Supporting Information for:

Diseleno[2,3-*b*:3′,2′-*d*]selenophene(DSS) and Diseleno[2,3-*b*:3′,2′-*d*] thiophene(DST): Building Blocks for the Construction of [7]Helicenes

Wan Xu[†], Longlong Wu[†], Maohong Fang, Zhiying Ma, Zhen Shan, Chunli Li[*] and Hua Wang[*]

Engineering Research Center for Nanomaterials, Henan University, Kaifeng, 475004, P. R. China

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NMR and HRMS Spectra

NMR and HRMS Spectra of 6

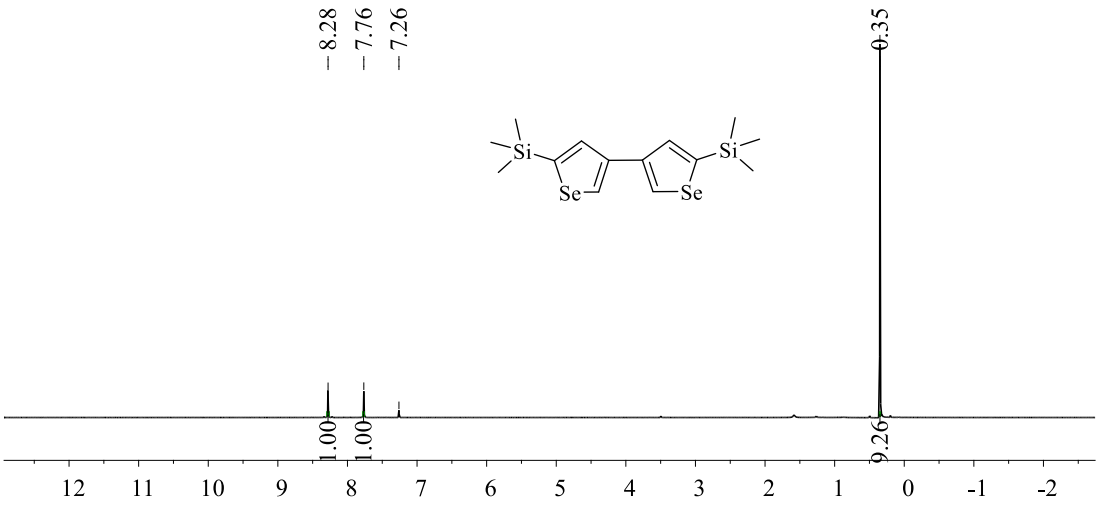


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **6**

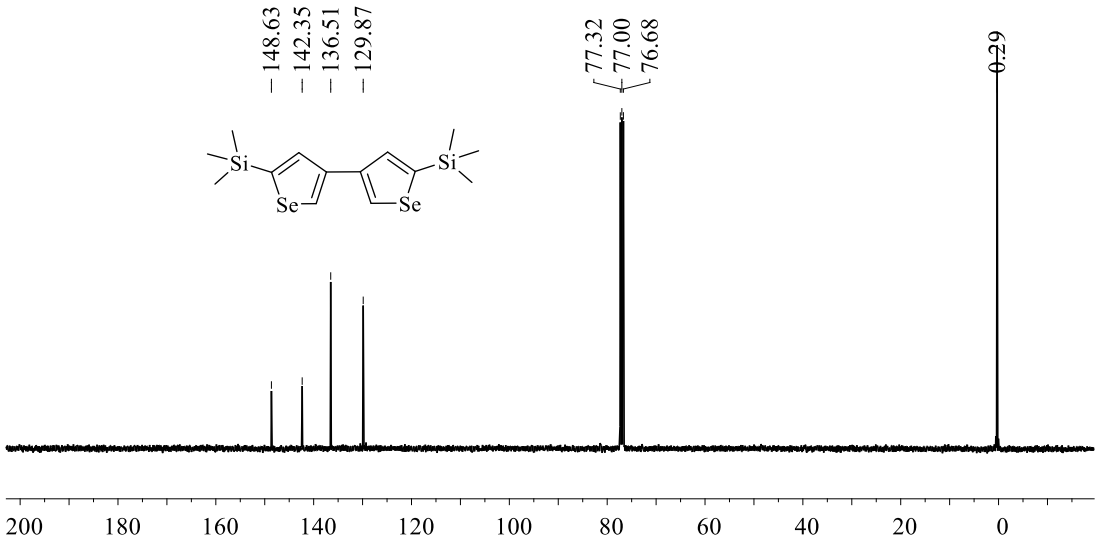


Figure S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of **6**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D152746

Sample Serial Number: wll-1-82-col

Operator : HUAQIN Date: 2015/10/28

Operation Mode: DART-Positive

Elemental composition search on mass 406.97

m/z= 401.97-411.97

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
406.9662	406.9663	-0.33	5.5	$C_{14}H_{23}Se_2Si_2$
	406.9659	0.68	6.5	$C_{15}H_{19}O_3Se_2$
	406.9669	-1.65	11.5	$C_{16}H_{15}O_4SeSi_2$
	406.9671	-2.21	11.5	$C_{17}H_{15}O_3SSeSi$
	406.9651	2.62	21.5	$C_{23}H_7O_2S_2Si$
	406.9673	-2.78	11.5	$C_{18}H_{15}O_2S_2Se$
	406.9649	3.18	21.5	$C_{22}H_7O_3SSi_2$

Figure S3. HRMS spectrum of **6**

NMR and HRMS Spectra of $(TMS)_2$-DST

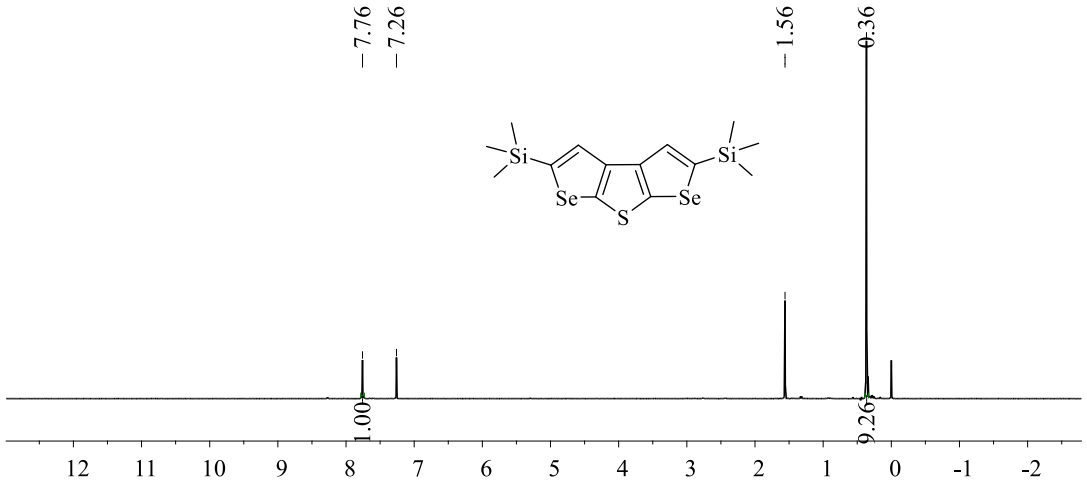


Figure S4. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of $(TMS)_2$-**DST**

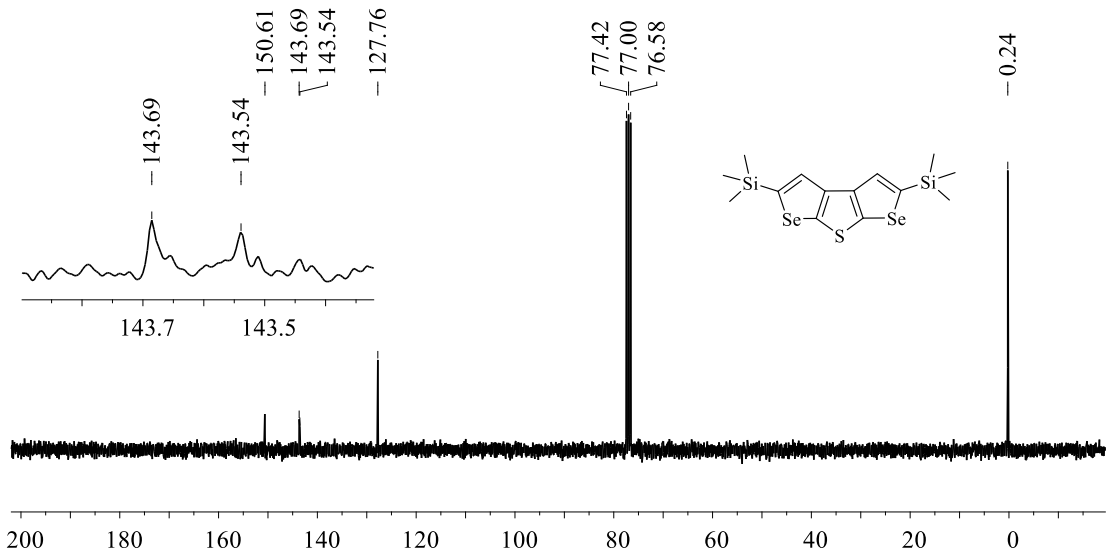


Figure S5. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of $(TMS)_2$-**DST**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D152747

Sample Serial Number: wll-3-182-col

Operator : HUAQIN Date: 2015/10/28

Operation Mode: DART-Positive

Elemental composition search on mass 436.92

m/z= 431.92-441.92

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
436.9229	436.9227	0.31	6.5	$C_{14}H_{21}SSe_2Si_2$
	436.9233	-0.92	12.5	$C_{16}H_{13}O_4SSeSi_2$
	436.9223	1.25	7.5	$C_{15}H_{17}O_3SSe_2$
	436.9235	-1.44	12.5	$C_{17}H_{13}O_3S_2SeSi$
	436.9221	1.77	7.5	$C_{14}H_{17}O_4Se_2Si$
	436.9213	3.58	22.5	$C_{22}H_5O_3S_2Si_2$

Figure S6. HRMS spectrum of $(TMS)_2$-**DST**

NMR and HRMS Spectra of $(TMS)_2$-DSS

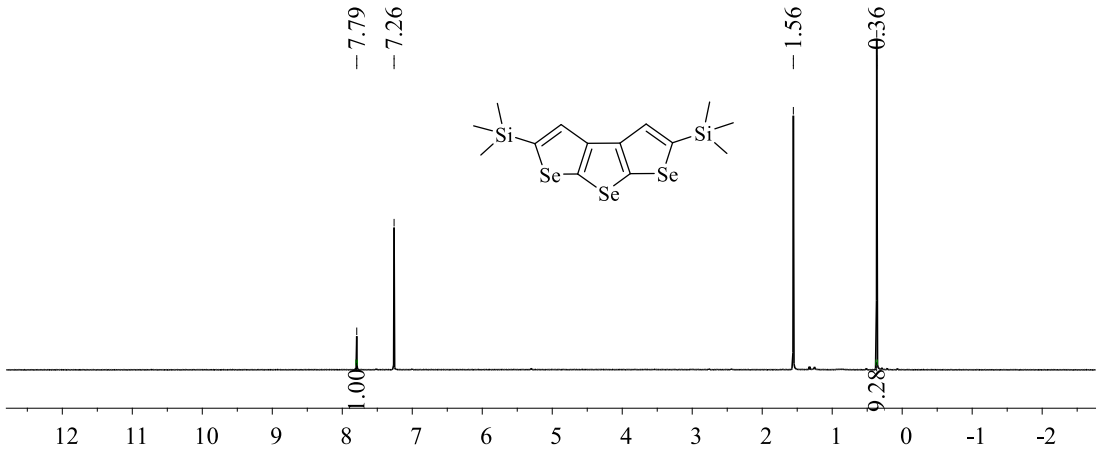


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of $(TMS)_2$-**DSS**

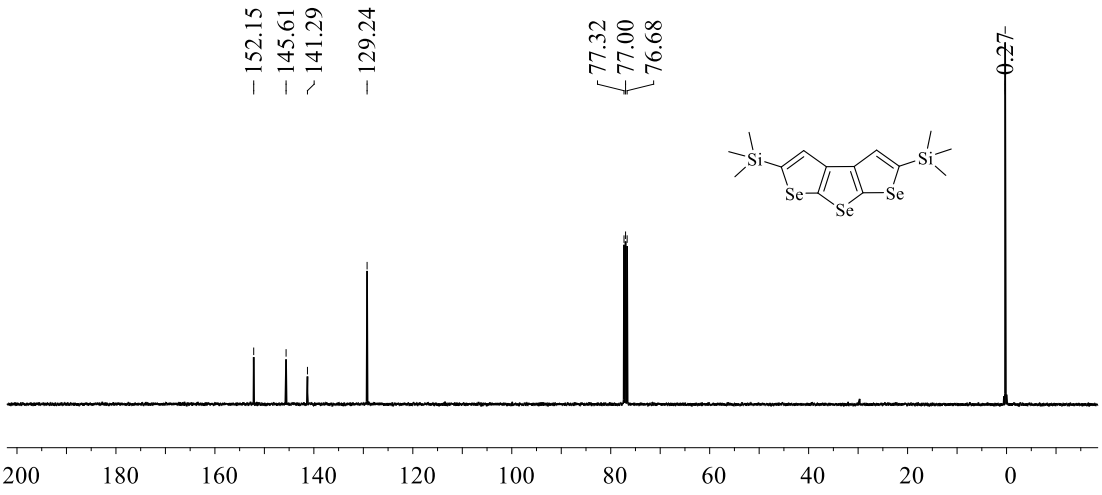


Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of $(TMS)_2$-**DSS**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: M162017

Sample Serial Number: wll-1-191-col

Operator: HUAQIN Date: 2016/07/21

Operation Mode: DART Positive

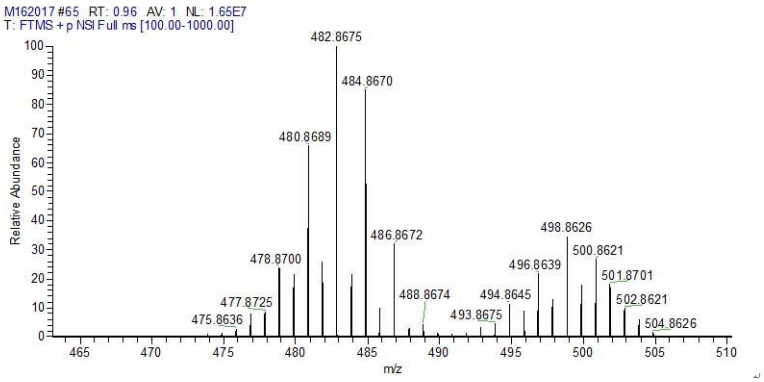


Figure S9. HRMS spectrum of $(TMS)_2$-**DSS**

NMR and HRMS Spectra of 8a

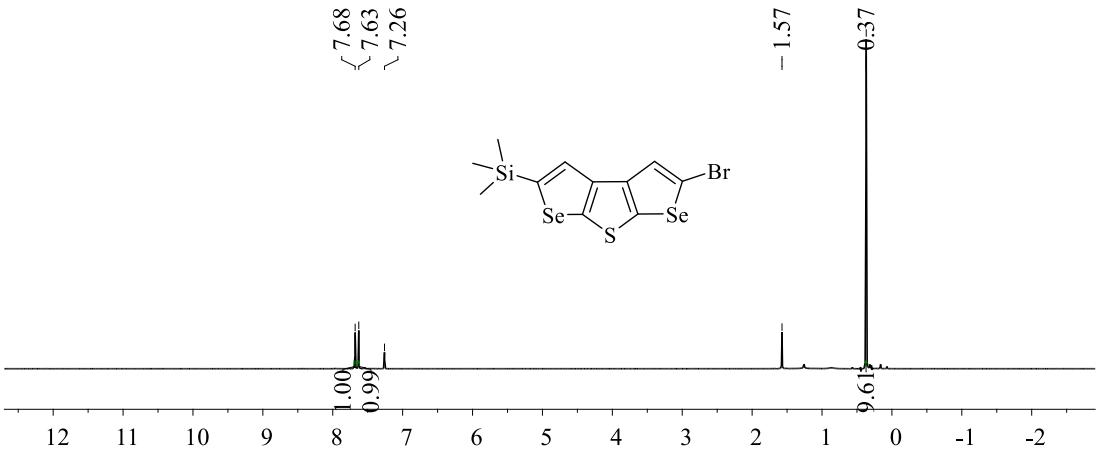


Figure S10. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **8a**

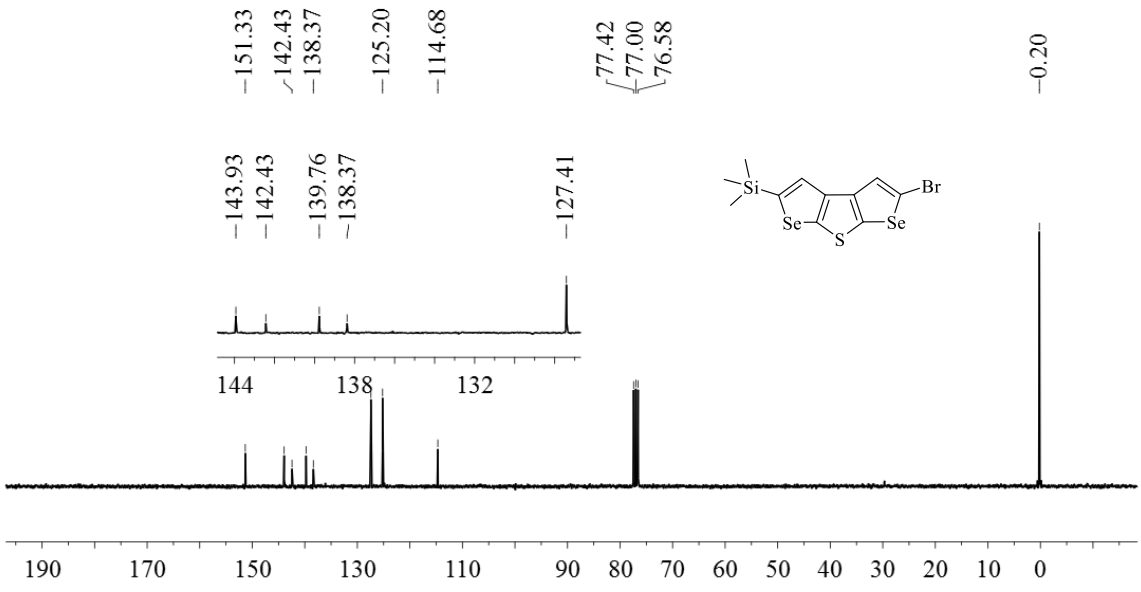


Figure S11. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **8a**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M162013

Sample Serial Number: wll-4-100-flt

Operator : HUAQIN Date: 2016/07/21

Operation Mode: DART Positive

Elemental composition search on mass 442.79

m/z= 437.79-447.79

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
442.7933	442.7937	-1.04	6.5	$C_{11}H_{12}BrSSe_2Si$

Figure S12. HRMS spectrum of **8a**

NMR and HRMS Spectra of 8b

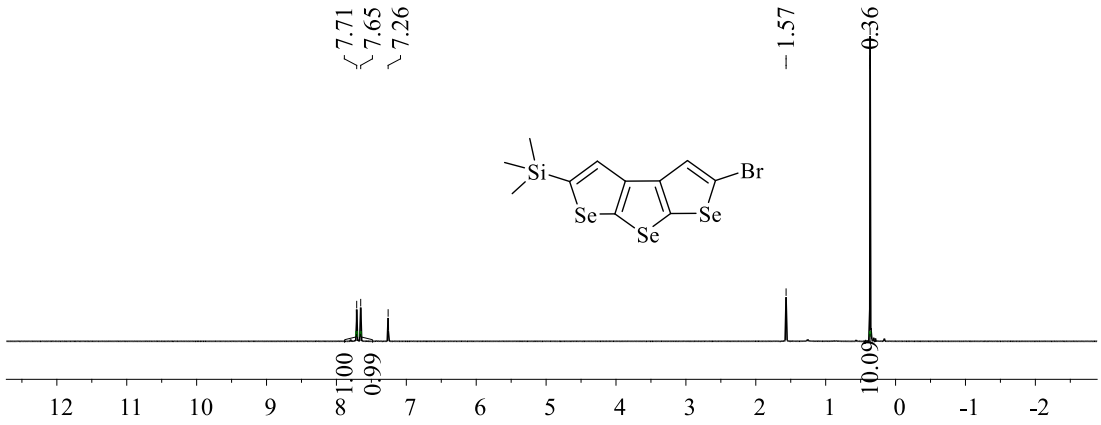


Figure S13. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **8b**

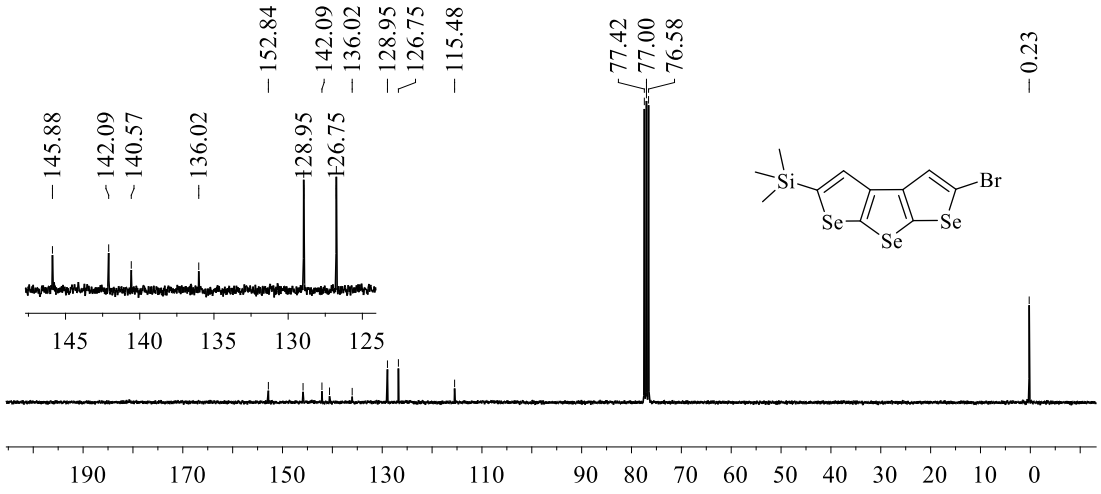


Figure S14. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **8b**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M163008

Sample Serial Number: xw-8-11-filt

Operator : HUAQIN Date: 2016/11/23

Operation Mode: MALDI-FT_DHB

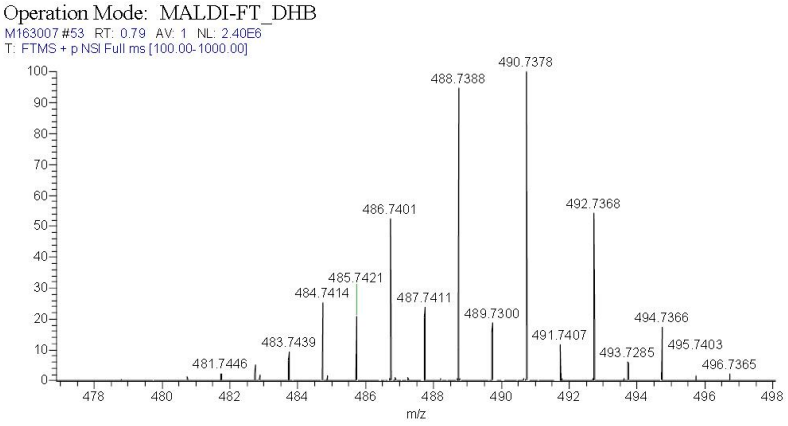


Figure S15. HRMS spectrum of **8b**

NMR and HRMS Spectra of 9a

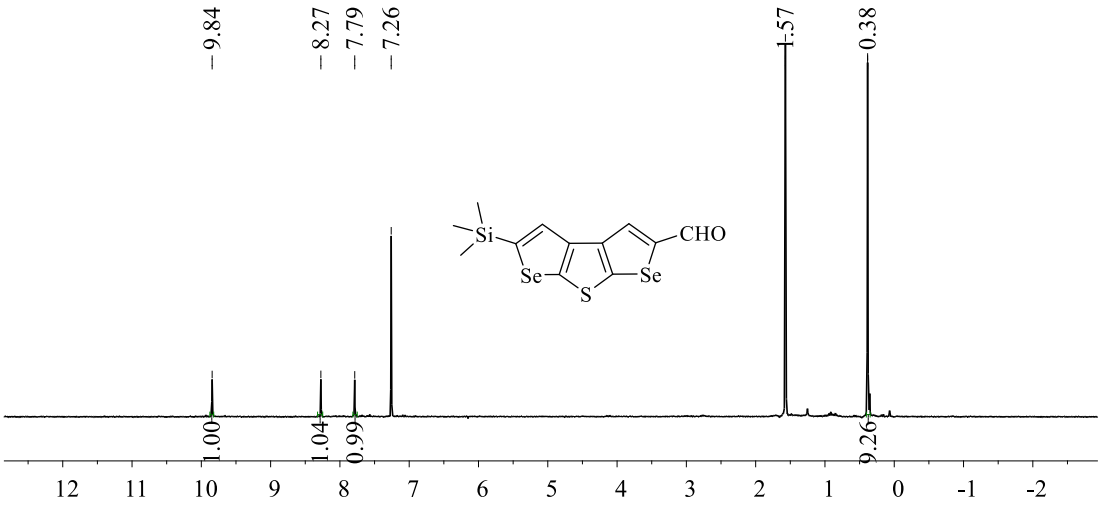


Figure S16. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **9a**

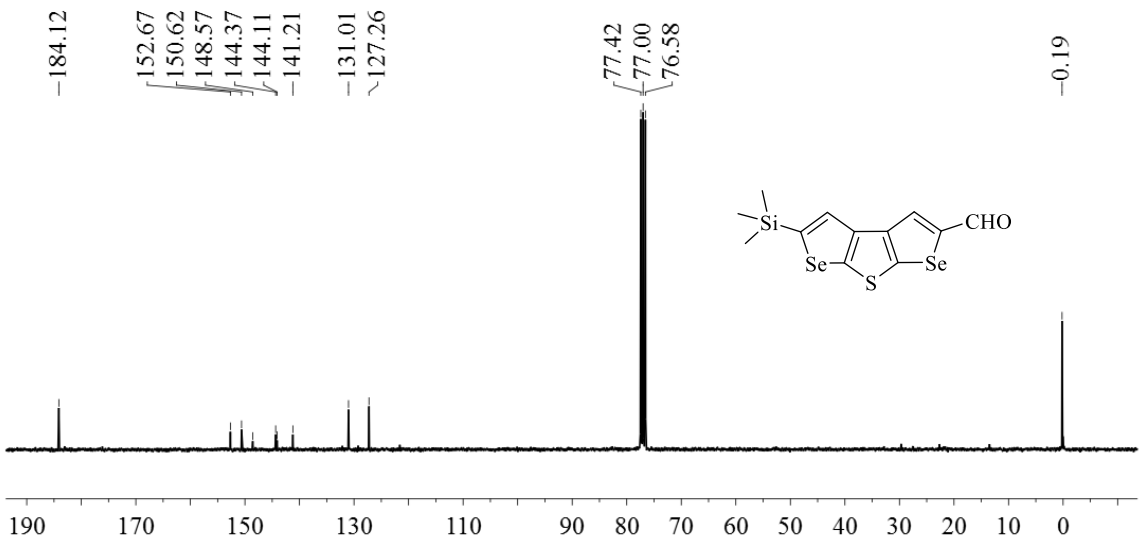


Figure S17. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **9a**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: M162015

Sample Serial Number: wll-4-89-col3

Operator: HUAQIN Date: 2016/07/21

Operation Mode: DART Positive

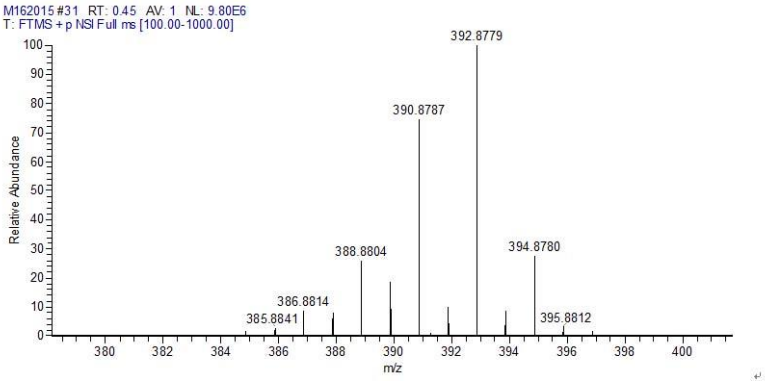


Figure S18. HRMS spectrum of **9a**

NMR and HRMS Spectra of 9b

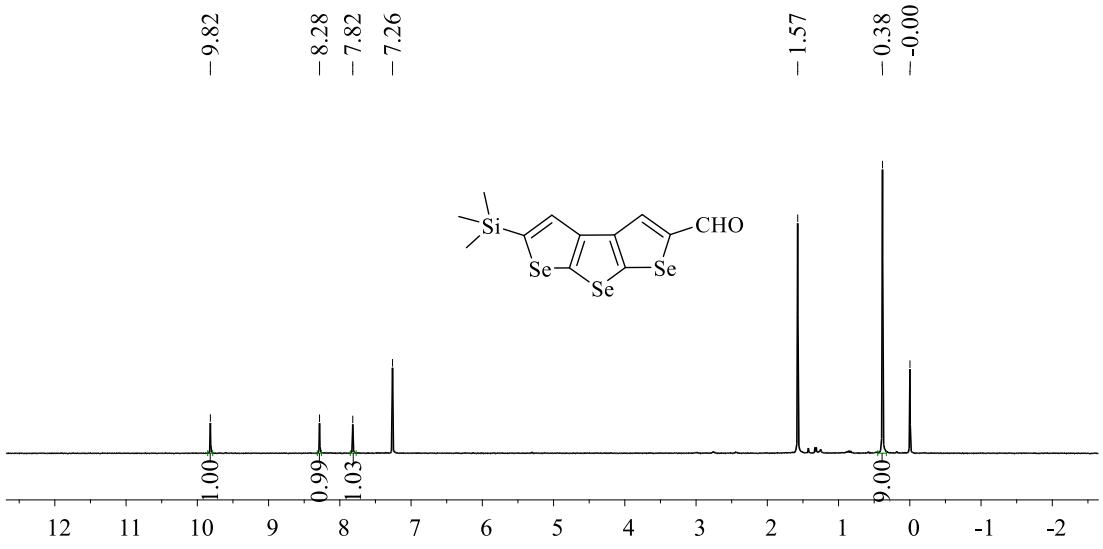


Figure S19. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **9b**

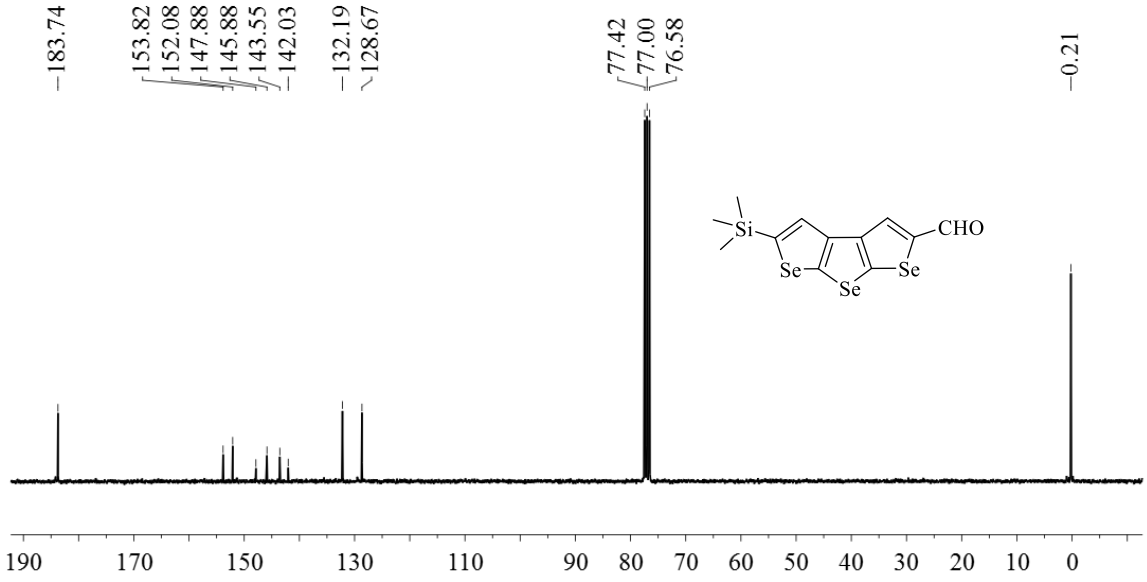


Figure S20. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **9b**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: M162019

Sample Serial Number: wll-4-90-col3

Operator: HUAQIN Date: 2016/07/21

Operation Mode: DART Positive

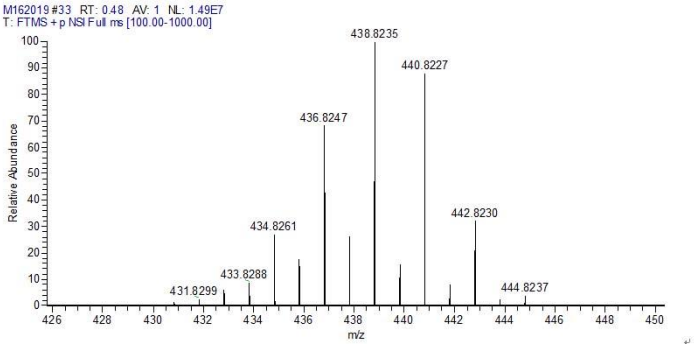


Figure S21. HRMS spectrum of **9b**

NMR and HRMS Spectra of 10a

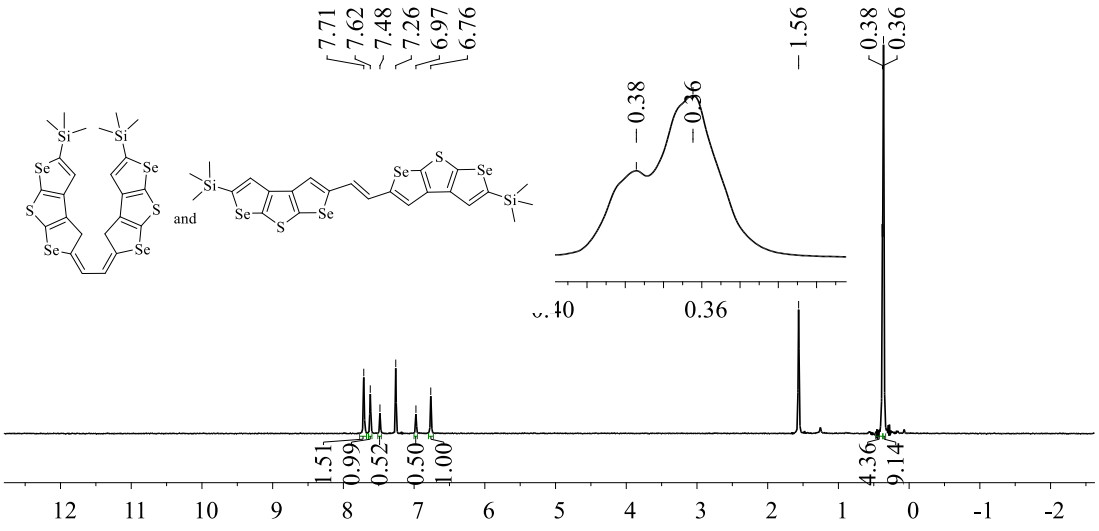


Figure S22. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **10a**

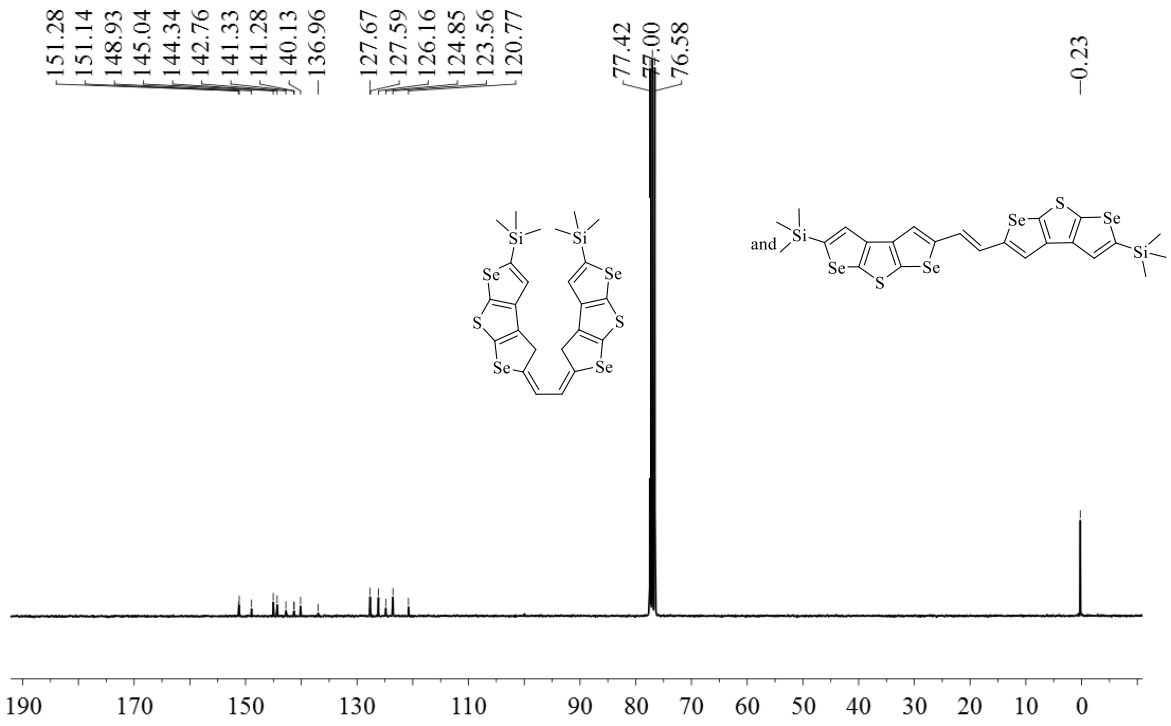


Figure S23. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **10a**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: D153073

Sample Serial Number: wll-3-196-pp

Operator: ZHUFJ Date: 2015/11/12

Operation Mode: DART Positive

Elemental composition search on mass 752.76

m/z= 747.76-757.76

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
752.7591	752.7592	-0.03	14.5	$C_{24}H_{25}S_2Se_4Si_2$
	752.7558	4.45	19.5	$C_{27}H_{21}SSe_4Si_2$

Figure S24. HRMS spectrum of **10a**

NMR and HRMS Spectra of 10b

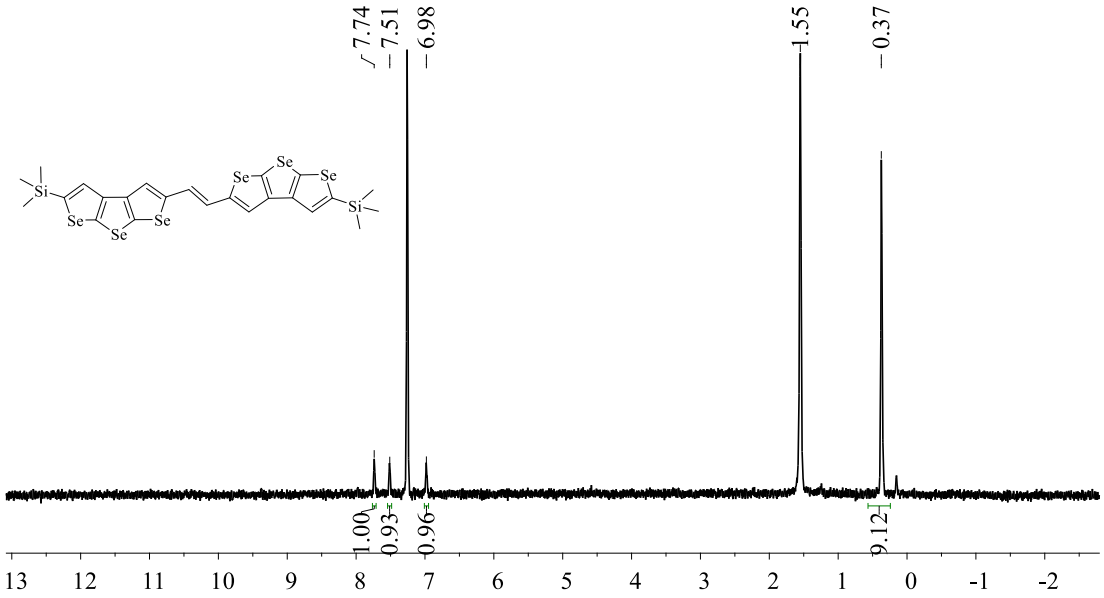


Figure S25. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of **10b**

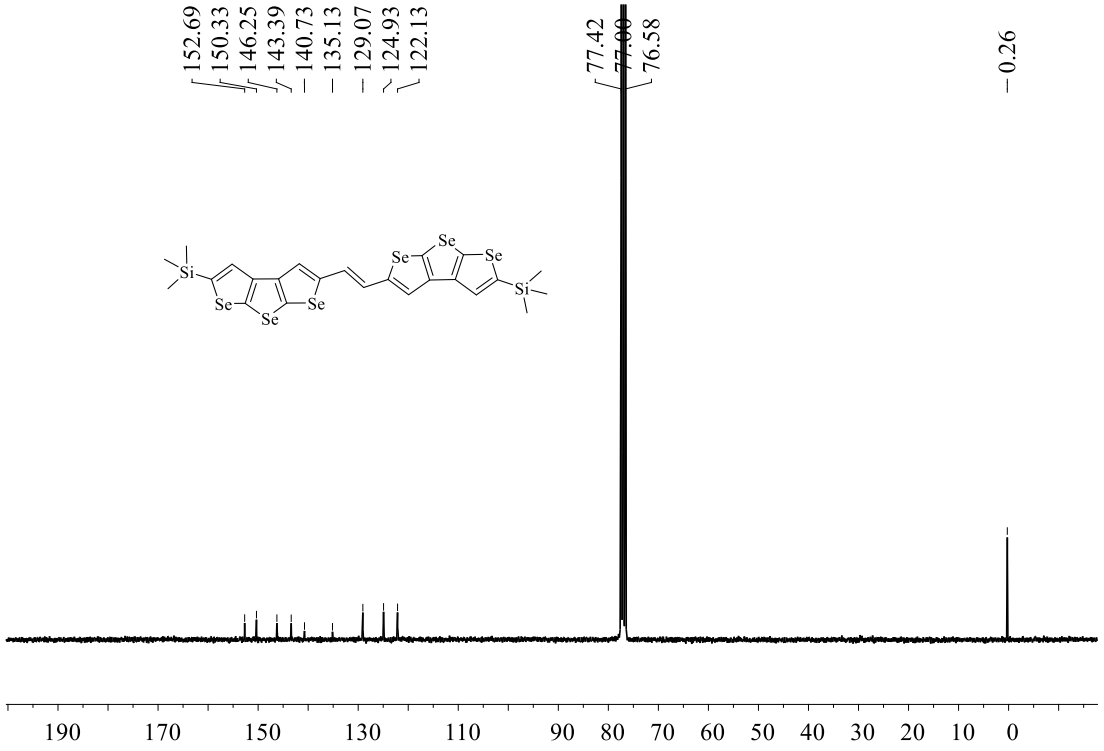


Figure S26. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of **10b**

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: M162024

Sample Serial Number: wll-4-49-pp

Operator: HUAQIN Date: 2016/07/21

Operation Mode: DART Positive

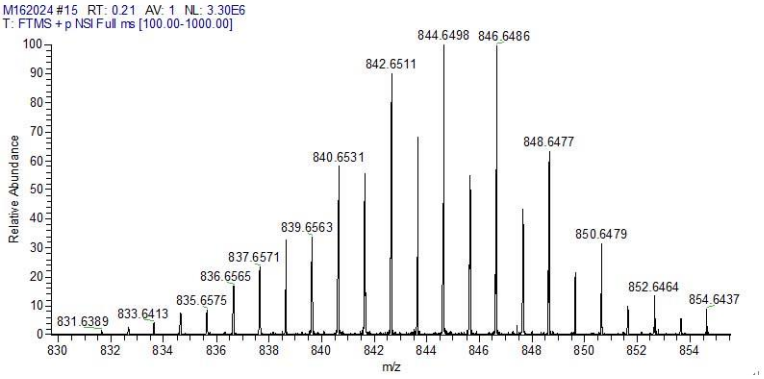


Figure S27. HRMS spectrum of **10b**

NMR and HRMS Spectra of *rac*-1

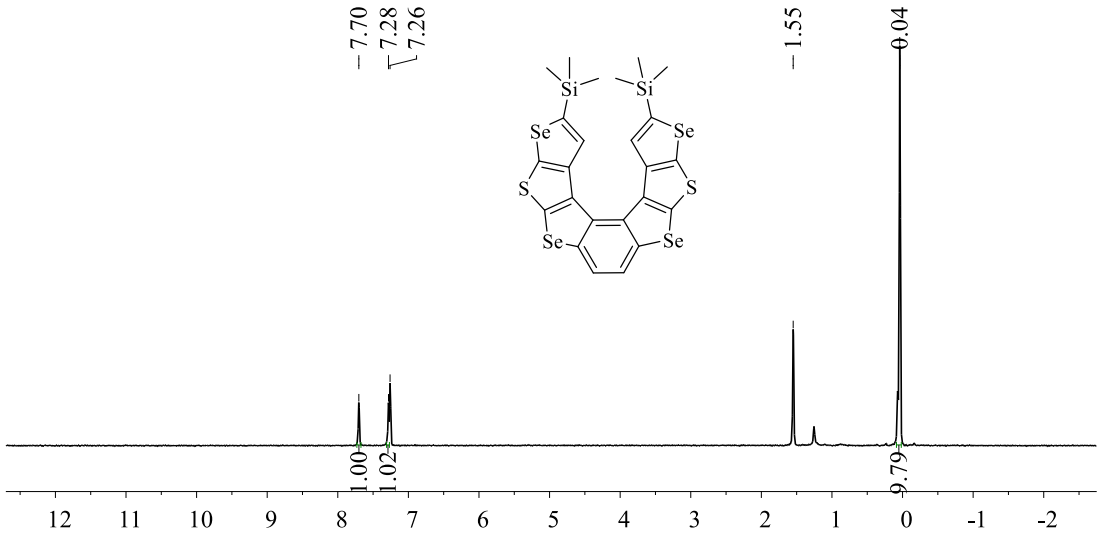


Figure S28. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of *rac*-**1**

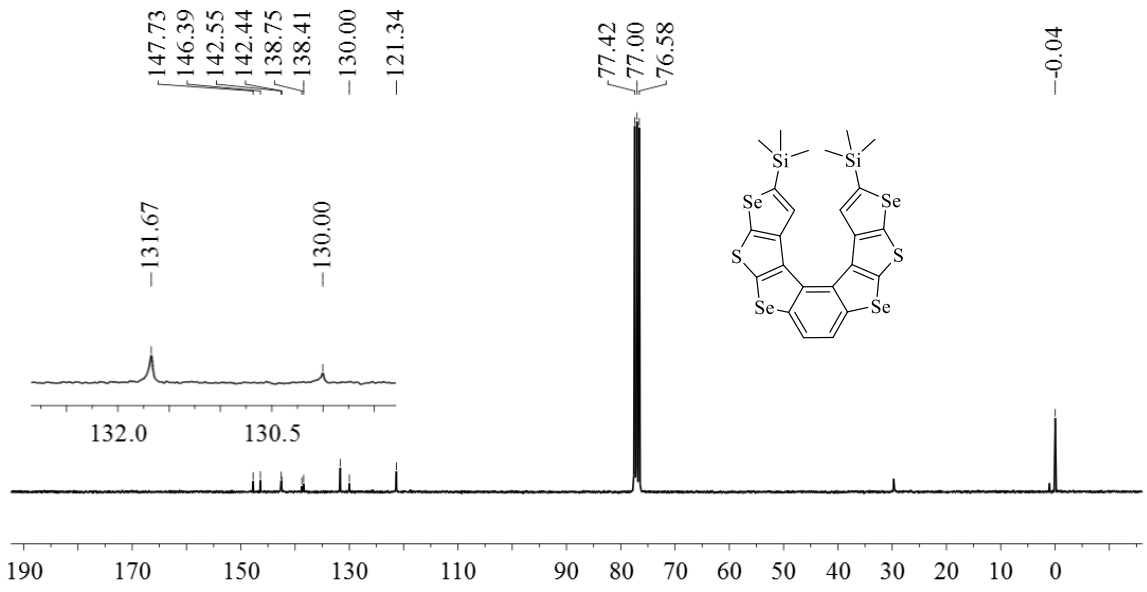


Figure S29. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of *rac*-**1**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: D153075

Sample Serial Number: wll-4-87-ptlc-1

Operator: ZHUFJ Date: 2015/11/12

Operation Mode: DART Positive

Elemental composition search on mass 750.74

m/z= 745.74-755.74

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
750.7435	750.7435	0.03	15.5	$C_{24}H_{23}S_2Se_4Si_2$
	750.7401	4.52	20.5	$C_{27}H_{19}SSe_4Si_2$

Figure S30. HRMS spectrum of *rac*-**1**

NMR and HRMS Spectra of *rac*-2

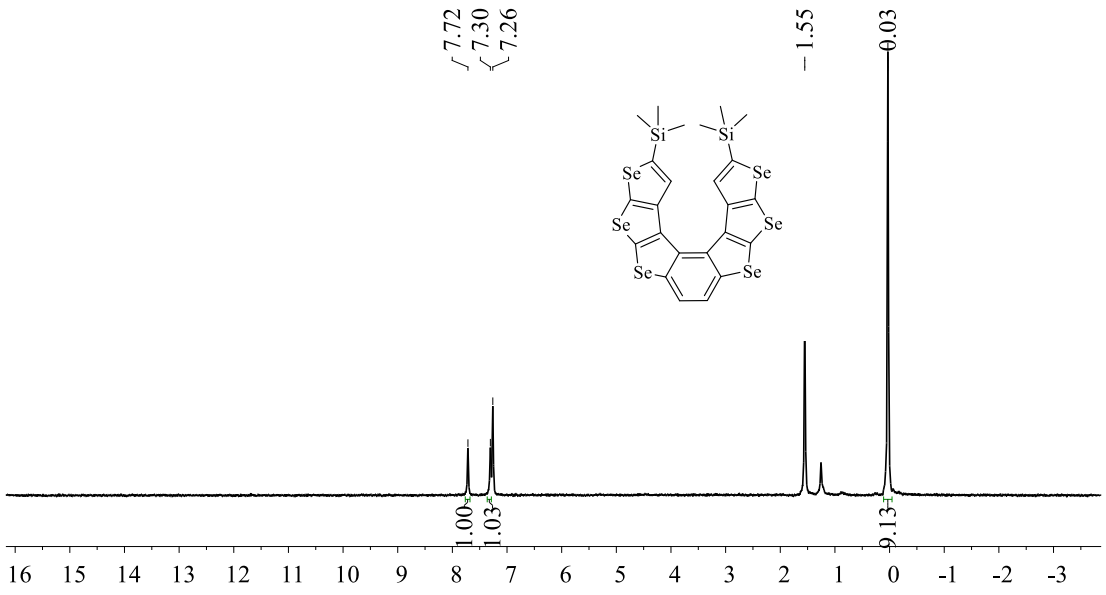


Figure S31. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of *rac*-**2**

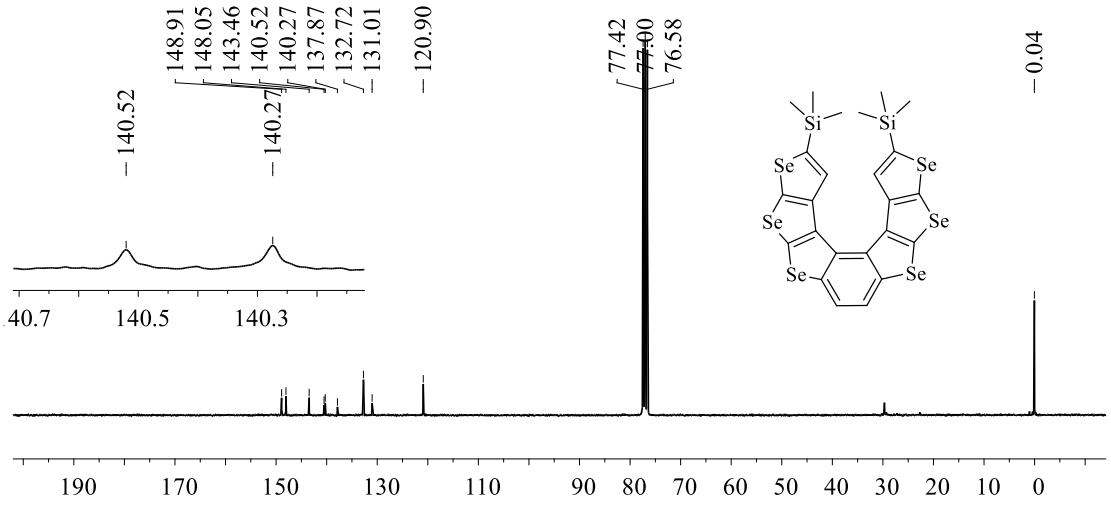


Figure S32. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of *rac*-**2**

Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number: D153076

Sample Serial Number: wll-4-129-ptlc-1

Operator :ZHUFJ Date: 2015/11/12

Operation Mode: DART Positive

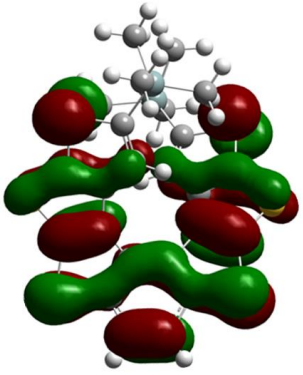
Elemental composition search on mass 846.63

m/z= 841.63-851.63

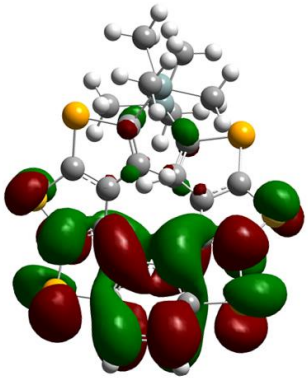
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
846.6323	846.6324	-0.07	15.5	$C_{24}H_{23}Se_6Si_2$
	846.6358	-4.05	10.5	$C_{21}H_{27}SSe_6Si_2$

Figure S33. HRMS spectrum of *rac*-**2**

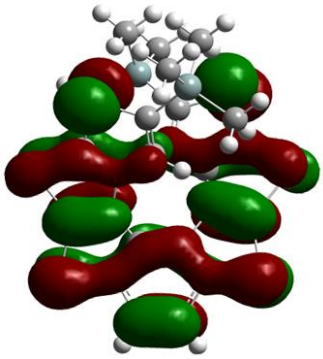
Quantum calculation



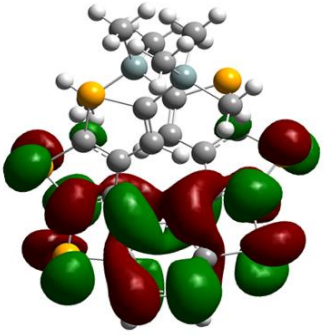
rac-1-HOMO



rac-1-LUMO



rac-**2**-HOMO



rac-**2**-LUMO

Figure S34. Distributions of the HOMO and LUMO distributions (b3lyp/6-31g*) for *rac*-**1** and *rac*-**2**.

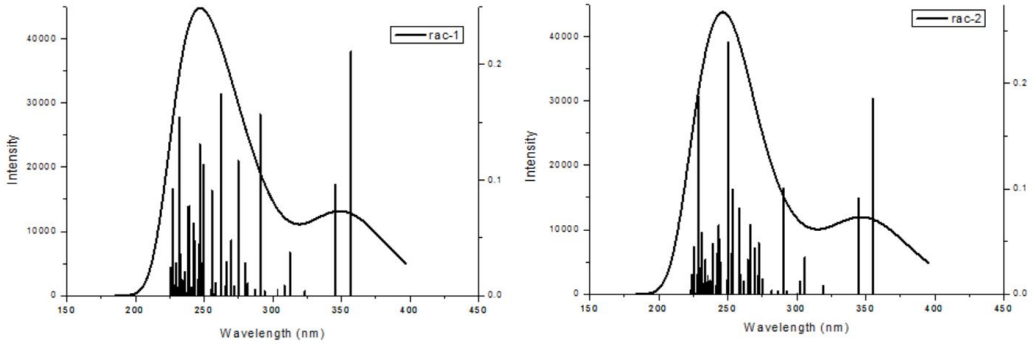


Figure S35. The prediction of UV-vis spectra of *rac*-**1** and *rac*-**2** at the PCM-TD-b3lyp/6-31g* level of theory.

Table S1. Selected computational absorption energies (nm), oscillator strength (f), and transition nature in dichloromethane solvent for *rac*-**1** and *rac*-**2** at the TD-b3lyp/6-31g* level of theory.

Compound	Excitation energies (eV)	Wavelength (nm)	*f*	Dominant transition contributions
rac-**1**	5.4621	226.99	0.0921	HOMO-3→LUMO+7 (51%) HOMO-2→LUMO+6 (15%)
	5.3504	231.73	0.1547	HOMO -1→LUMO+8 (12%) HOMO→LUMO+10 (37%)
	5.2090	238.02	0.0767	HOMO -4→ LUMO (82%)
	5.1809	239.31	0.0779	HOMO -3→ LUMO+4 (34%) HOMO-2→LUMO+5 (28%)
	5.1204	242.14	0.0630	HOMO -5→ LUMO+1 (11%) HOMO-1→LUMO+8 (50%)
	5.0231	246.83	0.1310	HOMO -4→ LUMO+1 (77%) HOMO→LUMO+8 (7%)
	4.9766	249.14	0.1133	HOMO -4→ LUMO+2 (13%) HOMO-2→LUMO+4 (12%) HOMO→LUMO+8 (57%)
	4.8502	255.63	0.0910	HOMO-3→LUMO+2 (82%) HOMO-5→LUMO (22%)
	4.7322	262.00	0.1748	HOMO-1→LUMO+3 (15%) HOMO-1→LUMO+5 (33%) HOMO-4→LUMO (24%)
	4.7284	262.21	0.0998	HOMO-2→LUMO+2 (28%) HOMO→LUMO+5 (16%)

				HOMO-2→LUMO+2 (10%)
	4.5104	274.89	0.1167	HOMO-1→LUMO+3 (48%) HOMO-1→LUMO+5 (12%)
				HOMO→LUMO+4 (14%)
				HOMO-3→LUMO (9%)
	4.2620	290.90	0.1569	HOMO→LUMO+3 (60%)
				HOMO→LUMO+5 (18%)
	3.5866	345.69	0.0963	HOMO-1→LUMO (94%) HOMO→LUMO+3 (2%)
	3.4740	356.89	0.2113	HOMO→LUMO (95%)
				HOMO-2→LUMO+5 (17%)
rac-**2**	5.1971	238.56	0.1879	HOMO-1→LUMO+9 (10%)
				HOMO-1→LUMO+11(16%)
	5.1421	241.12	0.0588	HOMO-5→LUMO+2(44%) HOMO-3→LUMO+4(20%)
				HOMO-4 →LUMO+1 (55%),
	4.8934	253.37	0.0658	HOMO-2 →LUMO+3 (15%)
				HOMO→ LUMO+3 (10%)
				HOMO-5→ LUMO+1 (37%)
	4.8777	254.19	0.0525	HOMO-3→ LUMO+3 (25%)
				HOMO-1→ LUMO+8 (19%)
				HOMO-3→ LUMO+2 (43%)
	4.7667	260.10	0.2391	HOMO-1→ LUMO+7 (12%)
				HOMO→ LUMO+9 (14%)
				HOMO-2→ LUMO+2 (16%)
	4.7072	263.39	0.0992	HOMO-1→ LUMO+6 (23%)
				HOMO→ LUMO+7 (19%)
				HOMO-3→ LUMO+2 (26%)
	4.6219	268.25	0.0818	HOMO-1→ LUMO+3 (11%)
				HOMO-1→ LUMO+5 (38%)
	4.4932	275.94	0.0660	HOMO-4→ LUMO (8%) HOMO-3→ LUMO+1 (75%)
	4.1246	300.60	0.1008	HOMO→ LUMO+2 (7%) HOMO→ LUMO+3 (78%)
	3.4974	354.51	0.0909	HOMO-1→ LUMO (94%) HOMO→ LUMO+3 (2%)
	3.3977	364.91	0.1858	HOMO→ LUMO (96%

Table S2. Cartesian coordinates and Energies for *rac*-**1** and *rac*-**2** at b3lyp/6-31g* level of theory.

rac-**1**				*rac*-**2**			
E = -11900.394472 a.u. NImag=0				E = -15902.782204 a.u. NImag=0			
C	3.869433	-1.29795	-0.44049	C	3.790289	-1.36724	-0.18939
C	5.091785	-0.64343	-0.26092	C	5.011259	0.682763	0.137682
C	5.09176	0.643644	0.260789	C	3.790468	1.366754	0.189411
C	3.869378	1.298102	0.440402	C	2.555379	0.709602	-0.00422
C	2.620346	0.698661	0.141254	C	2.555292	-0.70993	0.0043
C	2.620381	-0.69858	-0.14129	Se	3.54085	-3.23553	-0.4948
Se	3.690819	-3.08613	-1.06682	C	1.729081	-2.92778	-0.11667
C	1.874123	-2.89388	-0.66099	C	1.445383	-1.61854	0.217308
C	1.526462	-1.66073	-0.13147	C	0.141586	-1.45488	0.828482
C	0.196637	-1.71533	0.450249	C	-0.62788	-2.60683	0.813392
C	-0.41141	-2.94189	0.20908	Se	0.270425	-4.09298	0.09976
Se	-2.13362	-3.0489	0.910227	Se	-2.3118	-2.34714	1.569008
C	-1.83812	-1.31385	1.63834	C	-1.76527	-0.56577	1.962351
C	-0.60374	-0.84971	1.274083	C	-0.49315	-0.36098	1.507147
C	1.526372	1.660753	0.131475	C	1.44558	1.618344	-0.21722
C	1.873995	2.893921	0.660981	C	1.729471	2.927569	0.116668
Se	3.690695	3.086263	1.066751	Se	3.541283	3.235084	0.494786
C	-0.41156	2.941843	-0.20903	Se	0.270993	4.092967	-0.09985
C	0.196517	1.715292	-0.45019	C	-0.62753	2.606913	-0.81337
C	-0.60387	0.849635	-1.27398	C	0.141738	1.454829	-0.82835
C	-1.83824	1.313769	-1.63828	C	-0.49319	0.36097	-1.50691
Se	-2.13377	3.048814	-0.91019	C	-1.76522	0.565983	-1.96227
H	6.029051	-1.14464	-0.48085	Se	-2.31149	2.347446	-1.56899
H	6.029006	1.144909	0.480689	H	5.951442	-1.21066	-0.26425
H	-0.25063	0.121691	1.599723	H	5.951604	1.209897	0.264185
H	-0.25073	-0.12176	-1.59961	H	0.006848	0.587675	1.654207
Si	-3.16228	0.496948	-2.6931	H	0.006658	-0.58778	-1.6539
Si	-3.1622	-0.49704	2.693117	Si	-2.86306	-0.71729	-2.78681
C	-4.84796	0.997176	-1.99321	Si	-2.86299	0.717657	2.78681
H	-5.65411	0.627261	-2.63826	C	-4.30421	-1.16485	-1.64962
H	-5.00583	0.583713	-0.99093	H	-4.95181	-0.30166	-1.45508

H	-4.95701	2.086572	-1.9241	H	-4.92185	-1.94892	-2.1061
C	-3.04051	1.114638	-4.47753	H	-3.93582	-1.5368	-0.68791
H	-3.79712	0.628727	-5.1064	C	-3.54957	-0.0231	-4.40696
H	-3.20365	2.197142	-4.53584	H	-4.20674	-0.75534	-4.8922
H	-2.05643	0.899705	-4.90998	H	-4.13757	0.886953	-4.23707
C	-2.91746	-1.3759	-2.63602	H	-2.74521	0.223568	-5.10953
H	-2.01942	-1.67055	-3.19294	C	-1.80241	-2.24824	-3.12454
H	-2.81402	-1.76122	-1.61544	H	-1.00287	-2.02874	-3.84212
H	-3.77204	-1.8802	-3.10443	H	-1.33699	-2.66573	-2.22375
C	-4.84786	-0.99718	1.993125	H	-2.42961	-3.0342	-3.56426
H	-5.00568	-0.58366	0.990859	C	-4.30366	1.16582	1.649233
H	-4.95694	-2.08657	1.923942	H	-3.93482	1.537819	0.687712
H	-5.65402	-0.62728	2.638157	H	-4.95141	0.302822	1.454315
C	-3.04054	-1.11479	4.477534	H	-4.92125	1.949969	2.105616
H	-3.79715	-0.62885	5.106384	C	-3.55015	0.023321	4.406615
H	-3.20375	-2.19728	4.535814	H	-4.2073	0.755608	4.89182
H	-2.05646	-0.89993	4.910031	H	-4.13831	-0.88657	4.236355
C	-2.9173	1.375803	2.636127	H	-2.74605	-0.22369	5.109365
H	-2.01929	1.670396	3.193131	C	-1.80201	2.248256	3.125108
H	-2.81375	1.761162	1.615574	H	-1.00275	2.028412	3.842917
H	-3.7719	1.880121	3.10449	H	-1.33617	2.665722	2.224524
S	0.607358	-4.09119	-0.61619	H	-2.4291	3.034346	3.564736
S	0.607179	4.091181	0.61622	C	1.729081	-2.92778	-0.11667

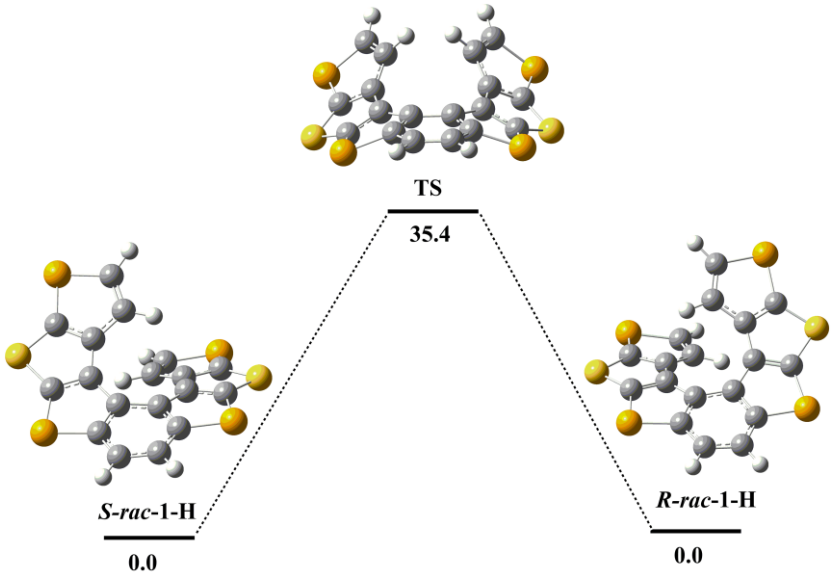


Figure S36. Isomerization process of *rac*-1-H from *S*-isomer to *R*-isomer. The relative energy (kcal/mol) was calculated at B3LYP/6-31G* level of theory.

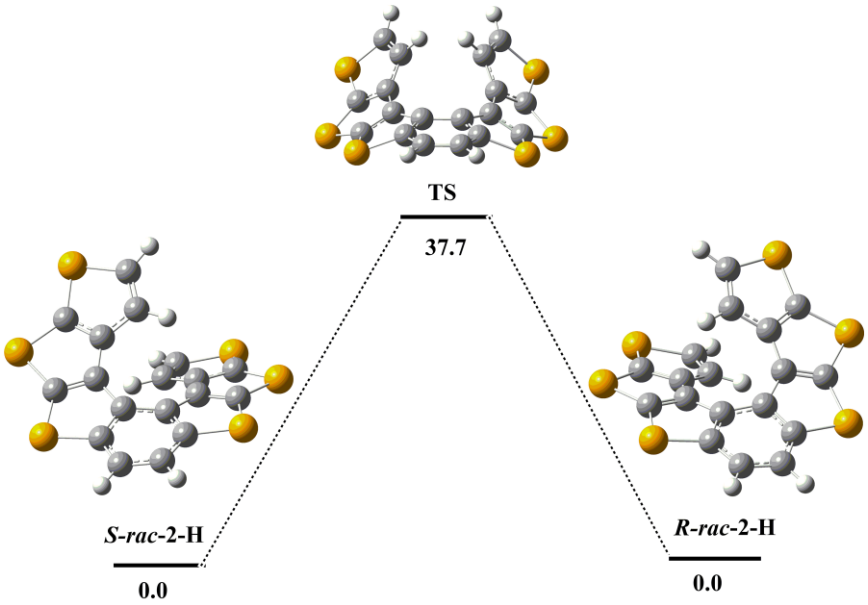


Figure S37. Isomerization process of *rac*-2-H from *S*-isomer to *R*-isomer. The relative energy (kcal/mol) was calculated at B3LYP/6-31G* level of theory.

X-ray crystallographic data

Complete crystal data for $(TMS)_2$-**DSS**

Table S3. Crystal data and structure refinement for $(TMS)_2$-**DSS**.

Identification code	$(TMS)_2$-**DSS**
Empirical formula	$C_{14}H_{20}Se_3Si_2$
Formula weight	481.36
Temperature	296(2)
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 6.4642(19) Å alpha = 90°
	b = 20.855(6) Å beta = 90.498(5)°
	c = 27.927(8) Å gamma = 90°
Volume	3764.8(19) $Å^3$
Z, Calculated density	8, 1.699 Mg/m^3
Absorption coefficient	5.976 mm^{-1}
F(000)	1872
Crystal size	0.43 x 0.16 x 0.14 mm
Theta range for data collection	1.46 to 25.00°
Limiting indices	-7<=h<=7, -20<=k<=24, -28<=l<=33
Reflections collected / unique	17875 / 6562 [R(int) = 0.0932]
Completeness to theta = 25.00	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4883 and 0.1832
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6562 / 0 / 343
Goodness-of-fit on F^2	0.923
Final R indices [I>2sigma(I)]	R1 = 0.0577, wR2 = 0.1149
R indices (all data)	R1 = 0.1338, wR2 = 0.1307
Largest diff. peak and hole	0.777 and -0.722 e $·Å^{-3}$

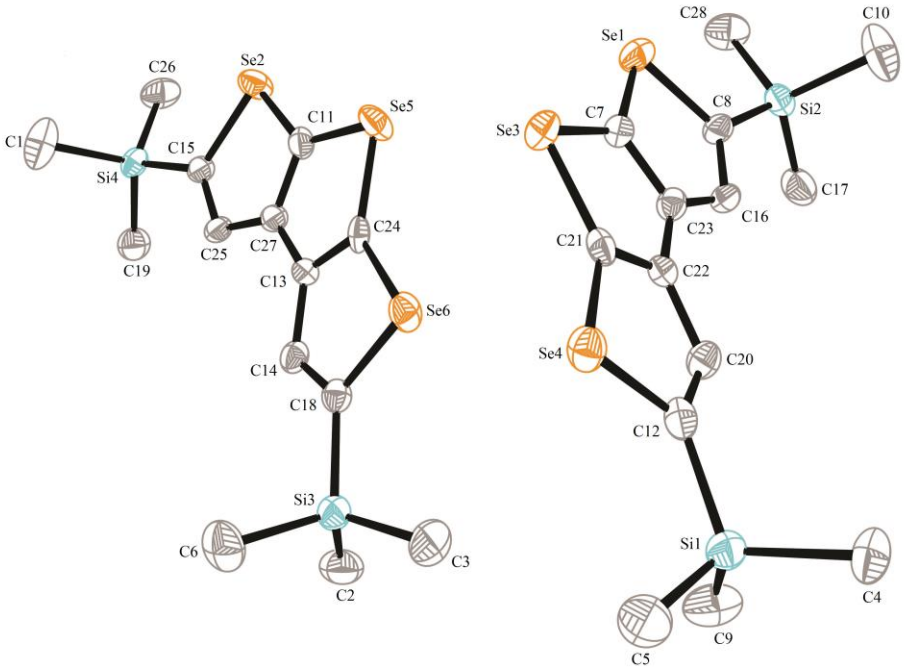


Figure S38. Molecular structures for compounds $(TMS)_2$-**DSS**, thermal ellipsoids set at 30% probability level.

Complete crystal data for *rac*-**1**

Table S4. Crystal data and structure refinement for *rac*-**1**.

Identification code	*rac*-**1**
Empirical formula	$C_{24}H_{22}S_2Se_4Si_2$
Formula weight	746.56
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Trigonal, R-3
Unit cell dimensions	a = 39.587(5) Å alpha = 90°
	b = 39.587(5) Å beta = 90°
	c = 9.490(3) Å gamma = 120°
Volume	12880(4) $Å^3$

Z, Calculated density	18, 1.733 Mg/m^3
Absorption coefficient	5.368 mm^{-1}
F(000)	6516
Crystal size	0.41 x 0.12 x 0.09 mm
Theta range for data collection	1.78 to 25.00^o
Limiting indices	-47<=h<=46, -33<=k<=46, -11<=l<=11
Reflections collected / unique	22199 / 5039 [R(int) = 0.0573]
Completeness to theta = 25.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6437 and 0.2169
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5039 / 0 / 289
Goodness-of-fit on F^2	1.000
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0770
R indices (all data)	R1 = 0.0697, wR2 = 0.0843
Largest diff. peak and hole	0.501 and -0.491 e $\cdot Å^{-3}$

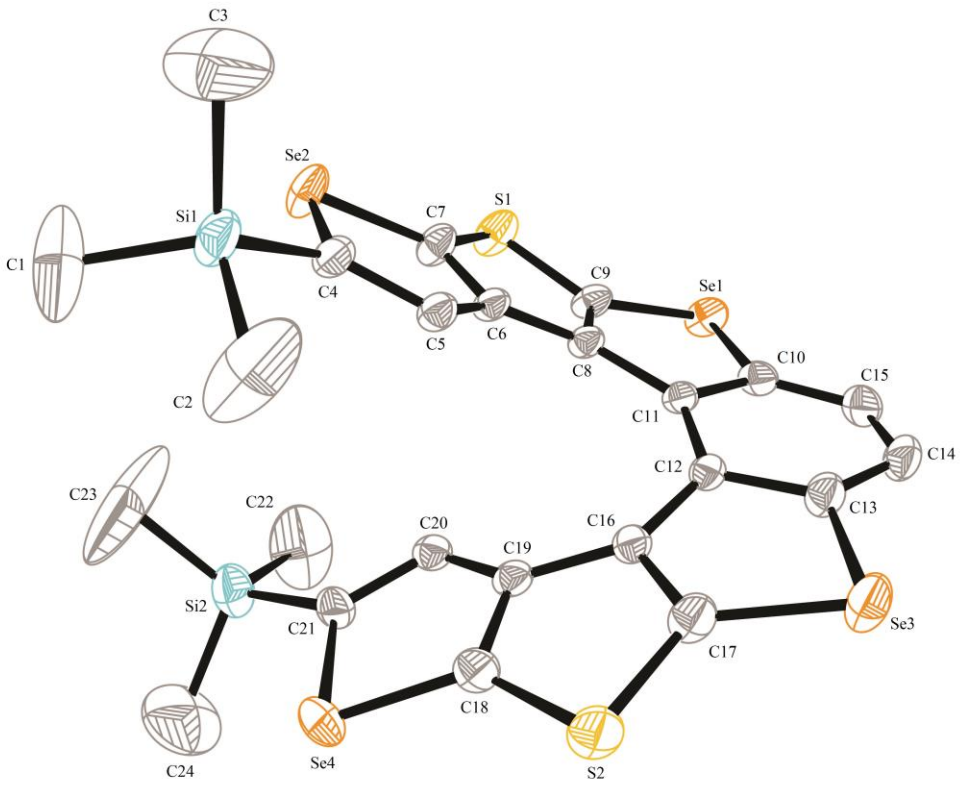


Figure S39. Molecular structures for compounds *rac*-**1**, thermal ellipsoids set at 30% probability level.

Complete crystal data for *rac*-**2**

Table S5. Crystal data and structure refinement for *rac*-**2**.

Identification code	*rac*-**2**
Empirical formula	$C_{24}H_{22}Se_6Si_2$
Formula weight	840.36
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 16.4144(11) Å alpha = 90°
	b = 10.1288(7) Å beta = 114.7190(10)°
	c = 18.9016(13) Å gamma = 90°
Volume	2854.6(3) $Å^3$
Z, Calculated density	4, 1.955 Mg/m^3
Absorption coefficient	7.787 mm^{-1}
F(000)	1592
Crystal size	0.34 x 0.25 x 0.06 mm
Theta range for data collection	2.15 to 24.99°
Limiting indices	-17<=h<=19, -12<=k<=11, -22<=l<=22
Reflections collected / unique	14245 / 5016 [R(int) = 0.0440]
Completeness to theta = 24.99	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6523 and 0.1771
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5016 / 30 / 289
Goodness-of-fit on F^2	1.176
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0980
R indices (all data)	R1 = 0.0611, wR2 = 0.1035
Largest diff. peak and hole	0.937 and -0.514 e $·Å^{-3}$

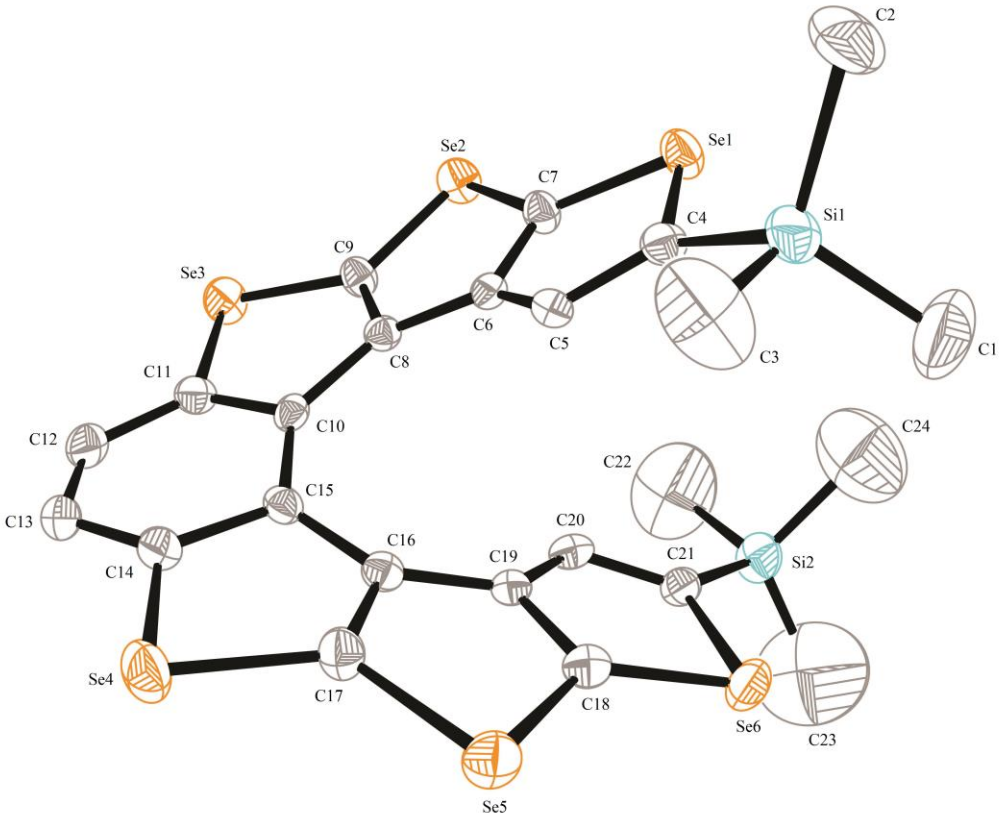


Figure S40. Molecular structures for compounds *rac*-**1**, thermal ellipsoids set at 30% probability level.

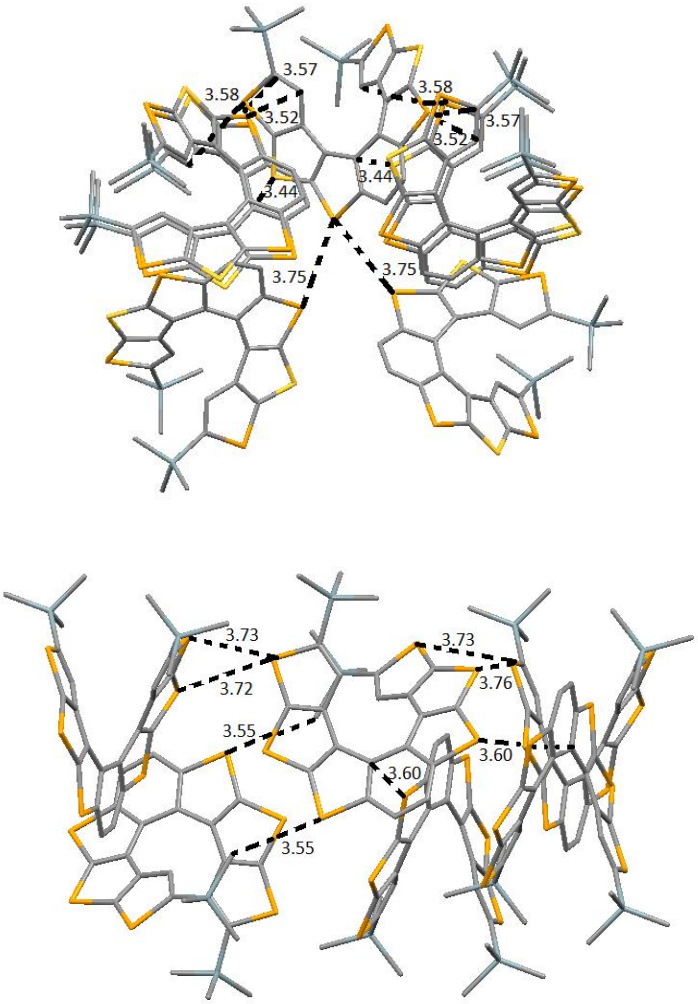


Figure S41. Multiple types of interaction in the crystal packing of *rac*-**1** and *rac*-**2**.