmin=0.265 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.371

R(reflections)= 0.0502(3806) wR2(reflections)= 0.1290(5134)

S = 1.034 Npar= 325

Table S1. Key bonds lengths and angles of (*S*,*S*,*S*)1 crystallographic data.

Atom	Length/Å	Atom	Length/Å	Atom	Angle/°	Atom	Angle/°
Pt1-O1	2.103(7)	C13-C14	1.414(18)	N1-Pt1-O1	94.2(3)	C12-C13-C14	122.0(13)
Pt1-N1	1.979(9)	C14-C15	1.39(2)	N1-Pt1-N2	175.9(4)	C15-C14-C13	118.4(15)
Pt1-N2	2.038(8)	C15-C16	1.33(2)	N2-Pt1-O1	84.4(3)	C16-C15-C14	121.7(14)
Pt1-C7	1.976(12)	C16-C17	1.390(18)	C7-Pt1-O1	170.5(4)	C15-C16-C17	119.1(15)
O1-C22	1.330(13)	C17-C18	1.41(2)	C7-Pt1-N1	80.7(5)	C16-C17-C12	121.8(14)
N1-C1	1.356(14)	C18-C19	1.367(16)	C7-Pt1-N2	101.3(4)	C16-C17-C18	121.5(12)
N1-C5	1.369(15)	C19-C20	1.413(14)	C22-O1-Pt1	107.1(6)	C18-C17-C12	116.4(11)
N2-C12	1.390(14)	C20-C21	1.491(15)	C1-N1-Pt1	123.6(8)	C19-C18-C17	119.5(11)
N2-C20	1.311(14)	C21-C22	1.471(12)	C1-N1-C5	119.3(11)	C18-C19-C20	121.8(13)
C1-C2	1.367(16)	C21-C30	1.346(17)	C5-N1-Pt1	117.0(8)	N2-C20-C19	120.0(10)
C2-C3	1.40(2)	C22-C23	1.374(14)	C12-N2-Pt1	121.6(8)	N2-C20-C21	122.5(9)
C3-C4	1.33(2)	C23-C23[1]	1.541(19)	C20-N2-Pt1	117.7(7)	C19-C20-C21	117.4(10)
C4-C5	1.407(19)	C23-C24	1.395(15)	C20-N2-C12	120.3(9)	C22-C21-C20	119.5(10)
C5-C6	1.470(19)	C24-C25	1.452(15)	N1-C1-C2	121.8(13)	C30-C21-C20	120.0(9)
C6-C7	1.394(17)	C24-C29	1.404(14)	C1-C2-C3	118.6(14)	C30-C21-C22	120.3(10)
C6-C11	1.373(19)	C25-C26	1.346(16)	C4-C3-C2	120.4(13)	O1-C22-C21	119.3(9)
C7-C8	1.405(17)	C26-C27	1.434(18)	C3-C4-C5	120.3(14)	O1-C22-C23	122.4(9)
C8-C9	1.381(18)	C27-C28	1.364(19)	N1-C5-C4	119.5(14)	C23-C22-C21	118.2(10)
C9-C10	1.40(2)	C28-C29	1.427(16)	N1-C5-C6	112.4(11)	C22-C23-C23[1]	118.3(11)
C10-C11	1.34(2)	C29-C30	1.417(15)	C4-C5-C6	128.0(13)	C22-C23-C24	120.4(9)
C12-C13	1.352(18)	O3-C31	1.57(3)	C7-C6-C5	113.8(11)	C24-C23-C23[1]	121.1(11)
C12-C17	1.427(15)			C11-C6-C5	123.6(13)	C23-C24-C25	121.8(10)
				C11-C6-C7	122.5(14)	C23-C24-C29	121.6(10)
				C6-C7-Pt1	115.5(9)	C29-C24-C25	116.6(11)
				C6-C7-C8	116.4(12)	C26-C25-C24	121.4(11)
				C8-C7-Pt1	127.3(10)	C25-C26-C27	121.1(12)
				C9-C8-C7	119.5(13)	C28-C27-C26	119.3(13)
				C8-C9-C10	122.7(14)	C27-C28-C29	120.3(12)
				C11-C10-C9	117.3(14)	C24-C29-C28	121.3(11)
				C10-C11-C6	121.6(15)	C24-C29-C30	117.9(10)
				N2-C12-C17	121.7(11)	C30-C29-C28	120.8(11)
				C13-C12-N2	121.6(10)	C21-C30-C29	121.4(10)
				C13-C12-C17	116.6(11)		

[1]+X,1-Y,3/2-Z

Table S2. Key bonds lengths and angles of (*R*,*R*,*R*)1 crystallographic data.

Atom	Length/Å	Atom	Length/Å	Atom	Angle/°	Atom	Angle/°
Pt1-O1	2.083(6)	C12-C12[1]	1.552(16)	N1-Pt1-O1	84.5(2)	C12-C11-C10	117.2(9)
Pt1-N1	2.028(6)	C12-C13	1.398(13)	N2-Pt1-O1	93.6(3)	C11-C12-C12[1]	116.6(9)
Pt1-N2	1.992(7)	C13-C14	1.430(12)	N2-Pt1-N1	175.7(3)	C13-C12-C11	121.2(8)
Pt1-C26	1.985(10)	C13-C18	1.388(12)	C26-Pt1-O1	170.6(3)	C13-C12-C12[1]	122.1(9)
O1-C11	1.318(11)	C14-C15	1.355(14)	C26-Pt1-N1	100.7(3)	C12-C13-C14	121.3(8)
N1-C1	1.388(11)	C15-C16	1.432(14)	C26-Pt1-N2	81.7(4)	C18-C13-C12	121.3(8)
N1-C9	1.310(12)	C16-C17	1.356(15)	C11-O1-Pt1	107.8(5)	C18-C13-C14	117.4(8)
N2-C20	1.326(12)	C17-C18	1.398(14)	C1-N1-Pt1	122.2(6)	C15-C14-C13	121.3(9)
N2-C24	1.374(12)	C18-C19	1.408(12)	C9-N1-Pt1	118.3(6)	C14-C15-C16	119.9(9)
C1-C2	1.357(15)	C20-C21	1.360(13)	C9-N1-C1	119.3(7)	C17-C16-C15	119.4(10)
C1-C6	1.409(12)	C21-C22	1.376(18)	C20-N2-Pt1	124.1(7)	C16-C17-C18	120.7(10)
C2-C3	1.416(15)	C22-C23	1.355(17)	C20-N2-C24	120.1(8)	C13-C18-C17	121.3(9)
C3-C4	1.375(18)	C23-C24	1.392(14)	C24-N2-Pt1	115.7(6)	C13-C18-C19	117.5(8)
C4-C5	1.318(19)	C24-C25	1.460(14)	N1-C1-C6	121.7(9)	C17-C18-C19	121.2(9)
C5-C6	1.409(15)	C25-C26	1.402(14)	C2-C1-N1	120.4(8)	C10-C19-C18	123.0(8)
C6-C7	1.406(17)	C25-C30	1.404(15)	C2-C1-C6	117.8(9)	N2-C20-C21	122.6(11)
C7-C8	1.332(14)	C26-C27	1.379(13)	C1-C2-C3	120.9(11)	C20-C21-C22	118.4(12)
C8-C9	1.410(12)	C27-C28	1.368(14)	C4-C3-C2	118.8(13)	C23-C22-C21	120.0(11)
C9-C10	1.497(12)	C28-C29	1.389(16)	C5-C4-C3	122.2(11)	C22-C23-C24	120.5(11)
C10-C11	1.453(11)	C29-C30	1.340(16)	C4-C5-C6	119.2(11)	N2-C24-C23	118.3(10)
C10-C19	1.358(13)	O2-C31	1.90(3)	C1-C6-C5	120.9(11)	N2-C24-C25	113.0(8)
C11-C12	1.400(12)	C31-C32	1.62(2)	C7-C6-C1	117.0(9)	C23-C24-C25	128.7(10)
				C7-C6-C5	122.1(10)	C26-C25-C24	115.3(9)
				C8-C7-C6	119.4(9)	C26-C25-C30	122.0(10)
				C7-C8-C9	122.0(11)	C30-C25-C24	122.7(10)
				N1-C9-C8	120.3(8)	C25-C26-Pt1	113.7(7)
				N1-C9-C10	121.3(8)	C27-C26-Pt1	128.8(8)
				C8-C9-C10	118.4(9)	C27-C26-C25	116.8(10)
				C11-C10-C9	119.3(9)	C28-C27-C26	120.0(10)
				C19-C10-C9	120.5(8)	C27-C28-C29	123.0(12)
				C19-C10-C11	119.7(8)	C30-C29-C28	118.2(11)
				O1-C11-C10	120.0(8)	C29-C30-C25	119.9(11)
				O1-C11-C12	122.7(8)	C32-C31-O2	109.4(15)

[1]1-X,+Y,1-Z

Table S3. Key bonds lengths and angles of (*Rac*)2 crystallographic data.

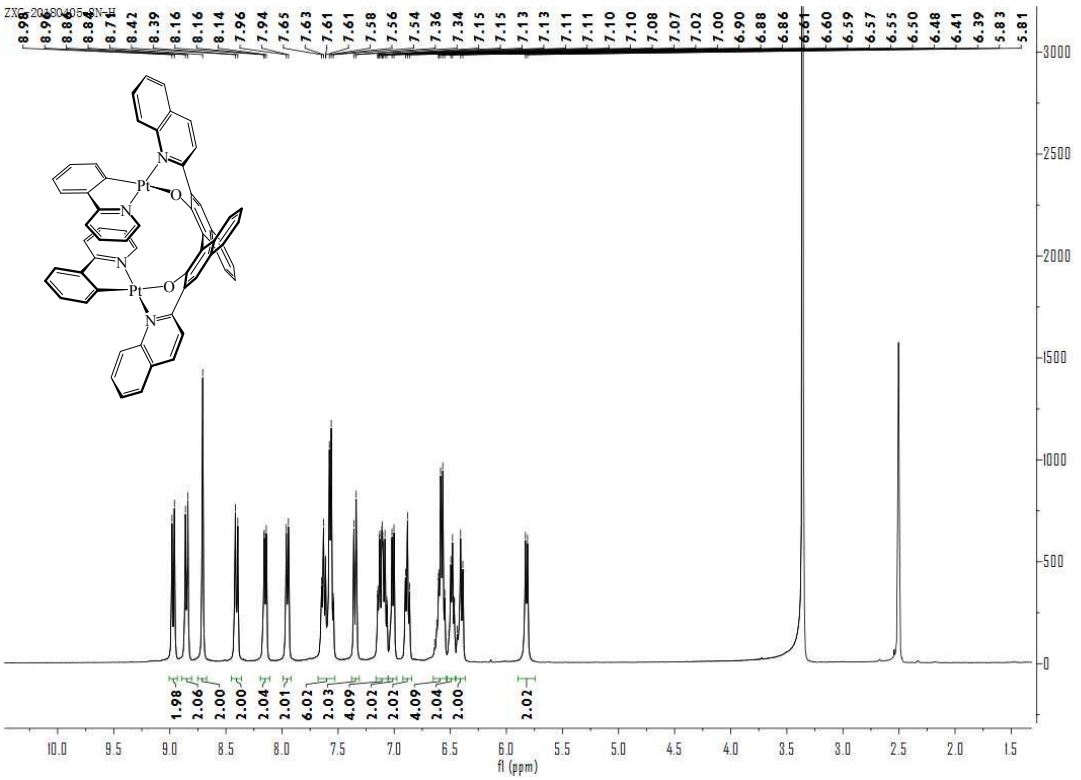
Atom	Length/Å	Atom	Length/Å	Atom	Angle/°	Atom	Angle/°
Pt1-O1	2.085(5)	C10-C19	1.378(11)	N1-Pt1-O1	84.1(2)	C13-C12-C11	121.5(7)
Pt1-N1	2.048(6)	C11-C12	1.406(11)	N2-Pt1-O1	93.4(3)	C13-C12-C12[1]	122.1(8)
Pt1-N2	1.998(6)	C12-C12[1]	1.521(14)	N2-Pt1-N1	175.3(2)	C12-C13-C14	123.7(8)
Pt1-C30	1.972(8)	C12-C13	1.394(11)	C30-Pt1-O1	172.3(3)	C12-C13-C18	119.8(7)
F1-C26	1.359(10)	C13-C14	1.426(12)	C30-Pt1-N1	101.1(3)	C14-C13-C18	116.4(8)
F2-C28	1.362(10)	C13-C18	1.430(11)	C30-Pt1-N2	81.8(3)	C15-C14-C13	122.3(9)
O1-C11	1.315(9)	C14-C15	1.358(12)	C11-O1-Pt1	109.6(5)	C14-C15-C16	120.2(10)
N1-C1	1.400(10)	C15-C16	1.390(13)	C1-N1-Pt1	120.6(5)	C17-C16-C15	120.3(10)
N1-C9	1.331(9)	C16-C17	1.352(14)	C9-N1-Pt1	118.6(5)	C16-C17-C18	121.6(9)
N2-C20	1.337(10)	C17-C18	1.415(12)	C9-N1-C1	120.7(6)	C17-C18-C13	119.1(8)
N2-C24	1.379(10)	C18-C19	1.401(12)	C20-N2-Pt1	123.2(6)	C19-C18-C13	118.9(8)
C1-C2	1.391(12)	C20-C21	1.364(11)	C20-N2-C24	119.8(7)	C19-C18-C17	122.0(8)
C1-C6	1.409(11)	C21-C22	1.358(13)	C24-N2-Pt1	116.8(5)	C10-C19-C18	121.8(7)
C2-C3	1.366(11)	C22-C23	1.358(12)	N1-C1-C6	120.1(8)	N2-C20-C21	122.2(8)
C3-C4	1.414(12)	C23-C24	1.399(10)	C2-C1-N1	120.6(7)	C22-C21-C20	119.0(9)
C4-C5	1.354(13)	C24-C25	1.454(11)	C2-C1-C6	119.3(8)	C23-C22-C21	120.4(8)
C5-C6	1.410(12)	C25-C26	1.347(12)	C3-C2-C1	120.1(8)	C22-C23-C24	120.2(8)
C6-C7	1.405(12)	C25-C30	1.456(11)	C2-C3-C4	120.7(9)	N2-C24-C23	118.3(7)
C7-C8	1.356(12)	C26-C27	1.405(13)	C5-C4-C3	120.0(9)	N2-C24-C25	113.0(7)
C8-C9	1.428(10)	C27-C28	1.353(12)	C4-C5-C6	120.1(9)	C23-C24-C25	128.6(8)
C9-C10	1.469(11)	C28-C29	1.377(12)	C1-C6-C5	119.7(9)	C24-C25-C30	114.5(7)
C10-C11	1.455(10)	C29-C30	1.388(11)	C7-C6-C1	118.1(8)	C26-C25-C24	125.4(8)
				C7-C6-C5	122.0(8)	C26-C25-C30	120.0(8)
				C8-C7-C6	120.5(8)	F1-C26-C27	115.9(8)
				C7-C8-C9	120.2(8)	C25-C26-F1	121.0(8)
				N1-C9-C8	119.9(8)	C25-C26-C27	123.1(9)
				N1-C9-C10	121.7(7)	C28-C27-C26	115.4(8)
				C8-C9-C10	118.3(7)	F2-C28-C29	117.5(8)
				C11-C10-C9	120.6(7)	C27-C28-F2	117.3(8)
				C19-C10-C9	119.6(7)	C27-C28-C29	125.2(9)
				C19-C10-C11	119.7(8)	C28-C29-C30	119.7(8)
				O1-C11-C10	121.2(7)	C25-C30-Pt1	113.8(6)
				O1-C11-C12	120.7(7)	C29-C30-Pt1	129.5(6)
				C12-C11-C10	118.1(7)	C29-C30-C25	116.6(8)
				C11-C12-C12[1]	115.9(8)		

[1]1-X,+Y,1/2-Z

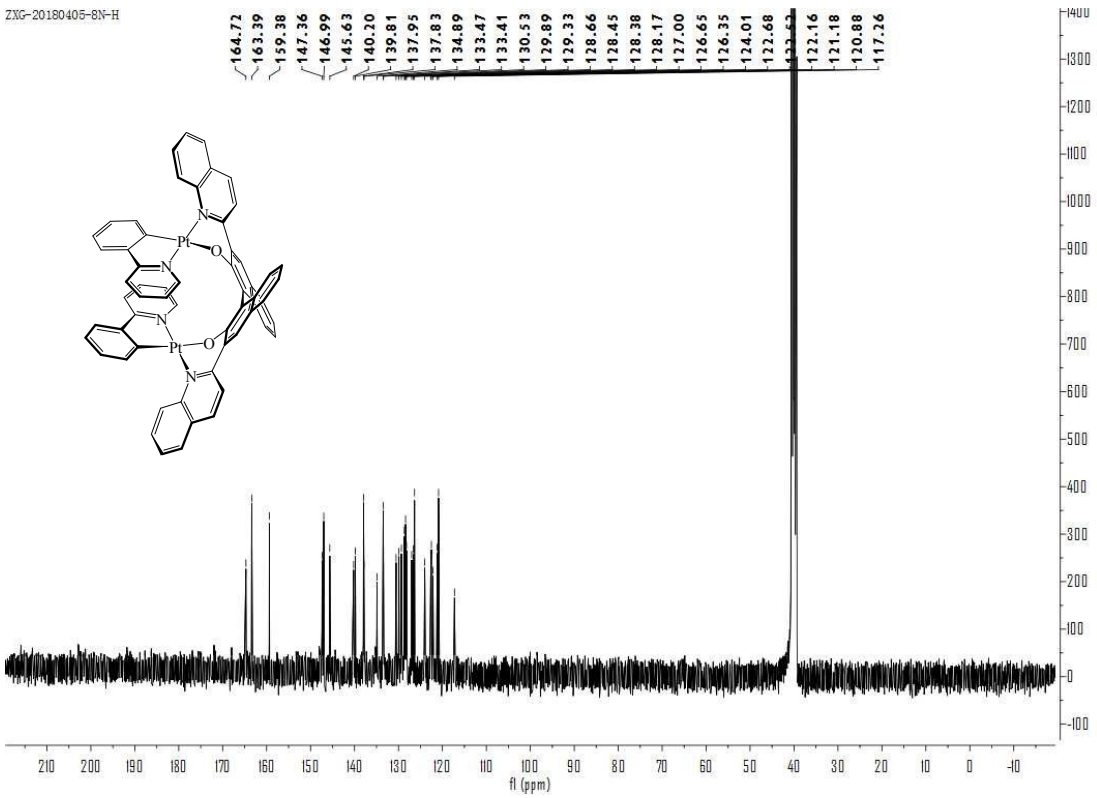
Table S4. Key bonds lengths and angles of (*Rac*)1 crystallographic data.

Atom	Length/Å	Atom	Length/Å	Atom	Angle/°	Atom	Angle/°
Pt1-O1	2.096(3)	C14-C15	1.365(8)	N1-Pt1-O1	83.30(15)	C13-C12-C12[1]	120.6(5)
Pt1-N1	2.034(4)	C15-C16	1.407(8)	N2-Pt1-O1	94.62(16)	C12-C13-C14	123.6(5)
Pt1-N2	1.997(4)	C16-C17	1.356(8)	N2-Pt1-N1	177.24(17)	C12-C13-C18	119.6(5)
Pt1-C26	1.985(6)	C17-C18	1.419(8)	C26-Pt1-O1	172.19(19)	C14-C13-C18	116.8(5)
O1-C11	1.324(6)	C18-C19	1.407(7)	C26-Pt1-N1	101.6(2)	C15-C14-C13	121.7(6)
N1-C1	1.388(7)	C20-C21	1.379(7)	C26-Pt1-N2	80.7(2)	C14-C15-C16	120.8(6)
N1-C9	1.347(7)	C21-C22	1.375(8)	C11-O1-Pt1	107.8(3)	C17-C16-C15	119.6(6)
N2-C20	1.352(6)	C22-C23	1.359(8)	C1-N1-Pt1	122.8(4)	C16-C17-C18	121.1(6)
N2-C24	1.364(7)	C23-C24	1.382(7)	C9-N1-Pt1	118.2(4)	C17-C18-C13	119.9(5)
C1-C2	1.387(8)	C24-C25	1.481(8)	C9-N1-C1	118.8(5)	C19-C18-C13	118.3(5)
C1-C6	1.418(7)	C25-C26	1.396(8)	C20-N2-Pt1	123.6(4)	C19-C18-C17	121.8(5)
C2-C3	1.366(8)	C25-C30	1.398(7)	C20-N2-C24	118.9(4)	C10-C19-C18	122.4(5)
C3-C4	1.376(9)	C26-C27	1.403(7)	C24-N2-Pt1	117.4(3)	N2-C20-C21	121.6(5)
C4-C5	1.374(9)	C27-C28	1.381(8)	N1-C1-C6	121.4(5)	C22-C21-C20	119.0(6)
C5-C6	1.397(8)	C28-C29	1.391(8)	C2-C1-N1	119.6(5)	C23-C22-C21	119.8(5)
C6-C7	1.401(8)	C29-C30	1.371(8)	C2-C1-C6	118.9(6)	C22-C23-C24	120.1(6)
C7-C8	1.356(8)	O2-C61	1.409(13)	C3-C2-C1	120.9(6)	N2-C24-C23	120.5(5)
C8-C9	1.399(7)	O2-O5[2]	1.604(16)	C2-C3-C4	120.4(7)	N2-C24-C25	111.9(5)
C9-C10	1.491(7)	C61-O3[3]	1.435(16)	C5-C4-C3	120.2(6)	C23-C24-C25	127.7(5)
C10-C11	1.443(7)	C61-C62	1.492(15)	C4-C5-C6	120.5(6)	C26-C25-C24	114.9(5)
C10-C19	1.369(7)	O3-C61[4]	1.435(16)	C5-C6-C1	118.8(6)	C26-C25-C30	122.4(6)
C11-C12	1.405(7)	O3-O4[5]	1.81(2)	C5-C6-C7	123.9(5)	C30-C25-C24	122.1(5)
C12-C12[1]	1.504(9)	O5-O2[6]	1.604(16)	C7-C6-C1	117.4(5)	C25-C26-Pt1	114.9(4)
C12-C13	1.416(8)	O5-O4[7]	1.63(2)	C8-C7-C6	120.3(5)	C25-C26-C27	116.5(5)
C13-C14	1.420(7)	O4-O3[8]	1.81(2)	C7-C8-C9	120.7(6)	C27-C26-Pt1	128.4(4)
C13-C18	1.429(7)	O4-O5[9]	1.63(2)	N1-C9-C8	121.0(5)	C28-C27-C26	121.4(6)
				N1-C9-C10	120.2(5)	C27-C28-C29	120.6(6)
				C8-C9-C10	118.6(5)	C30-C29-C28	119.7(6)
				C11-C10-C9	120.1(5)	C29-C30-C25	119.3(6)
				C19-C10-C9	119.7(5)	C61-O2-O52	112.4(11)
				C19-C10-C11	119.9(5)	O2-C61-O33	114.5(12)
				O1-C11-C10	121.0(5)	O2-C61-C62	118.5(16)
				O1-C11-C12	120.5(5)	O3[3]-C61-C62	127.0(14)
				C12-C11-C10	118.4(5)	C61[4]-O3-O4[5]	107.2(10)
				C11-C12-C12[1]	118.0(5)	O2[6]-O5-O4[7]	106.5(11)
				C11-C12-C13	120.9(5)	O5[8]-O4-O3[9]	99.3(9)

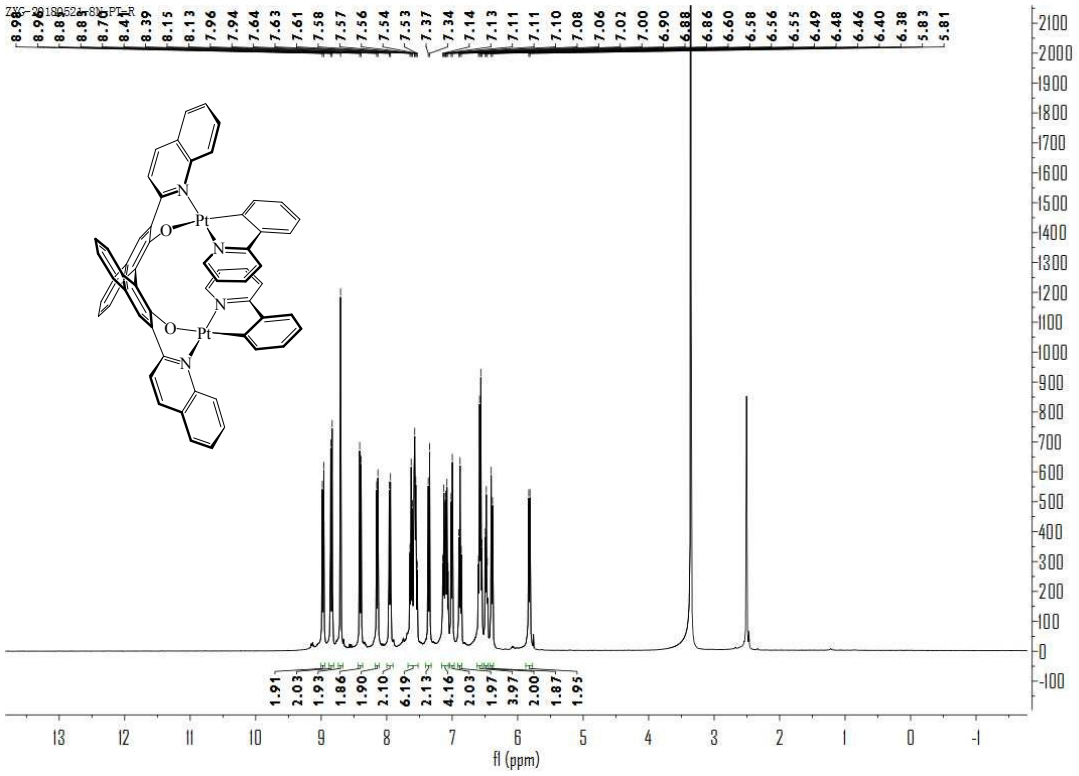
[1]1-X,+Y,1/2-Z; [2]+X,-Y,1/2+Z; [3]1/2-X,1/2+Y,1-Z; [4]1/2-X,-1/2+Y,1-Z; [5]-1/2+X,1/2-Y,+Z; [6]+X,-Y,-1/2+Z; [7]1-X,-1+Y,1/2-Z; [8]1/2+X,1/2-Y,+Z; [9]1-X,1+Y,1/2-Z



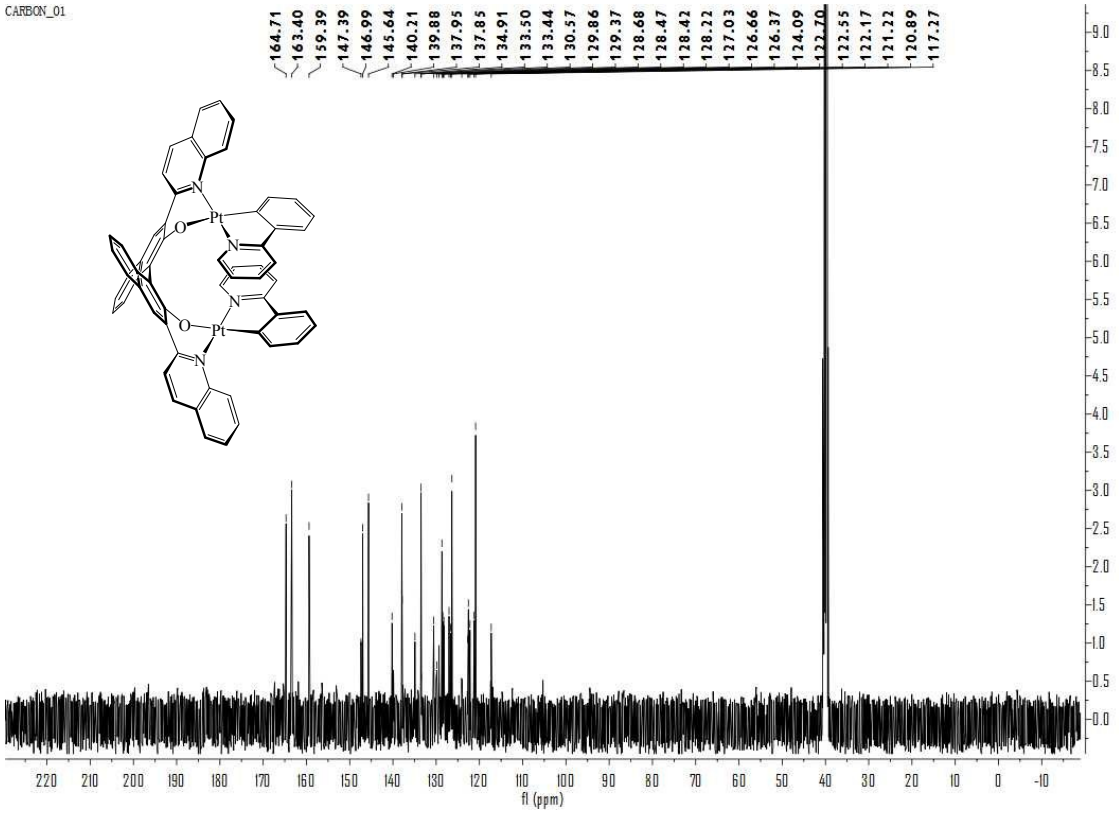
^{1}H NMR of **(*S*,*S*,*S*)1** in DMSO-d$_6$



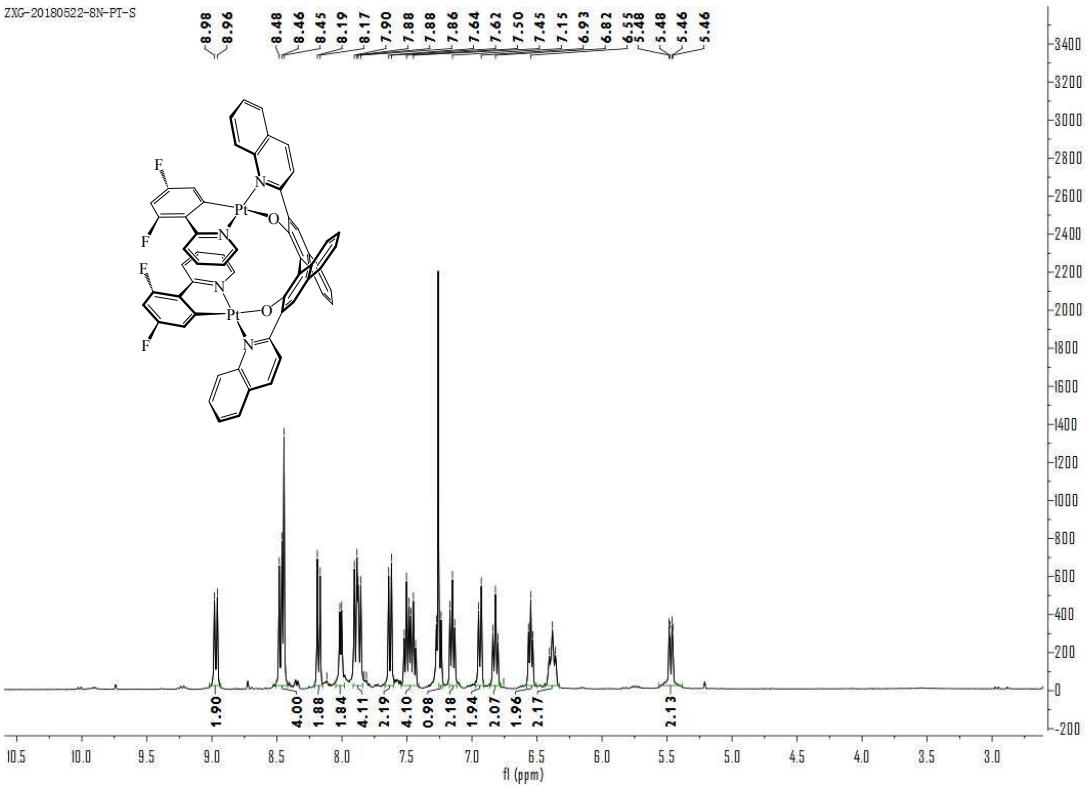
^{13}C NMR of **(*S*,*S*,*S*)1** in DMSO-d$_6$



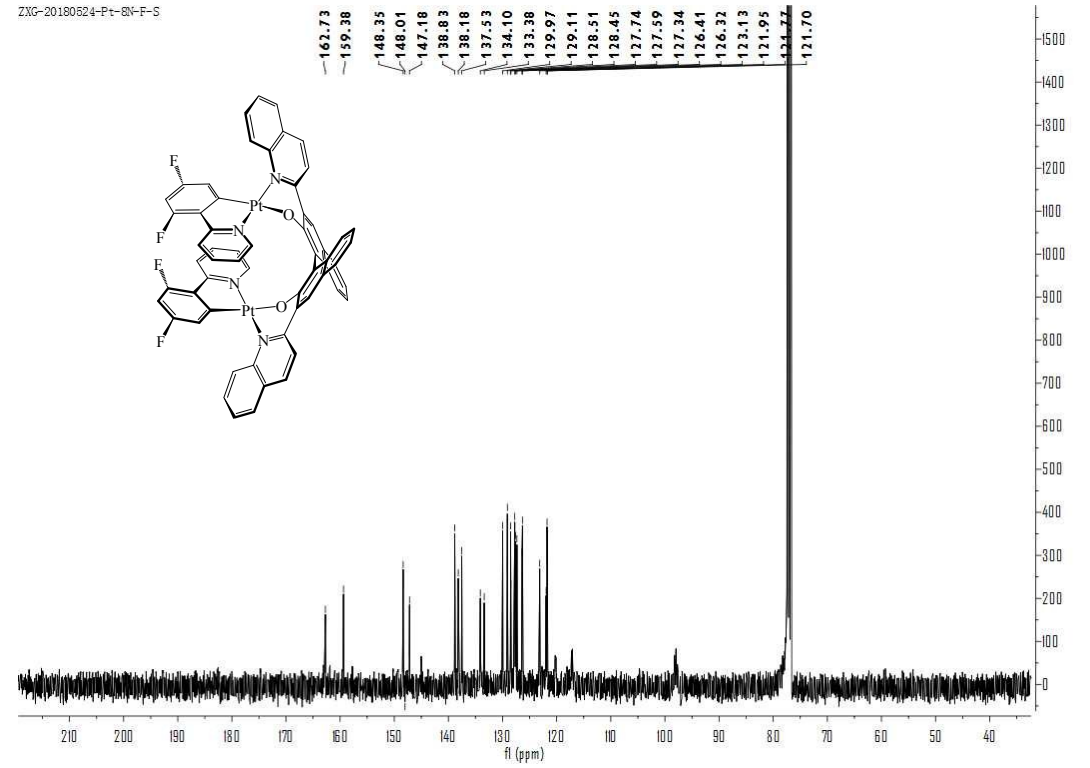
^{1}H NMR of ***(R,R,R)*1** in DMSO-d_6



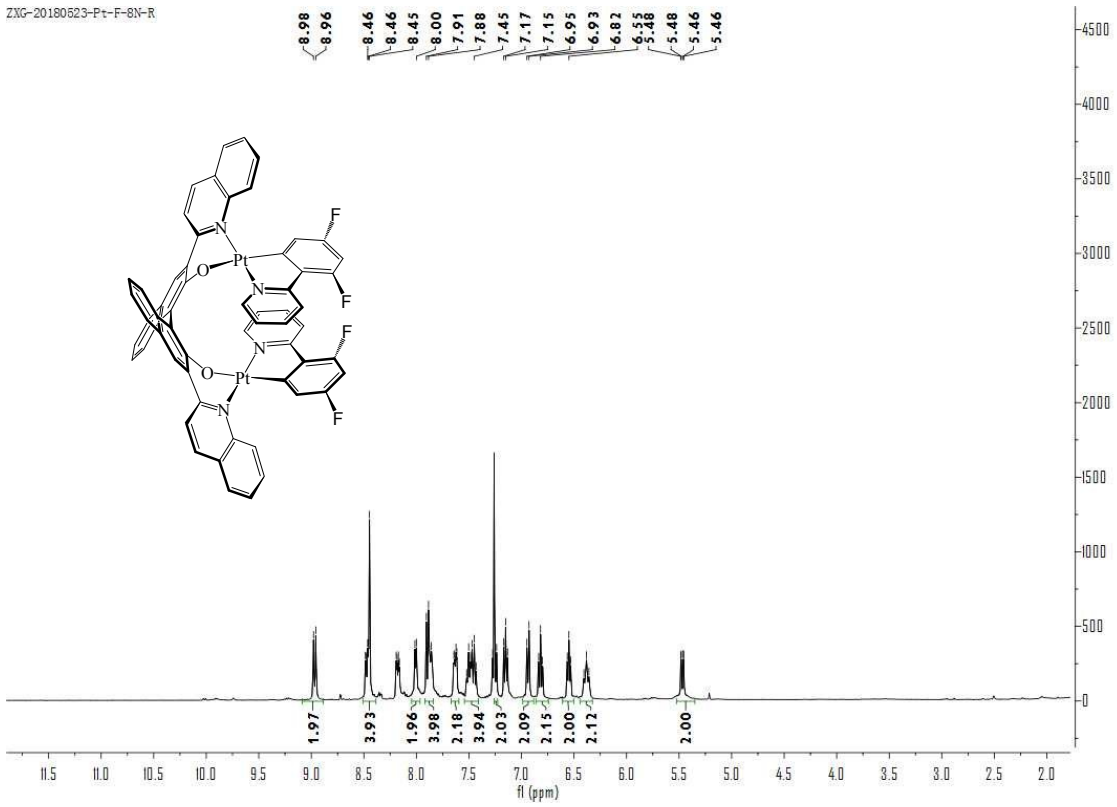
^{13}C NMR of ***(R,R,R)*1** in DMSO-d_6



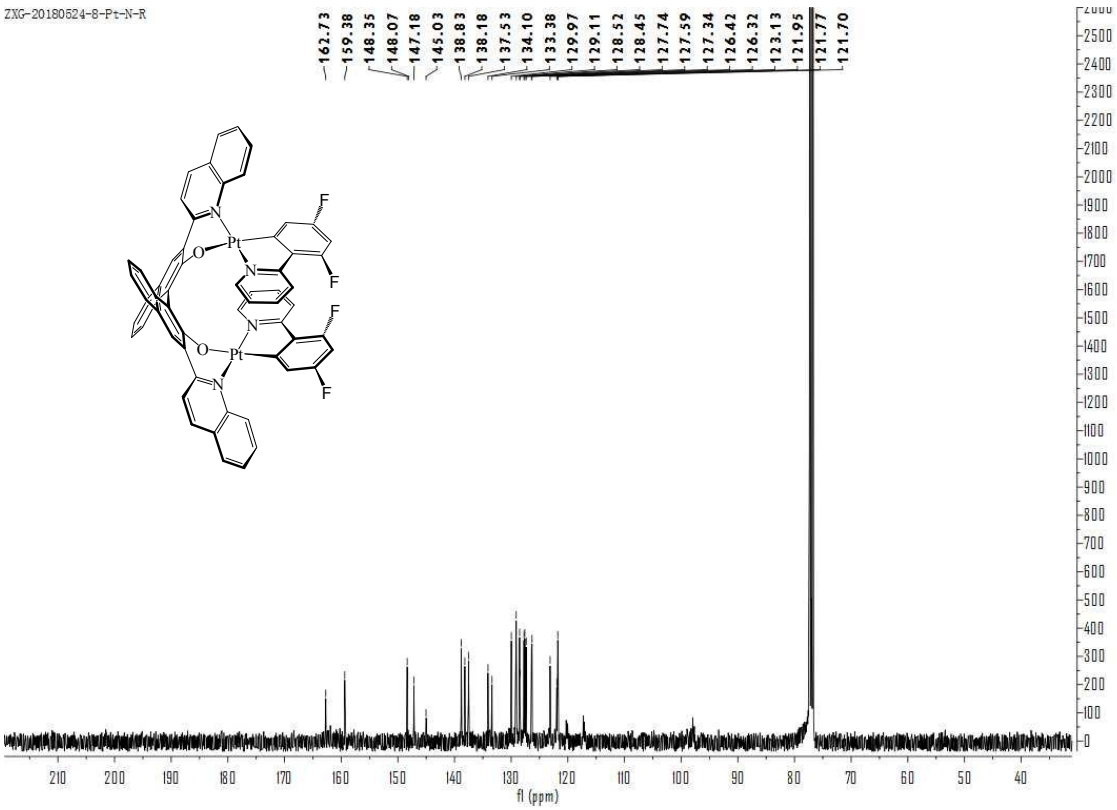
^{1}H NMR of ***(S,S,S)*2** in $CDCl_3$-d



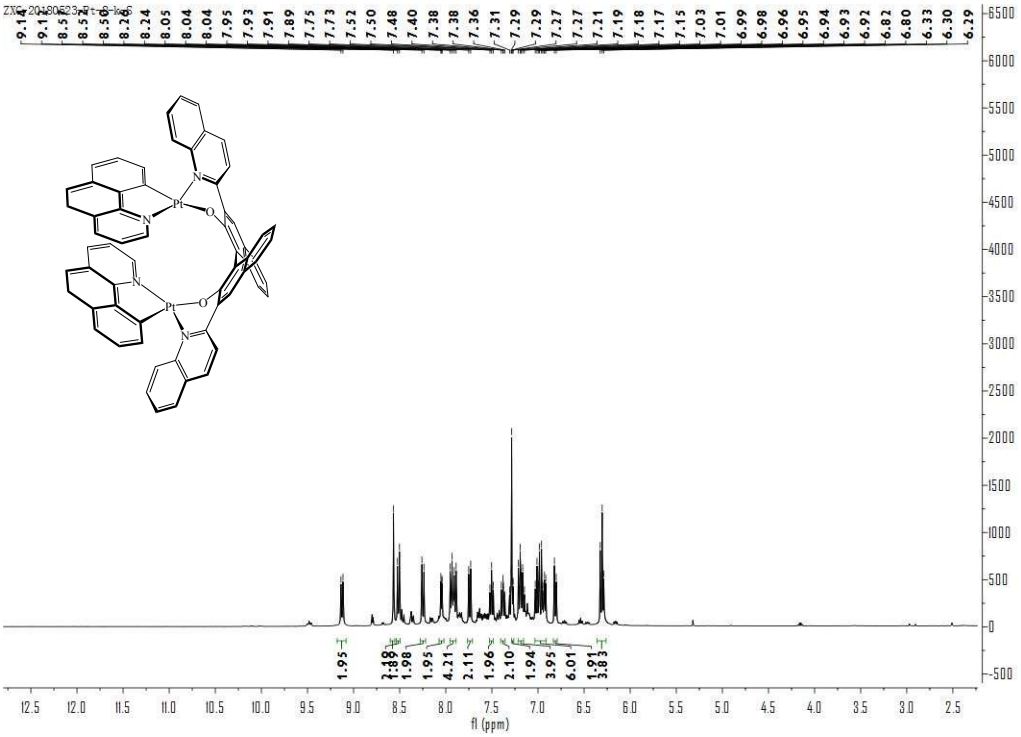
^{13}C NMR of ***(S,S,S)*2** in $CDCl_3$-d



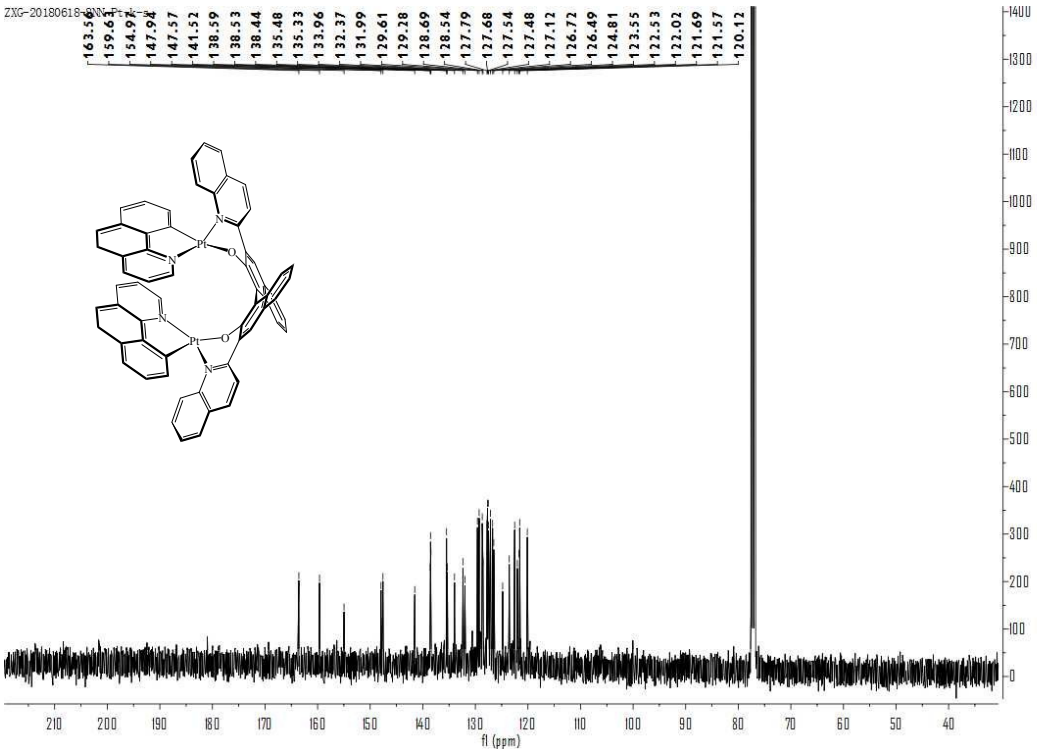
^{1}H NMR of **(*R*,*R*,*R*)2** in $CDCl_3$-d



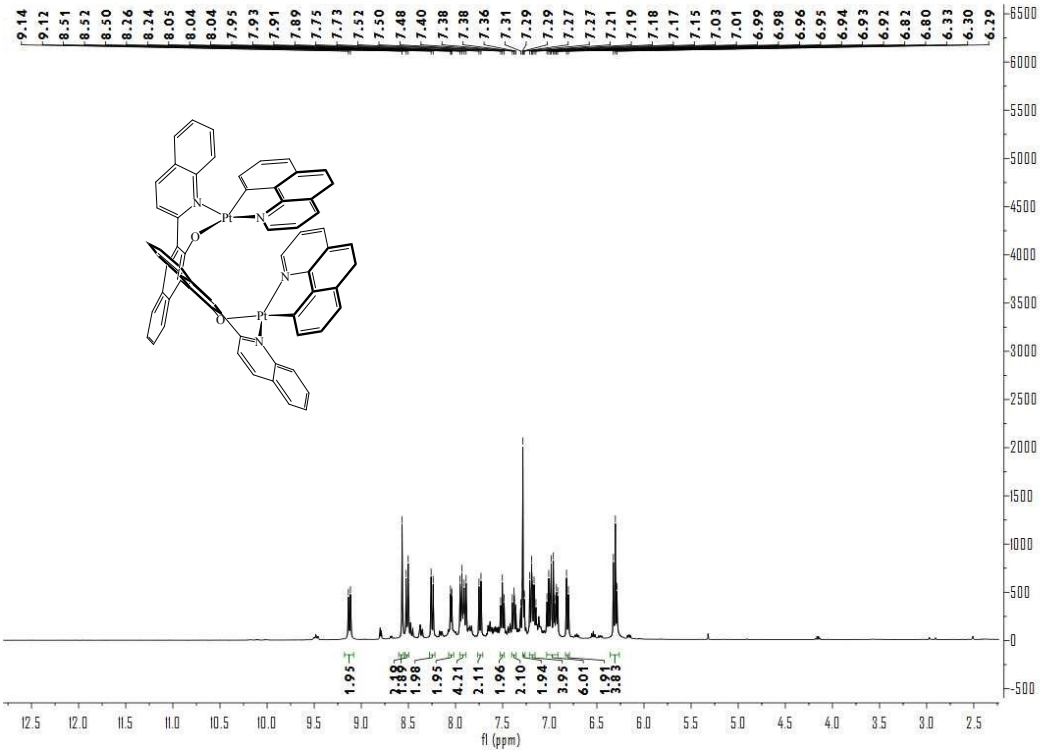
^{13}C NMR of **(*R*,*R*,*R*)2** in $CDCl_3$-d



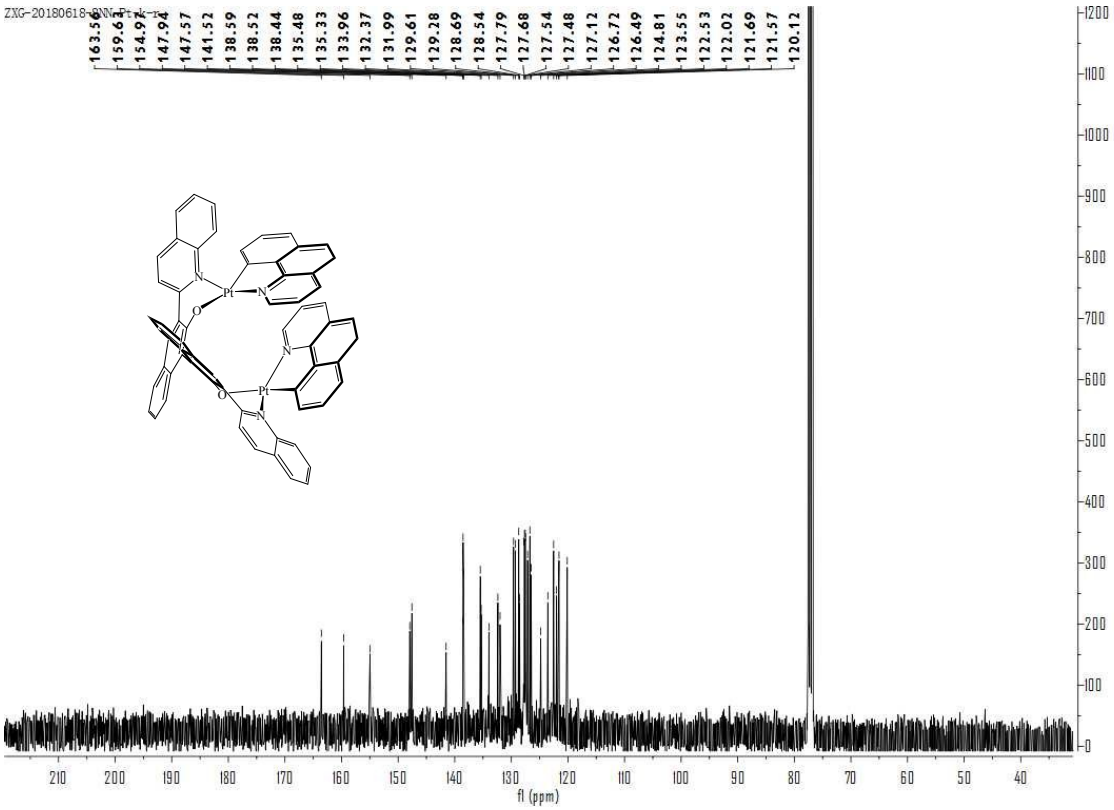
^{1}H NMR of ***(S,S,S)*3** in $CDCl_3$-d



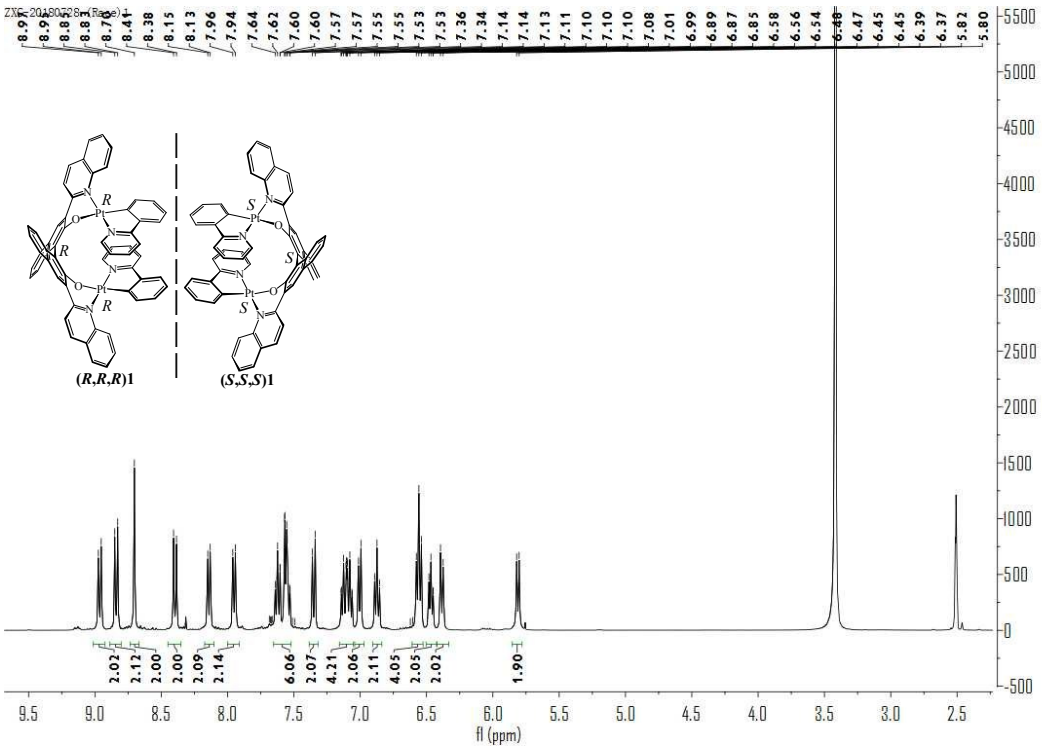
^{13}C NMR of ***(S,S,S)*3** in $CDCl_3$-d



^{1}H NMR of ***(R,R,R)*3** in $CDCl_3$-d



^{13}C NMR of ***(R,R,R)*3** in $CDCl_3$-d



^{1}H NMR of **(*Rac*)1** in DMSO-d_6

(*S,S,S*)1:PLATON/SQUEEZE

Cycle	R(F)	Nref(Heml)	R(F)>4жslg(F)	Nref	El(Sol v)/cell
1	0.048	24788	0.038	18097	0
2	0.046	24788	0.037	18097	8
3	0.046	24788	0.037	18097	22
4	0.046	24788	0.037	18097	27
5	0.046	24788	0.037	18097	28

(*R,R,R*)1:PLATON/SQUEEZE

Cycle	R(F)	Nref(Heml)	R(F)>4жslg(F)	Nref	El(Sol v)/cell
1	0.036	24820	0.028	18109	0
2	0.035	24820	0.027	18109	6
3	0.035	24820	0.027	18109	17
4	0.035	24820	0.027	18109	21
5	0.035	24820	0.027	18109	23