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Supporting Information

for

Thiophene/selenophene-based S-shaped double helicenes: regioselective synthesis and structures

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Supporting crystallographic information for compounds DH-1 and DH-2

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Complete crystal data for DH-1

Table S1. Crystal data and structure refinement for **DH-1**.

Identification code	**DH-1**	
Empirical formula	$C_{32}H_{26}S_6Si_2$	
Formula weight	659.07	
Temperature	150.0 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.1290(7) Å	α = 108.362(2)°
	b = 12.1240(7) Å	β = 111.318(2)°
	c = 13.7363(9) Å	γ = 100.961(2)°
Volume	1538.32(17) $Å^3$	
Z	2	
Density (calculated)	1.423 Mg/m^3	
Absorption coefficient	0.546 mm^{-1}	
F(000)	684	
Crystal size	0.14 x 0.12 x 0.08 mm^3	
Theta range for data collection	2.284 to 25.499°	
Index ranges	$-13 \leq h \leq 13$, $-14 \leq k \leq 13$, $-16 \leq l \leq 16$	
Reflections collected	19274	
Independent reflections	5716 [R(int) = 0.1014]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6783	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5716 / 0 / 367	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0562, wR2 = 0.0872	
R indices (all data)	R1 = 0.1093, wR2 = 0.1101	
Extinction coefficient	n / a	
Largest diff. peak and hole	0.476 and -0.451 $e.Å^{-3}$	

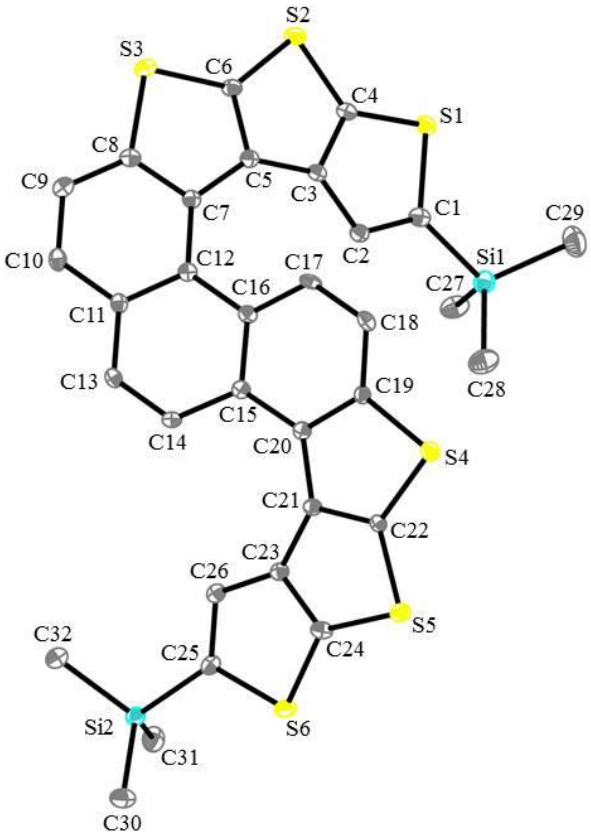

Figure S1. The crystal structures for compound **DH-1**. Carbon, sulfur, and silicon atoms are depicted with thermal ellipsoids set at 30% probability level, and all hydrogen atoms are omitted for clarity.

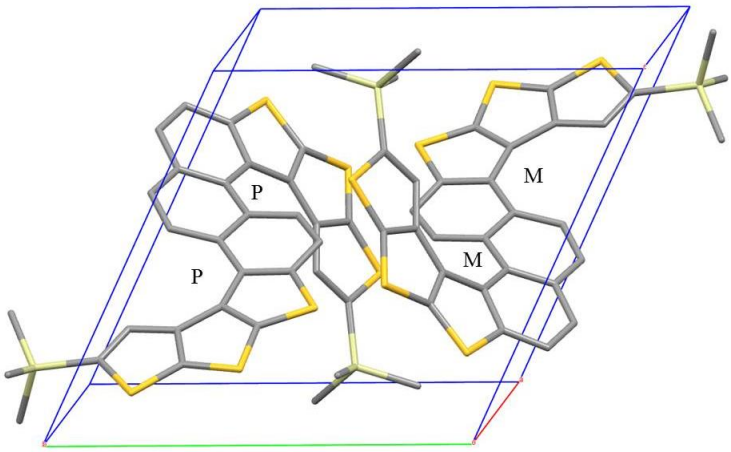

Figure S2. Molecular configuration of **DH-1** in one unit cell.

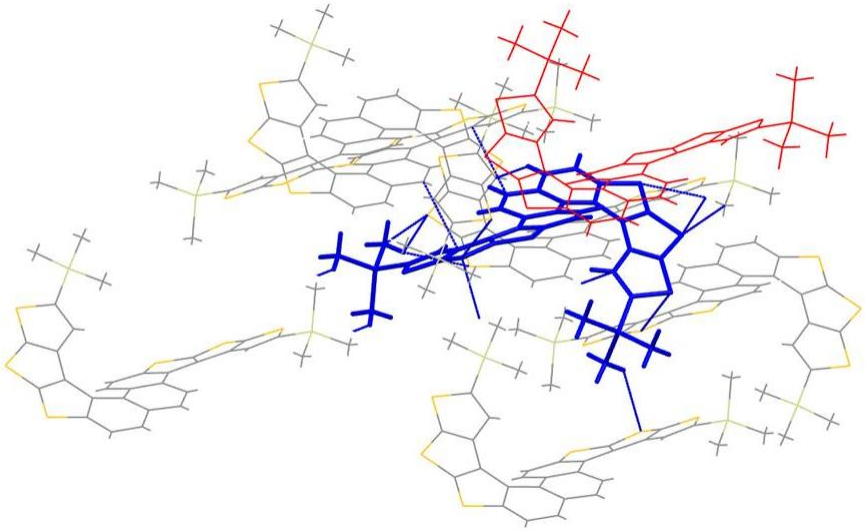

Figure S3. Multiple interactions in the crystal packings of **DH-1**.

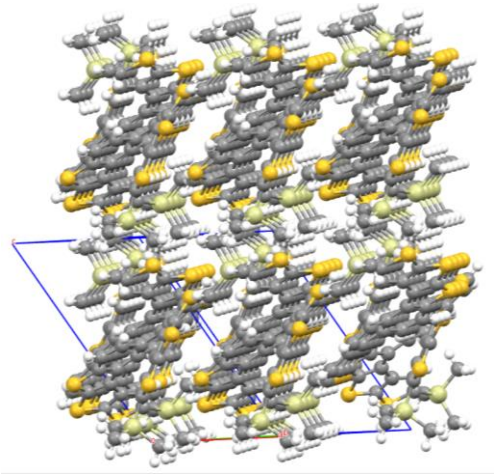

Figure S4. Molecular packing of **DH-1**.

Complete crystal data for DH-2

Table S2. Crystal data and structure refinement for **DH-2**.

Identification code	**DH-2**	
Empirical formula	$C_{32}H_{26}S_2Se_4Si_2$	
Formula weight	846.67	
Temperature	149.98 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.0959(11) Å	□α = 112.217(4)°.
	b = 12.2773(12) Å	□β = 106.495(3)°.
	c = 13.5535(13) Å	□γ = 99.898(3)°.
Volume	1555.7(3) Å^3	
Z	2	
Density (calculated)	1.807 Mg/m^3	
Absorption coefficient	4.951 mm^{-1}	
F(000)	828	
Crystal size	0.21 x 0.17 x 0.12 mm^3	
Theta range for data collection	2.288 to 28.326°.	
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 16$, $-18 \le l \le 18$	
Reflections collected	23440	
Independent reflections	7708 [R(int) = 0.0726]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.5103	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7708 / 0 / 367	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.0999	
R indices (all data)	R1 = 0.0690, wR2 = 0.1133	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.175 and -0.880 e.Å^{-3}	

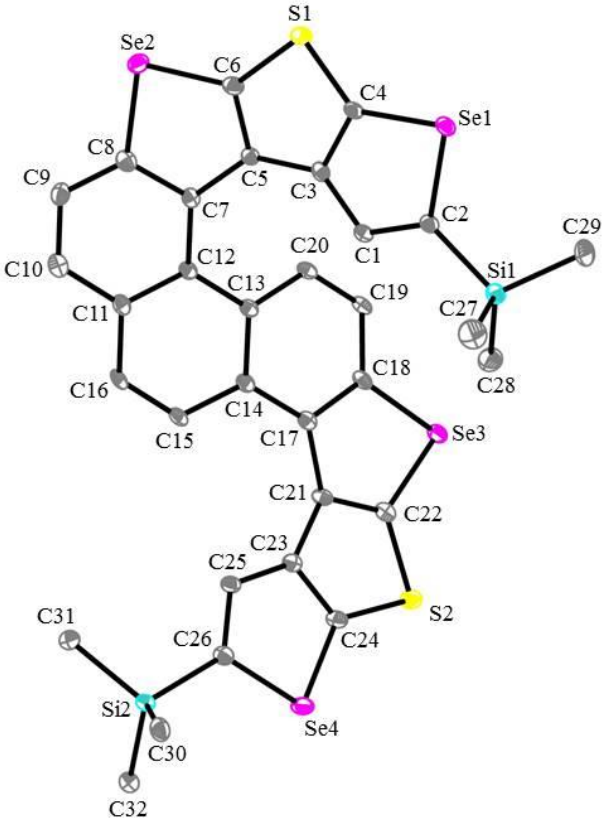

Figure S5. The crystal structures for compound **DH-2**. Carbon, selenium, sulfur, and silicon atoms are depicted with thermal ellipsoids set at 30% probability level, and all hydrogen atoms are omitted for clarity.

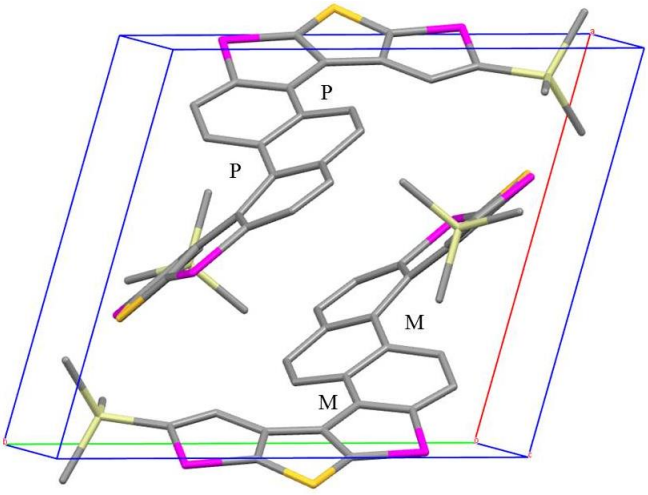

Figure S6. Molecular configuration of **DH-2** in one unit cell.

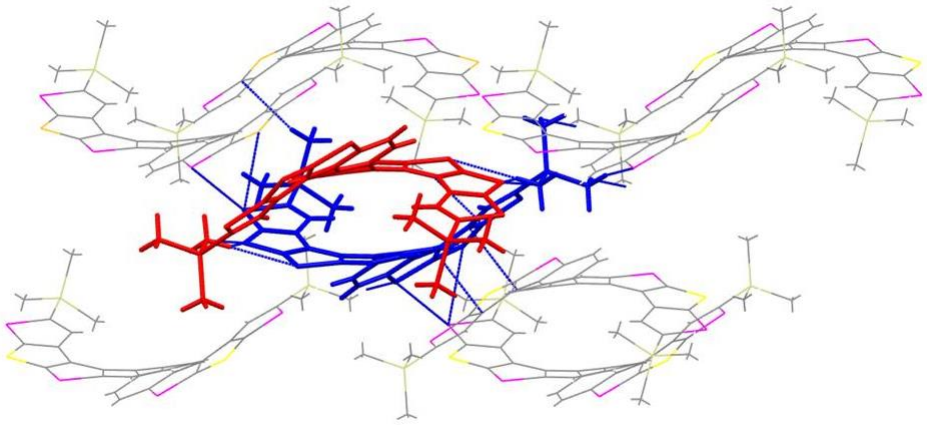

Figure S7. Multiple interactions in the crystal packings of **DH-2**

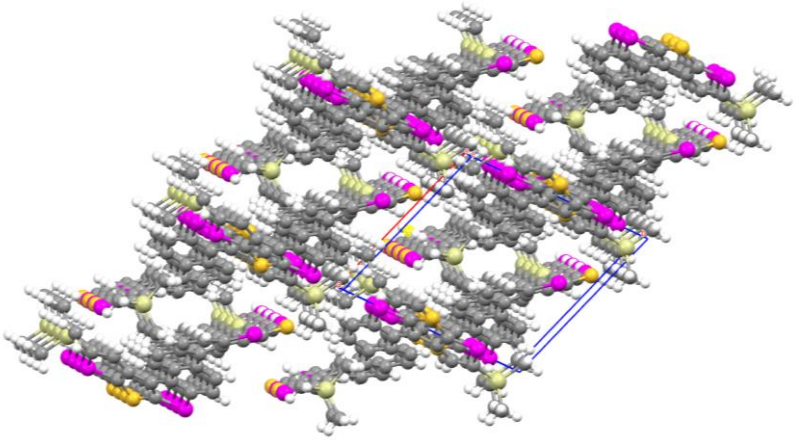

Figure S8. Molecular packing of **DH-2**.