Supporting Information

Synthesis and Properties of Novel Oligothiophenes Surrounded by Bicyclo[2.2.2]octene Frameworks

Atsushi Wakamiya, Daisuke Yamazaki, Tohru Nishinaga, Toshikazu Kitagawa
and Koichi Komatsu*

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Figure S1. ¹H NMR spectrum of 1(2T) in CDCl₃.

Figure S2. ¹³C NMR spectrum of 1(2T) in CDCl₃.

Figure S3. ^1H NMR spectrum of 1(3T) in C_6D_6 .

Figure S4. ^{13}C NMR spectrum of 1(3T) in C_6D_6 .

Figure S5. ^1H NMR spectrum of 1(4T) in CD_2Cl_2

Figure S6. ^{13}C NMR spectrum of 1(4T) in CD_2Cl_2

Figure S7. ^1H NMR spectrum of 1(6T) in C_6D_6 .

Figure S8. ^{13}C NMR spectrum of 1(6T) in C_6D_6 .

Figure S9. ¹H NMR spectrum of **8** in CDCl₃.

Figure S10. ¹³C NMR spectrum of **1(2T)** in CDCl₃.

Figure S11. ¹H NMR spectrum of **9** in CDCl₃.

Figure S12. ¹³C NMR spectrum of **1(2T)** in CDCl₃.

Table S1. Crystal data and structure refinement for **1(2T)**.

Identification code	1(2T) .	
Empirical formula	C₂₇ H₃₀ S₂	
Formula weight	418.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	<i>a</i> = 6.3159(6) Å	<i>a</i> = 74.183(2)°.
	<i>b</i> = 10.5969(10) Å	<i>b</i> = 88.992(2)°.
	<i>c</i> = 16.9425(17) Å	<i>g</i> = 85.741(2)°.
Volume	1087.99(18) Å ³	
<i>Z</i>	2	
Density (calculated)	1.278 Mg/m ³	
Absorption coefficient	0.256 mm ⁻¹	
<i>F</i> (000)	448	

Crystal size	0.30 x 0.30 x 0.30 mm ³
Theta range for data collection	1.25 to 25.00°.
Index ranges	-7<= <i>h</i> <=7, -12<= <i>k</i> <=11, -20<= <i>l</i> <=12
Reflections collected	6204
Independent reflections	3830 [R(int) = 0.0209]
Completeness to theta = 25.00°	99.7 %
Absorption correction	Emprical (SADABS)
Max. and min. transmission	0.9271 and 0.9271
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3830 / 6 / 365
Goodness-of-fit on F ²	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1490
R indices (all data)	R1 = 0.0680, wR2 = 0.1601
Largest diff. peak and hole	0.421 and -0.225 e.Å ⁻³

Table S2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **1(2T)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(2B)	7935(3)	8078(2)	1812(1)	22(1)
S(1B)	2184(3)	6894(2)	3262(1)	28(1)
C(3B)	5652(12)	7693(6)	3556(4)	29(2)
C(6B)	4408(13)	7283(10)	1471(6)	40(3)
S(1A)	6450(2)	8067(1)	3596(1)	20(1)
S(2A)	3627(3)	7103(2)	1492(1)	27(1)
C(3A)	3083(9)	7027(4)	3392(3)	26(1)
C(6A)	7193(11)	7939(7)	1687(4)	32(2)
C(19)	5251(3)	7282(2)	-129(1)	26(1)
C(13)	4802(3)	7753(2)	5215(1)	30(1)

C(5)	5403(3)	7563(2)	2122(1)	22(1)
C(4)	4756(3)	7481(2)	2962(1)	23(1)
C(2)	2823(4)	7093(2)	4216(1)	30(1)
C(8)	5470(3)	7468(2)	712(1)	26(1)
C(7)	7346(3)	7890(2)	865(1)	27(1)
C(1)	4628(3)	7600(2)	4369(1)	30(1)
C(14)	2857(3)	8656(2)	5333(1)	30(1)
C(20)	7092(3)	6287(2)	-219(1)	28(1)
C(17)	9235(3)	6802(2)	-80(1)	29(1)
C(11)	2582(4)	5792(2)	5648(1)	33(1)
C(16)	8862(3)	8116(2)	153(1)	29(1)
C(12)	798(3)	8049(2)	5186(1)	31(1)
C(10)	1339(4)	6768(2)	4932(1)	31(1)
C(21)	5624(3)	8607(2)	-761(1)	31(1)
C(15)	4603(4)	6394(2)	5829(1)	32(1)
C(18)	7728(4)	9120(2)	-576(1)	34(1)
C(31)	8299(11)	7213(6)	7365(4)	32(1)
C(32)	11558(16)	7882(13)	7656(6)	59(3)
C(33)	9601(5)	8261(3)	7407(2)	22(1)
C(37)	8798(8)	9680(5)	7112(3)	41(1)
C(34)	11460(30)	5712(9)	7963(6)	61(3)
C(35)	12553(5)	6732(5)	7969(2)	41(1)
C(36)	9357(12)	5940(5)	7656(3)	61(2)
C(44)	10390(30)	6766(14)	7606(7)	85(6)
C(41)	7970(40)	9219(19)	7028(9)	72(5)
C(45)	7440(30)	8260(30)	7056(10)	108(7)
C(47)	11240(70)	5430(30)	7850(20)	79(9)
C(46)	8880(30)	7150(40)	7403(17)	91(13)
C(42)	10770(50)	9060(20)	7396(12)	136(10)
C(43)	11770(20)	8089(12)	7735(9)	1(2)

Table S3. Bond lengths [$\approx$] and angles [∞] for **1(2T)**.

S(2B)-C(7)	1.719(3)
S(2B)-C(5)	1.754(3)
S(1B)-C(2)	1.745(3)
S(1B)-C(4)	1.798(3)
C(3B)-C(4)	1.243(7)
C(3B)-C(1)	1.493(7)
C(6B)-C(5)	1.389(11)
C(6B)-C(8)	1.412(10)
S(1A)-C(1)	1.721(2)
S(1A)-C(4)	1.785(2)
S(2A)-C(8)	1.727(3)
S(2A)-C(5)	1.745(2)
C(3A)-C(4)	1.318(6)
C(3A)-C(2)	1.423(6)
C(6A)-C(5)	1.363(7)
C(6A)-C(7)	1.409(7)
C(19)-C(8)	1.501(3)
C(19)-C(20)	1.545(3)
C(19)-C(21)	1.547(3)
C(13)-C(1)	1.494(3)
C(13)-C(15)	1.542(3)
C(13)-C(14)	1.545(3)
C(5)-C(4)	1.455(3)
C(2)-C(1)	1.353(3)
C(2)-C(10)	1.500(3)
C(8)-C(7)	1.351(3)

C(7)-C(16)	1.506(3)
C(14)-C(12)	1.546(3)
C(20)-C(17)	1.541(3)
C(17)-C(16)	1.549(3)
C(11)-C(15)	1.541(3)
C(11)-C(10)	1.544(3)
C(16)-C(18)	1.540(3)
C(12)-C(10)	1.545(3)
C(21)-C(18)	1.541(3)
C(31)-C(36)	1.423(11)
C(31)-C(33)	1.448(7)
C(32)-C(35)	1.307(12)
C(32)-C(33)	1.311(10)
C(33)-C(37)	1.501(6)
C(34)-C(35)	1.329(15)
C(34)-C(36)	1.412(18)
C(44)-C(46)	1.03(3)
C(44)-C(47)	1.43(3)
C(44)-C(43)	1.77(2)
C(41)-C(45)	1.08(3)
C(41)-C(42)	1.87(3)
C(45)-C(46)	1.43(3)
C(42)-C(43)	1.17(3)
C(7)-S(2B)-C(5)	87.16(13)
C(2)-S(1B)-C(4)	84.54(13)
C(4)-C(3B)-C(1)	124.2(6)
C(5)-C(6B)-C(8)	119.3(7)
C(1)-S(1A)-C(4)	87.30(12)
C(8)-S(2A)-C(5)	88.27(12)
C(4)-C(3A)-C(2)	120.8(4)

C(5)-C(6A)-C(7)	119.4(5)
C(8)-C(19)-C(20)	106.21(16)
C(8)-C(19)-C(21)	107.77(17)
C(20)-C(19)-C(21)	107.36(17)
C(1)-C(13)-C(15)	108.02(17)
C(1)-C(13)-C(14)	106.41(16)
C(15)-C(13)-C(14)	107.69(17)
C(6A)-C(5)-C(6B)	94.1(4)
C(6A)-C(5)-C(4)	133.2(3)
C(6B)-C(5)-C(4)	132.7(4)
C(6A)-C(5)-S(2A)	109.0(3)
C(6B)-C(5)-S(2A)	15.0(4)
C(4)-C(5)-S(2A)	117.74(16)
C(6A)-C(5)-S(2B)	15.0(3)
C(6B)-C(5)-S(2B)	109.0(4)
C(4)-C(5)-S(2B)	118.27(16)
S(2A)-C(5)-S(2B)	123.97(14)
C(3B)-C(4)-C(3A)	93.8(4)
C(3B)-C(4)-C(5)	133.3(4)
C(3A)-C(4)-C(5)	132.5(3)
C(3B)-C(4)-S(1A)	15.8(4)
C(3A)-C(4)-S(1A)	108.8(3)
C(5)-C(4)-S(1A)	118.68(16)
C(3B)-C(4)-S(1B)	110.0(4)
C(3A)-C(4)-S(1B)	16.4(2)
C(5)-C(4)-S(1B)	116.60(16)
S(1A)-C(4)-S(1B)	124.57(13)
C(1)-C(2)-C(3A)	103.5(3)
C(1)-C(2)-C(10)	114.20(19)
C(3A)-C(2)-C(10)	142.3(3)

C(1)-C(2)-S(1B)	123.75(19)
C(3A)-C(2)-S(1B)	20.7(2)
C(10)-C(2)-S(1B)	121.99(18)
C(7)-C(8)-C(6B)	102.8(5)
C(7)-C(8)-C(19)	115.12(18)
C(6B)-C(8)-C(19)	141.9(5)
C(7)-C(8)-S(2A)	118.90(17)
C(6B)-C(8)-S(2A)	16.1(4)
C(19)-C(8)-S(2A)	125.87(17)
C(8)-C(7)-C(6A)	104.4(3)
C(8)-C(7)-C(16)	114.12(18)
C(6A)-C(7)-C(16)	141.5(3)
C(8)-C(7)-S(2B)	121.67(18)
C(6A)-C(7)-S(2B)	17.3(3)
C(16)-C(7)-S(2B)	124.15(17)
C(2)-C(1)-C(3B)	97.1(3)
C(2)-C(1)-C(13)	114.95(19)
C(3B)-C(1)-C(13)	147.9(3)
C(2)-C(1)-S(1A)	119.55(18)
C(3B)-C(1)-S(1A)	23.0(3)
C(13)-C(1)-S(1A)	125.46(17)
C(13)-C(14)-C(12)	109.58(17)
C(17)-C(20)-C(19)	110.00(16)
C(20)-C(17)-C(16)	110.10(16)
C(15)-C(11)-C(10)	109.86(16)
C(7)-C(16)-C(18)	107.21(18)
C(7)-C(16)-C(17)	107.32(16)
C(18)-C(16)-C(17)	107.48(17)
C(10)-C(12)-C(14)	110.21(17)
C(2)-C(10)-C(11)	107.18(18)

C(2)-C(10)-C(12)	107.17(17)
C(11)-C(10)-C(12)	107.57(17)
C(18)-C(21)-C(19)	110.32(16)
C(11)-C(15)-C(13)	110.18(17)
C(16)-C(18)-C(21)	109.92(16)
C(36)-C(31)-C(33)	113.2(5)
C(35)-C(32)-C(33)	133.4(9)
C(32)-C(33)-C(31)	115.1(6)
C(32)-C(33)-C(37)	123.1(6)
C(31)-C(33)-C(37)	121.6(4)
C(35)-C(34)-C(36)	119.2(7)
C(32)-C(35)-C(34)	114.8(7)
C(34)-C(36)-C(31)	123.8(6)
C(46)-C(44)-C(47)	130(3)
C(46)-C(44)-C(43)	106(3)
C(47)-C(44)-C(43)	123(2)
C(45)-C(41)-C(42)	109.9(19)
C(41)-C(45)-C(46)	117(3)
C(44)-C(46)-C(45)	150(4)
C(43)-C(42)-C(41)	127.5(15)
C(42)-C(43)-C(44)	106.7(14)

Symmetry transformations used to generate equivalent atoms:

Table S4. Torsion angles [°] for **1**(2T)..

C(7)-C(6A)-C(5)-C(6B)	-0.8(6)
C(7)-C(6A)-C(5)-C(4)	179.2(3)
C(7)-C(6A)-C(5)-S(2A)	-0.7(6)
C(7)-C(6A)-C(5)-S(2B)	174.3(17)

C(8)-C(6B)-C(5)-C(6A)	-0.1(8)
C(8)-C(6B)-C(5)-C(4)	179.9(4)
C(8)-C(6B)-C(5)-S(2A)	-180(2)
C(8)-C(6B)-C(5)-S(2B)	-1.5(8)
C(8)-S(2A)-C(5)-C(6A)	-0.2(3)
C(8)-S(2A)-C(5)-C(6B)	0.1(17)
C(8)-S(2A)-C(5)-C(4)	179.93(16)
C(8)-S(2A)-C(5)-S(2B)	-1.70(18)
C(7)-S(2B)-C(5)-C(6A)	-4.1(13)
C(7)-S(2B)-C(5)-C(6B)	1.1(4)
C(7)-S(2B)-C(5)-C(4)	179.95(16)
C(7)-S(2B)-C(5)-S(2A)	1.59(19)
C(1)-C(3B)-C(4)-C(3A)	-8.8(5)
C(1)-C(3B)-C(4)-C(5)	177.2(3)
C(1)-C(3B)-C(4)-S(1A)	152.9(14)
C(1)-C(3B)-C(4)-S(1B)	-5.7(6)
C(2)-C(3A)-C(4)-C(3B)	7.2(5)
C(2)-C(3A)-C(4)-C(5)	-178.7(2)
C(2)-C(3A)-C(4)-S(1A)	2.0(4)
C(2)-C(3A)-C(4)-S(1B)	-162.7(11)
C(6A)-C(5)-C(4)-C(3B)	-2.4(6)
C(6B)-C(5)-C(4)-C(3B)	177.6(6)
S(2A)-C(5)-C(4)-C(3B)	177.5(4)
S(2B)-C(5)-C(4)-C(3B)	-0.9(5)
C(6A)-C(5)-C(4)-C(3A)	-174.3(5)
C(6B)-C(5)-C(4)-C(3A)	5.7(7)
S(2A)-C(5)-C(4)-C(3A)	5.6(4)
S(2B)-C(5)-C(4)-C(3A)	-172.9(3)
C(6A)-C(5)-C(4)-S(1A)	5.0(5)
C(6B)-C(5)-C(4)-S(1A)	-175.1(5)

S(2A)-C(5)-C(4)-S(1A)	-175.14(12)
S(2B)-C(5)-C(4)-S(1A)	6.4(2)
C(6A)-C(5)-C(4)-S(1B)	-179.3(4)
C(6B)-C(5)-C(4)-S(1B)	0.6(6)
S(2A)-C(5)-C(4)-S(1B)	0.6(2)
S(2B)-C(5)-C(4)-S(1B)	-177.87(14)
C(1)-S(1A)-C(4)-C(3B)	-19.1(11)
C(1)-S(1A)-C(4)-C(3A)	0.2(2)
C(1)-S(1A)-C(4)-C(5)	-179.19(16)
C(1)-S(1A)-C(4)-S(1B)	5.46(15)
C(2)-S(1B)-C(4)-C(3B)	1.3(3)
C(2)-S(1B)-C(4)-C(3A)	12.1(8)
C(2)-S(1B)-C(4)-C(5)	178.94(16)
C(2)-S(1B)-C(4)-S(1A)	-5.62(16)
C(4)-C(3A)-C(2)-C(1)	-3.6(4)
C(4)-C(3A)-C(2)-C(10)	179.0(3)
C(4)-C(3A)-C(2)-S(1B)	165.8(9)
C(4)-S(1B)-C(2)-C(1)	3.5(2)
C(4)-S(1B)-C(2)-C(3A)	-8.9(6)
C(4)-S(1B)-C(2)-C(10)	-179.42(18)
C(5)-C(6B)-C(8)-C(7)	0.9(8)
C(5)-C(6B)-C(8)-C(19)	176.1(3)
C(5)-C(6B)-C(8)-S(2A)	180(2)
C(20)-C(19)-C(8)-C(7)	57.7(2)
C(21)-C(19)-C(8)-C(7)	-57.1(2)
C(20)-C(19)-C(8)-C(6B)	-117.0(7)
C(21)-C(19)-C(8)-C(6B)	128.2(7)
C(20)-C(19)-C(8)-S(2A)	-118.35(19)
C(21)-C(19)-C(8)-S(2A)	126.86(18)
C(5)-S(2A)-C(8)-C(7)	1.06(19)

C(5)-S(2A)-C(8)-C(6B)	-0.1(15)
C(5)-S(2A)-C(8)-C(19)	177.01(17)
C(6B)-C(8)-C(7)-C(6A)	-1.2(5)
C(19)-C(8)-C(7)-C(6A)	-177.9(3)
S(2A)-C(8)-C(7)-C(6A)	-1.5(4)
C(6B)-C(8)-C(7)-C(16)	177.6(4)
C(19)-C(8)-C(7)-C(16)	0.9(3)
S(2A)-C(8)-C(7)-C(16)	177.27(16)
C(6B)-C(8)-C(7)-S(2B)	0.1(5)
C(19)-C(8)-C(7)-S(2B)	-176.62(16)
S(2A)-C(8)-C(7)-S(2B)	-0.3(3)
C(5)-C(6A)-C(7)-C(8)	1.4(6)
C(5)-C(6A)-C(7)-C(16)	-176.8(3)
C(5)-C(6A)-C(7)-S(2B)	-174.9(15)
C(5)-S(2B)-C(7)-C(8)	-0.7(2)
C(5)-S(2B)-C(7)-C(6A)	3.4(10)
C(5)-S(2B)-C(7)-C(16)	-177.99(18)
C(3A)-C(2)-C(1)-C(3B)	-1.5(3)
C(10)-C(2)-C(1)-C(3B)	176.7(3)
S(1B)-C(2)-C(1)-C(3B)	-6.1(3)
C(3A)-C(2)-C(1)-C(13)	-178.8(2)
C(10)-C(2)-C(1)-C(13)	-0.5(3)
S(1B)-C(2)-C(1)-C(13)	176.74(16)
C(3A)-C(2)-C(1)-S(1A)	3.7(3)
C(10)-C(2)-C(1)-S(1A)	-178.04(15)
S(1B)-C(2)-C(1)-S(1A)	-0.8(3)
C(4)-C(3B)-C(1)-C(2)	7.4(5)
C(4)-C(3B)-C(1)-C(13)	-177.3(3)
C(4)-C(3B)-C(1)-S(1A)	-160.8(10)
C(15)-C(13)-C(1)-C(2)	57.2(2)

C(14)-C(13)-C(1)-C(2)	-58.2(2)
C(15)-C(13)-C(1)-C(3B)	-117.6(5)
C(14)-C(13)-C(1)-C(3B)	127.0(5)
C(15)-C(13)-C(1)-S(1A)	-125.47(18)
C(14)-C(13)-C(1)-S(1A)	119.13(18)
C(4)-S(1A)-C(1)-C(2)	-2.53(18)
C(4)-S(1A)-C(1)-C(3B)	10.9(6)
C(4)-S(1A)-C(1)-C(13)	-179.79(18)
C(1)-C(13)-C(14)-C(12)	56.9(2)
C(15)-C(13)-C(14)-C(12)	-58.7(2)
C(8)-C(19)-C(20)-C(17)	-57.1(2)
C(21)-C(19)-C(20)-C(17)	58.0(2)
C(19)-C(20)-C(17)-C(16)	3.1(2)
C(8)-C(7)-C(16)-C(18)	57.3(2)
C(6A)-C(7)-C(16)-C(18)	-124.5(5)
S(2B)-C(7)-C(16)-C(18)	-125.23(19)
C(8)-C(7)-C(16)-C(17)	-57.9(2)
C(6A)-C(7)-C(16)-C(17)	120.2(5)
S(2B)-C(7)-C(16)-C(17)	119.56(19)
C(20)-C(17)-C(16)-C(7)	52.9(2)
C(20)-C(17)-C(16)-C(18)	-62.1(2)
C(13)-C(14)-C(12)-C(10)	-2.4(2)
C(1)-C(2)-C(10)-C(11)	-57.4(2)
C(3A)-C(2)-C(10)-C(11)	119.8(4)
S(1B)-C(2)-C(10)-C(11)	125.31(18)
C(1)-C(2)-C(10)-C(12)	57.8(2)
C(3A)-C(2)-C(10)-C(12)	-124.9(4)
S(1B)-C(2)-C(10)-C(12)	-119.45(18)
C(15)-C(11)-C(10)-C(2)	56.4(2)
C(15)-C(11)-C(10)-C(12)	-58.5(2)

C(14)-C(12)-C(10)-C(2)	-53.4(2)
C(14)-C(12)-C(10)-C(11)	61.6(2)
C(8)-C(19)-C(21)-C(18)	52.1(2)
C(20)-C(19)-C(21)-C(18)	-61.9(2)
C(10)-C(11)-C(15)-C(13)	-2.6(2)
C(1)-C(13)-C(15)-C(11)	-52.6(2)
C(14)-C(13)-C(15)-C(11)	61.9(2)
C(7)-C(16)-C(18)-C(21)	-56.9(2)
C(17)-C(16)-C(18)-C(21)	58.2(2)
C(19)-C(21)-C(18)-C(16)	3.1(2)
C(35)-C(32)-C(33)-C(31)	-9.3(12)
C(35)-C(32)-C(33)-C(37)	175.9(8)
C(36)-C(31)-C(33)-C(32)	3.8(8)
C(36)-C(31)-C(33)-C(37)	178.6(4)
C(33)-C(32)-C(35)-C(34)	8.3(13)
C(36)-C(34)-C(35)-C(32)	-2.1(11)
C(35)-C(34)-C(36)-C(31)	-1.6(12)
C(33)-C(31)-C(36)-C(34)	0.7(9)
C(42)-C(41)-C(45)-C(46)	4(2)
C(47)-C(44)-C(46)-C(45)	-171(4)
C(43)-C(44)-C(46)-C(45)	17(6)
C(41)-C(45)-C(46)-C(44)	-13(6)
C(45)-C(41)-C(42)-C(43)	-12(2)
C(41)-C(42)-C(43)-C(44)	14.7(17)
C(46)-C(44)-C(43)-C(42)	-15(2)
C(47)-C(44)-C(43)-C(42)	172(2)

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for **1(3T)**.

Identification code	1(3T)	
Empirical formula	C ₃₀ H ₃₂ S ₃	
Formula weight	488.74	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.1988(8) Å	a = 90°.
	b = 10.1717(7) Å	b = 96.436(2)°.
	c = 17.8654(11) Å	g = 90°.
Volume	2383.4(3) Å ³	
Z	4	
Density (calculated)	1.362 Mg/m ³	
Absorption coefficient	0.329 mm ⁻¹	
F(000)	1040	
Crystal size	0.20 x 0.20 x 0.10 mm ³	

Theta range for data collection	1.82 to 27.50°.
Index ranges	-11<=h<=17, -11<=k<=13, -23<=l<=23
Reflections collected	16015
Independent reflections	5443 [R(int) = 0.0403]
Completeness to theta = 27.50°	99.4 %
Absorption correction	Empirical (SADABS)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5443 / 0 / 336
Goodness-of-fit on F ²	0.927
Final R indices [I>2sigma(I)]	R1 = 0.0392, wR2 = 0.0843
R indices (all data)	R1 = 0.0536, wR2 = 0.0879
Largest diff. peak and hole	0.383 and -0.226 e.Å ⁻³

Table S6. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **1**(3T). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8640(1)	11042(1)	2310(1)	20(1)
C(4)	8811(3)	9691(4)	1130(2)	25(1)
S(11)	8799(3)	9366(4)	897(2)	20(1)
C(44)	8647(16)	10671(18)	1977(10)	80(8)
S(3)	4633(1)	6300(1)	688(1)	20(1)
C(10)	3526(3)	8312(3)	335(2)	23(1)
S(33)	3312(4)	8788(4)	252(3)	23(1)
C(50)	4230(14)	6800(20)	634(9)	99(11)
S(2)	6558(1)	8448(1)	949(1)	22(1)
C(6)	6183(1)	10578(2)	1628(1)	19(1)
C(22)	4335(1)	10771(2)	1601(1)	20(1)
C(20)	5424(1)	12788(2)	1501(1)	24(1)

C(7)	5221(1)	10004(2)	1376(1)	19(1)
C(12)	3392(1)	6085(2)	289(1)	23(1)
C(13)	10814(1)	11424(2)	2320(1)	31(1)
C(9)	4460(1)	8004(2)	658(1)	19(1)
C(2)	9821(1)	10123(2)	1374(1)	24(1)
C(18)	11261(1)	11365(2)	977(1)	28(1)
C(25)	2810(1)	4853(2)	93(1)	27(1)
C(19)	6090(1)	11862(2)	2034(1)	21(1)
C(1)	9806(1)	10870(2)	2001(1)	24(1)
C(28)	1808(1)	7018(2)	-235(1)	28(1)
C(11)	2884(1)	7221(2)	121(1)	24(1)
C(23)	4375(1)	12149(2)	1263(1)	23(1)
C(21)	5512(1)	11586(2)	2717(1)	27(1)
C(27)	2461(1)	4901(2)	-757(1)	29(1)
C(5)	6994(1)	9849(2)	1445(1)	20(1)
C(24)	4488(1)	10898(2)	2467(1)	26(1)
C(15)	11218(1)	12230(2)	1685(1)	31(1)
C(3)	8085(1)	10093(2)	1555(1)	20(1)
C(16)	10862(1)	9973(2)	1126(1)	29(1)
C(17)	11544(1)	9376(2)	1793(1)	38(1)
C(26)	1847(1)	4904(2)	505(1)	35(1)
C(29)	1849(1)	6178(2)	-947(1)	30(1)
C(30)	1260(1)	6199(2)	323(1)	35(1)
C(8)	5285(1)	8856(2)	990(1)	20(1)
C(14)	11535(1)	10256(2)	2493(1)	40(1)

Table S7. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **1**(3T).

S(1)-C(1)	1.7007(17)
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S(1)-C(3)	1.7512(18)
C(4)-C(3)	1.351(4)
C(4)-C(2)	1.425(4)
S(11)-C(2)	1.698(5)
S(11)-C(3)	1.750(4)
C(44)-C(3)	1.16(3)
C(44)-C(1)	1.54(2)
S(3)-C(12)	1.7256(17)
S(3)-C(9)	1.7487(18)
C(10)-C(9)	1.338(4)
C(10)-C(11)	1.423(4)
S(33)-C(11)	1.699(5)
S(33)-C(9)	1.792(5)
C(50)-C(9)	1.27(3)
C(50)-C(12)	1.40(2)
S(2)-C(8)	1.7398(16)
S(2)-C(5)	1.7416(16)
C(6)-C(5)	1.371(2)
C(6)-C(7)	1.424(2)
C(6)-C(19)	1.506(2)
C(22)-C(7)	1.498(2)
C(22)-C(23)	1.530(2)
C(22)-C(24)	1.544(2)
C(20)-C(19)	1.543(2)
C(20)-C(23)	1.546(2)
C(7)-C(8)	1.363(2)
C(12)-C(11)	1.352(2)
C(12)-C(25)	1.491(2)
C(13)-C(1)	1.497(2)
C(13)-C(14)	1.532(3)

C(13)-C(15)	1.543(2)
C(9)-C(8)	1.465(2)
C(2)-C(1)	1.355(2)
C(2)-C(16)	1.498(2)
C(18)-C(16)	1.544(2)
C(18)-C(15)	1.546(2)
C(25)-C(27)	1.538(2)
C(25)-C(26)	1.540(3)
C(19)-C(21)	1.535(2)
C(28)-C(11)	1.504(2)
C(28)-C(29)	1.540(2)
C(28)-C(30)	1.540(2)
C(21)-C(24)	1.544(2)
C(27)-C(29)	1.548(2)
C(5)-C(3)	1.452(2)
C(16)-C(17)	1.535(3)
C(17)-C(14)	1.540(3)
C(26)-C(30)	1.544(3)
C(1)-S(1)-C(3)	90.53(8)
C(3)-C(4)-C(2)	115.6(3)
C(2)-S(11)-C(3)	85.89(19)
C(3)-C(44)-C(1)	130.3(12)
C(12)-S(3)-C(9)	89.88(8)
C(9)-C(10)-C(11)	115.2(2)
C(11)-S(33)-C(9)	83.7(2)
C(9)-C(50)-C(12)	133.5(11)
C(8)-S(2)-C(5)	92.80(8)
C(5)-C(6)-C(7)	113.28(14)
C(5)-C(6)-C(19)	133.78(14)
C(7)-C(6)-C(19)	112.93(13)

C(7)-C(22)-C(23)	107.98(13)
C(7)-C(22)-C(24)	107.15(13)
C(23)-C(22)-C(24)	108.24(13)
C(19)-C(20)-C(23)	110.10(13)
C(8)-C(7)-C(6)	114.01(14)
C(8)-C(7)-C(22)	132.59(15)
C(6)-C(7)-C(22)	113.38(14)
C(11)-C(12)-C(50)	90.2(7)
C(11)-C(12)-C(25)	115.87(15)
C(50)-C(12)-C(25)	153.5(7)
C(11)-C(12)-S(3)	114.08(13)
C(50)-C(12)-S(3)	24.4(7)
C(25)-C(12)-S(3)	130.05(14)
C(1)-C(13)-C(14)	106.87(15)
C(1)-C(13)-C(15)	106.61(14)
C(14)-C(13)-C(15)	107.62(15)
C(50)-C(9)-C(10)	90.4(7)
C(50)-C(9)-C(8)	138.8(7)
C(10)-C(9)-C(8)	130.1(2)
C(50)-C(9)-S(3)	21.3(7)
C(10)-C(9)-S(3)	110.86(17)
C(8)-C(9)-S(3)	119.04(12)
C(50)-C(9)-S(33)	103.3(7)
C(10)-C(9)-S(33)	12.9(2)
C(8)-C(9)-S(33)	117.21(18)
S(3)-C(9)-S(33)	123.74(17)
C(1)-C(2)-C(4)	109.0(2)
C(1)-C(2)-C(16)	113.62(15)
C(4)-C(2)-C(16)	137.3(2)
C(1)-C(2)-S(11)	125.79(19)

C(4)-C(2)-S(11)	16.81(19)
C(16)-C(2)-S(11)	120.57(19)
C(16)-C(18)-C(15)	109.71(14)
C(12)-C(25)-C(27)	107.14(14)
C(12)-C(25)-C(26)	106.93(14)
C(27)-C(25)-C(26)	107.41(14)
C(6)-C(19)-C(21)	107.43(13)
C(6)-C(19)-C(20)	107.64(13)
C(21)-C(19)-C(20)	107.67(13)
C(2)-C(1)-C(13)	115.50(15)
C(2)-C(1)-C(44)	90.6(8)
C(13)-C(1)-C(44)	153.9(8)
C(2)-C(1)-S(1)	115.03(13)
C(13)-C(1)-S(1)	129.46(14)
C(44)-C(1)-S(1)	24.5(8)
C(11)-C(28)-C(29)	107.86(14)
C(11)-C(28)-C(30)	106.86(14)
C(29)-C(28)-C(30)	107.28(15)
C(12)-C(11)-C(10)	109.9(2)
C(12)-C(11)-C(28)	113.48(15)
C(10)-C(11)-C(28)	136.6(2)
C(12)-C(11)-S(33)	128.5(2)
C(10)-C(11)-S(33)	18.53(18)
C(28)-C(11)-S(33)	118.1(2)
C(22)-C(23)-C(20)	110.26(13)
C(19)-C(21)-C(24)	110.49(13)
C(25)-C(27)-C(29)	109.53(14)
C(6)-C(5)-C(3)	131.60(15)
C(6)-C(5)-S(2)	109.95(11)
C(3)-C(5)-S(2)	118.33(12)

C(22)-C(24)-C(21)	109.85(13)
C(13)-C(15)-C(18)	110.23(15)
C(44)-C(3)-C(4)	94.4(7)
C(44)-C(3)-C(5)	136.7(7)
C(4)-C(3)-C(5)	128.9(2)
C(44)-C(3)-S(11)	107.4(7)
C(4)-C(3)-S(11)	13.0(2)
C(5)-C(3)-S(11)	115.94(19)
C(44)-C(3)-S(1)	15.3(7)
C(4)-C(3)-S(1)	109.74(19)
C(5)-C(3)-S(1)	121.38(13)
S(11)-C(3)-S(1)	122.68(17)
C(2)-C(16)-C(17)	106.79(14)
C(2)-C(16)-C(18)	107.38(14)
C(17)-C(16)-C(18)	108.30(15)
C(16)-C(17)-C(14)	110.08(15)
C(25)-C(26)-C(30)	110.44(14)
C(28)-C(29)-C(27)	110.52(14)
C(28)-C(30)-C(26)	109.71(15)
C(7)-C(8)-C(9)	128.77(15)
C(7)-C(8)-S(2)	109.94(12)
C(9)-C(8)-S(2)	121.27(12)
C(13)-C(14)-C(17)	110.36(15)

Symmetry transformations used to generate equivalent atoms:

Table S8. Torsion angles [°] for **1**(3T).

C(4)-C(3)-C(5)-S(2)	25.8(3)
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C(4)-C(3)-C(5)-C(6)	-149.7(3)
S(2)-C(5)-C(3)-S(1)	-155.14(10)
C(10)-C(9)-C(8)-C(7)	34.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S9. Crystal data and structure refinement for **10**.

Identification code	10	
Empirical formula	C ₂₀ H ₂₀ Br ₂ S ₂	
Formula weight	484.30	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5907(18) Å	α = 93.242(4)°.
	b = 9.505(2) Å	β = 107.154(4)°.
	c = 12.059(3) Å	γ = 102.644(4)°.
Volume	910.3(3) Å ³	
Z	2	
Density (calculated)	1.767 Mg/m ³	
Absorption coefficient	4.681 mm ⁻¹	
F(000)	484	

Crystal size	0.20 x 0.20 x 0.20 mm ³
Theta range for data collection	1.78 to 27.50°.
Index ranges	-11<=h<=11, -12<=k<=9, -15<=l<=15
Reflections collected	6123
Independent reflections	4078 [R(int) = 0.0485]
Completeness to theta = 27.50°	97.4 %
Absorption correction	Empirical (SADABS)
Max. and min. transmission	0.4545 and 0.4545
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4078 / 0 / 217
Goodness-of-fit on F ²	0.958
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1648
R indices (all data)	R1 = 0.0919, wR2 = 0.1814
Largest diff. peak and hole	2.363 and -1.356 e.Å ⁻³

Table S10. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å²x 10³) for **10**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(2)	4622(1)	2258(1)	640(1)	20(1)
Br(1)	11776(1)	4298(1)	9027(1)	19(1)
S(2)	5999(2)	3015(2)	3347(1)	13(1)
S(1)	10485(2)	3773(2)	6290(1)	13(1)
C(8)	6301(8)	2353(7)	2073(5)	13(1)
C(1)	10018(8)	3722(7)	7602(5)	13(1)
C(3)	7410(8)	2807(7)	6220(5)	13(1)
C(15)	10322(8)	1712(7)	3755(5)	15(1)
C(7)	7779(8)	1962(7)	2290(5)	12(1)
C(6)	8688(7)	2154(7)	3512(5)	9(1)

C(20)	8834(9)	-163(7)	1928(6)	18(1)
C(5)	7885(7)	2698(6)	4210(5)	9(1)
C(11)	5964(9)	3795(8)	7878(6)	19(1)
C(4)	8384(7)	3020(6)	5478(5)	9(1)
C(2)	8363(8)	3205(7)	7425(5)	12(1)
C(16)	11331(9)	2620(8)	3056(6)	22(2)
C(10)	6425(9)	1300(7)	8011(6)	18(1)
C(19)	10344(8)	2337(8)	1727(6)	19(1)
C(12)	5549(8)	2194(7)	6019(6)	15(1)
C(13)	4922(9)	3348(8)	6576(6)	22(2)
C(17)	9898(9)	90(7)	3252(6)	17(1)
C(14)	5406(9)	865(7)	6695(6)	19(1)
C(9)	7322(8)	2946(7)	8245(6)	16(1)
C(18)	8587(9)	1306(7)	1511(5)	18(1)

Table S11. Bond lengths [Å] and angles [°] for **10**.

Br(2)-C(8)	1.879(6)
Br(1)-C(1)	1.881(6)
S(2)-C(8)	1.738(6)
S(2)-C(5)	1.747(6)
S(1)-C(4)	1.744(6)
S(1)-C(1)	1.744(6)
C(8)-C(7)	1.357(9)
C(1)-C(2)	1.346(9)
C(3)-C(4)	1.389(8)
C(3)-C(2)	1.423(8)
C(3)-C(12)	1.517(9)
C(15)-C(6)	1.504(8)

C(15)-C(16)	1.547(9)
C(15)-C(17)	1.548(9)
C(7)-C(6)	1.429(8)
C(7)-C(18)	1.504(9)
C(6)-C(5)	1.378(8)
C(20)-C(18)	1.547(9)
C(20)-C(17)	1.563(9)
C(5)-C(4)	1.456(8)
C(11)-C(9)	1.534(9)
C(11)-C(13)	1.541(10)
C(2)-C(9)	1.514(8)
C(16)-C(19)	1.552(9)
C(10)-C(14)	1.550(9)
C(10)-C(9)	1.554(9)
C(19)-C(18)	1.549(9)
C(12)-C(13)	1.528(9)
C(12)-C(14)	1.544(9)
C(8)-S(2)-C(5)	91.6(3)
C(4)-S(1)-C(1)	91.6(3)
C(7)-C(8)-S(2)	112.1(5)
C(7)-C(8)-Br(2)	129.4(5)
S(2)-C(8)-Br(2)	118.4(3)
C(2)-C(1)-S(1)	112.0(5)
C(2)-C(1)-Br(1)	128.6(5)
S(1)-C(1)-Br(1)	119.3(3)
C(4)-C(3)-C(2)	113.4(5)
C(4)-C(3)-C(12)	133.5(6)
C(2)-C(3)-C(12)	113.1(5)
C(6)-C(15)-C(16)	106.5(5)
C(6)-C(15)-C(17)	107.3(5)

C(16)-C(15)-C(17)	108.3(5)
C(8)-C(7)-C(6)	112.4(5)
C(8)-C(7)-C(18)	132.7(6)
C(6)-C(7)-C(18)	114.8(5)
C(5)-C(6)-C(7)	113.6(5)
C(5)-C(6)-C(15)	134.0(5)
C(7)-C(6)-C(15)	112.4(5)
C(18)-C(20)-C(17)	109.7(5)
C(6)-C(5)-C(4)	130.1(5)
C(6)-C(5)-S(2)	110.3(4)
C(4)-C(5)-S(2)	119.7(4)
C(9)-C(11)-C(13)	111.1(5)
C(3)-C(4)-C(5)	129.6(6)
C(3)-C(4)-S(1)	110.0(4)
C(5)-C(4)-S(1)	120.4(4)
C(1)-C(2)-C(3)	113.0(5)
C(1)-C(2)-C(9)	133.1(6)
C(3)-C(2)-C(9)	113.9(5)
C(15)-C(16)-C(19)	111.0(6)
C(14)-C(10)-C(9)	109.9(5)
C(18)-C(19)-C(16)	109.9(5)
C(3)-C(12)-C(13)	107.3(6)
C(3)-C(12)-C(14)	106.4(5)
C(13)-C(12)-C(14)	108.3(5)
C(12)-C(13)-C(11)	110.7(5)
C(15)-C(17)-C(20)	110.9(5)
C(12)-C(14)-C(10)	111.0(5)
C(2)-C(9)-C(11)	106.8(5)
C(2)-C(9)-C(10)	106.8(5)
C(11)-C(9)-C(10)	107.7(5)

C(7)-C(18)-C(20)	107.2(5)
C(7)-C(18)-C(19)	106.8(5)
C(20)-C(18)-C(19)	108.2(5)

Symmetry transformations used to generate equivalent atoms:

Table S12. Torsion angles [°] for **10**.

C(5)-S(2)-C(8)-C(7)	-2.0(5)
C(5)-S(2)-C(8)-Br(2)	177.5(4)
C(4)-S(1)-C(1)-C(2)	-1.8(5)
C(4)-S(1)-C(1)-Br(1)	176.4(4)
S(2)-C(8)-C(7)-C(6)	1.7(7)
Br(2)-C(8)-C(7)-C(6)	-177.8(5)
S(2)-C(8)-C(7)-C(18)	178.0(6)
Br(2)-C(8)-C(7)-C(18)	-1.4(11)
C(8)-C(7)-C(6)-C(5)	-0.3(8)
C(18)-C(7)-C(6)-C(5)	-177.3(5)
C(8)-C(7)-C(6)-C(15)	179.7(6)
C(18)-C(7)-C(6)-C(15)	2.6(7)
C(16)-C(15)-C(6)-C(5)	-123.4(7)
C(17)-C(15)-C(6)-C(5)	120.7(7)
C(16)-C(15)-C(6)-C(7)	56.7(7)
C(17)-C(15)-C(6)-C(7)	-59.2(7)
C(7)-C(6)-C(5)-C(4)	179.0(6)
C(15)-C(6)-C(5)-C(4)	-0.9(11)
C(7)-C(6)-C(5)-S(2)	-1.2(7)
C(15)-C(6)-C(5)-S(2)	178.8(6)
C(8)-S(2)-C(5)-C(6)	1.8(5)
C(8)-S(2)-C(5)-C(4)	-178.4(5)

C(2)-C(3)-C(4)-C(5)	177.6(6)
C(12)-C(3)-C(4)-C(5)	-0.1(11)
C(2)-C(3)-C(4)-S(1)	-1.9(7)
C(12)-C(3)-C(4)-S(1)	-179.5(6)
C(6)-C(5)-C(4)-C(3)	-141.0(7)
S(2)-C(5)-C(4)-C(3)	39.3(8)
C(6)-C(5)-C(4)-S(1)	38.4(8)
S(2)-C(5)-C(4)-S(1)	-141.3(4)
C(1)-S(1)-C(4)-C(3)	2.0(5)
C(1)-S(1)-C(4)-C(5)	-177.5(5)
S(1)-C(1)-C(2)-C(3)	1.0(7)
Br(1)-C(1)-C(2)-C(3)	-176.9(5)
S(1)-C(1)-C(2)-C(9)	-180.0(6)
Br(1)-C(1)-C(2)-C(9)	2.1(11)
C(4)-C(3)-C(2)-C(1)	0.6(8)
C(12)-C(3)-C(2)-C(1)	178.7(6)
C(4)-C(3)-C(2)-C(9)	-178.6(5)
C(12)-C(3)-C(2)-C(9)	-0.5(8)
C(6)-C(15)-C(16)-C(19)	-59.0(7)
C(17)-C(15)-C(16)-C(19)	56.2(7)
C(15)-C(16)-C(19)-C(18)	3.8(8)
C(4)-C(3)-C(12)-C(13)	-124.5(7)
C(2)-C(3)-C(12)-C(13)	57.8(7)
C(4)-C(3)-C(12)-C(14)	119.7(7)
C(2)-C(3)-C(12)-C(14)	-57.9(7)
C(3)-C(12)-C(13)-C(11)	-55.5(7)
C(14)-C(12)-C(13)-C(11)	59.0(7)
C(9)-C(11)-C(13)-C(12)	-0.5(8)
C(6)-C(15)-C(17)-C(20)	55.0(7)
C(16)-C(15)-C(17)-C(20)	-59.6(7)

C(18)-C(20)-C(17)-C(15)	2.1(7)
C(3)-C(12)-C(14)-C(10)	57.2(7)
C(13)-C(12)-C(14)-C(10)	-57.8(7)
C(9)-C(10)-C(14)-C(12)	-1.4(8)
C(1)-C(2)-C(9)-C(11)	124.3(8)
C(3)-C(2)-C(9)-C(11)	-56.7(7)
C(1)-C(2)-C(9)-C(10)	-120.7(8)
C(3)-C(2)-C(9)-C(10)	58.3(7)
C(13)-C(11)-C(9)-C(2)	55.8(7)
C(13)-C(11)-C(9)-C(10)	-58.7(7)
C(14)-C(10)-C(9)-C(2)	-55.2(7)
C(14)-C(10)-C(9)-C(11)	59.3(7)
C(8)-C(7)-C(18)-C(20)	-119.8(7)
C(6)-C(7)-C(18)-C(20)	56.5(7)
C(8)-C(7)-C(18)-C(19)	124.4(7)
C(6)-C(7)-C(18)-C(19)	-59.3(7)
C(17)-C(20)-C(18)-C(7)	-56.5(7)
C(17)-C(20)-C(18)-C(19)	58.3(7)
C(16)-C(19)-C(18)-C(7)	53.0(7)
C(16)-C(19)-C(18)-C(20)	-62.0(7)

Symmetry transformations used to generate equivalent atoms:

Table S13. Cartesian Coordinates from the Optimized Structure of **1(2T)** at B3LYP/6-31G(d).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.315345	5.265468	-1.300760
2	6	0	0.668077	2.961944	0.127859
3	6	0	-0.668077	3.134953	-0.126497
4	1	0	2.476336	4.117907	0.490461
5	6	0	1.053238	1.594903	0.202278
6	1	0	-0.576431	4.847041	-2.278160
7	16	0	-1.493414	1.618842	-0.300500
8	6	0	-1.147521	4.555430	-0.193110
9	1	0	-0.587575	6.328069	-1.322517
10	6	0	-0.785865	5.222311	1.166384
11	1	0	-2.219472	4.642561	-0.396239
12	1	0	-1.058887	6.284185	1.125639
13	6	0	0.738006	5.053114	1.450314

14	1	0	-1.382124	4.768364	1.964594
15	6	0	1.409742	4.265050	0.289382
16	1	0	0.897280	4.521483	2.394206
17	1	0	1.223974	6.031776	1.547739
18	6	0	1.207561	5.090330	-1.013620
19	1	0	1.700773	4.582394	-1.848905
20	1	0	1.694293	6.066844	-0.899795
21	6	0	0.000758	0.724514	-0.000082
22	6	0	1.147521	-4.555430	-0.193110
23	1	0	2.060756	1.253101	0.418091
24	16	0	1.493414	-1.618842	-0.300500
25	6	0	-0.668077	-2.961944	0.127859
26	1	0	0.576431	-4.847041	-2.278160
27	6	0	0.668077	-3.134953	-0.126497
28	6	0	-1.207561	-5.090330	-1.013620
29	1	0	0.587575	-6.328069	-1.322517
30	1	0	-2.060756	-1.253101	0.418091
31	1	0	1.382124	-4.768364	1.964594
32	6	0	-0.000758	-0.724514	-0.000082
33	1	0	-0.897280	-4.521483	2.394206
34	1	0	-1.700773	-4.582394	-1.848905
35	1	0	2.219472	-4.642561	-0.396239
36	6	0	-1.409742	-4.265050	0.289382
37	1	0	-2.476336	-4.117907	0.490461
38	1	0	-1.694293	-6.066844	-0.899795
39	1	0	-1.223974	-6.031776	1.547739
40	1	0	1.058887	-6.284185	1.125639
41	6	0	-0.738006	-5.053114	1.450314
42	6	0	-1.053238	-1.594903	0.202278
43	6	0	0.315345	-5.265468	-1.300760

44 6 0 0.785865 -5.222311 1.166384

HF=-1571.7509393 hartree

Table S14. Cartesian Coordinates from the Optimized Structure of **1(3T)** at B3LYP/6-31G(d).

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
<hr/>					
1	6	0	2.956081	-0.659825	6.271050
2	6	0	2.491029	0.652787	5.578330
3	6	0	0.362543	-0.363937	5.125493
4	6	0	0.594743	0.804658	7.277559
5	6	0	0.429166	-0.590544	6.607536
6	6	0	1.822619	1.544332	6.664251
7	6	0	1.431651	0.289406	4.567701

8	6	0	0.106784	0.007138	2.658814
9	1	0	-0.320632	1.388419	7.135982
10	1	0	1.630397	-2.405490	6.460380
11	1	0	2.561176	1.778440	7.440904
12	16	0	-0.843833	-0.751670	3.942508
13	1	0	3.342245	1.171534	5.124498
14	6	0	-0.336124	0.006110	1.276351
15	1	0	0.723498	0.666627	8.358365
16	1	0	-0.446539	-1.111981	7.006456
17	1	0	1.515734	2.495863	6.217759
18	6	0	1.291860	0.501791	3.169340
19	1	0	2.019692	1.016790	2.550428
20	1	0	3.688644	-0.414149	7.049806
21	1	0	3.466336	-1.297802	5.542017
22	6	0	1.728992	-1.401131	6.884648
23	1	0	1.848239	-1.519672	7.968801
24	16	0	0.876248	-0.095262	0.000000
25	6	0	0.106784	0.007138	-2.658814
26	6	0	-1.593094	0.069082	0.715093
27	6	0	-3.832063	-0.979079	0.779942
28	6	0	-2.973366	0.200532	-1.310649
29	6	0	-3.832063	-0.979079	-0.779942
30	6	0	-1.593094	0.069082	-0.715093
31	6	0	-2.973366	0.200532	1.310649
32	1	0	-3.436627	-1.924258	1.166966
33	1	0	-2.959836	0.204139	-2.403423
34	1	0	-4.853005	-0.878238	-1.168299
35	6	0	-0.336124	0.006110	-1.276351
36	6	0	-3.590206	1.523012	0.779003
37	1	0	-2.959836	0.204139	2.403423

38	1	0	-4.853005	-0.878238	1.168299
39	1	0	-3.020184	2.373423	-1.167825
40	1	0	-3.436627	-1.924258	-1.166966
41	1	0	-4.611481	1.619179	1.167926
42	6	0	-3.590206	1.523012	-0.779003
43	1	0	-3.020184	2.373423	1.167825
44	1	0	-4.611481	1.619179	-1.167926
45	6	0	1.291860	0.501791	-3.169340
46	1	0	3.342245	1.171534	-5.124498
47	1	0	-0.320632	1.388419	-7.135982
48	1	0	2.019692	1.016790	-2.550428
49	1	0	2.561176	1.778440	-7.440904
50	6	0	1.431651	0.289406	-4.567701
51	6	0	1.822619	1.544332	-6.664251
52	6	0	0.429166	-0.590544	-6.607536
53	6	0	0.594743	0.804658	-7.277559
54	6	0	0.362543	-0.363937	-5.125493
55	6	0	2.491029	0.652787	-5.578330
56	1	0	1.515734	2.495863	-6.217759
57	1	0	-0.446539	-1.111981	-7.006456
58	1	0	0.723498	0.666627	-8.358365
59	16	0	-0.843833	-0.751670	-3.942508
60	1	0	3.688644	-0.414149	-7.049806
61	6	0	1.728992	-1.401131	-6.884648
62	1	0	1.630397	-2.405490	-6.460380
63	6	0	2.956081	-0.659825	-6.271050
64	1	0	1.848239	-1.519672	-7.968801
65	1	0	3.466336	-1.297802	-5.542017

HF=-2357.0330409

Table S15. Cartesian Coordinates from the Optimized Structure of **13** at B3LYP/6-31G(d).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.399551	-1.298601	0.271241
2	16	0	-1.846103	-1.191415	-0.226390
3	6	0	-0.715687	0.119710	0.069053
4	6	0	-1.399551	1.298601	0.271241
5	6	0	-2.814872	1.155424	0.201248
6	6	0	-3.207808	-0.129789	-0.051526
7	6	0	3.207808	0.129789	-0.051527
8	16	0	1.846103	1.191415	-0.226390
9	6	0	0.715687	-0.119710	0.069053
10	1	0	3.510160	-1.975697	0.343278
11	1	0	-0.899537	2.237264	0.485599
12	1	0	-3.510160	1.975697	0.343278

13	1	0	4.212069	0.520155	-0.146726
14	1	0	-4.212069	-0.520155	-0.146726
15	1	0	0.899537	-2.237264	0.485599
16	6	0	2.814872	-1.155424	0.201248

HF=-1104.8167055

Table S16. Cartesian Coordinates from the Optimized Structure of **14** at B3LYP/6-31G(d).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.708129	-1.522640	-0.019563
2	16	0	3.922895	-1.036028	0.321834
3	6	0	2.660620	0.121858	-0.071693
4	6	0	3.219710	1.343185	-0.384341
5	6	0	4.641609	1.352480	-0.319264
6	6	0	5.166001	0.141593	0.040438
7	6	0	-1.264992	-0.261176	0.037124

8	16	0	-0.000126	0.957480	-0.001446
9	6	0	1.264978	-0.261059	-0.035822
10	1	0	-1.304033	-2.428721	0.054256
11	1	0	2.626202	2.204798	-0.671532
12	1	0	5.247993	2.224307	-0.539611
13	6	0	-2.660677	0.121676	0.072467
14	1	0	6.205334	-0.133401	0.159034
15	1	0	1.304287	-2.428683	-0.046948
16	6	0	-0.707978	-1.522704	0.024026
17	6	0	-3.220073	1.342394	0.386910
18	6	0	-4.641926	1.351737	0.320550
19	6	0	-5.165942	0.141518	-0.041963
20	1	0	-5.248561	2.223092	0.542069
21	16	0	-3.922518	-1.035495	-0.324448
22	1	0	-2.626820	2.203385	0.676468
23	1	0	-6.205167	-0.133275	-0.161995

HF = -1656.63166708 hartree

Table S17. Cartesian Coordinates from the Optimized Structure of **15** at B3LYP/6-31G(d).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-1.199608	-0.000295	0.000030
2	6	0	0.011022	1.243564	-0.000088
3	6	0	1.272265	0.715319	0.000011
4	6	0	1.272988	-0.714781	-0.000076
5	6	0	0.011947	-1.243527	-0.000146
6	1	0	-0.280705	2.285122	0.000166
7	1	0	2.172207	1.321001	0.000338
8	1	0	2.173179	-1.319843	0.000256
9	1	0	-0.280279	-2.285016	0.000566

HF = -553.002628314

Table S18. Cartesian Coordinates from the Optimized Structure of **16** at B3LYP/6-31G(d).

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	1	0	0.000000	2.293228	1.915581
2	1	0	0.000000	-2.293228	1.915581
3	6	0	0.000000	1.253229	1.616189
4	6	0	0.000000	0.718470	0.361743
5	6	0	0.000000	-0.718470	0.361743
6	6	0	0.000000	-1.253229	1.616189
7	16	0	0.000000	0.000000	2.830096
8	1	0	0.000000	2.410559	-1.003176
9	6	0	0.000000	-1.315376	-1.020954
10	6	0	1.255177	-0.780860	-1.763185
11	1	0	0.000000	-2.410559	-1.003176
12	6	0	-1.255177	-0.780860	-1.763185
13	1	0	1.253076	-1.167120	-2.789871
14	1	0	2.158334	-1.166312	-1.278538
15	6	0	1.255177	0.780860	-1.763185
16	1	0	2.158334	1.166312	-1.278538
17	6	0	0.000000	1.315376	-1.020954
18	1	0	1.253076	1.167120	-2.789871
19	1	0	-2.158334	1.166312	-1.278538
20	1	0	-1.253076	-1.167120	-2.789871
21	6	0	-1.255177	0.780860	-1.763185
22	1	0	-2.158334	-1.166312	-1.278538
23	1	0	-1.253076	1.167120	-2.789871

Table S19. Cartesian Coordinates from the Optimized Structure of **17** at B3LYP/6-31G(d).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	0.235147	-1.750111	2.159158
2	1	0	-3.344993	1.841261	0.000000
3	6	0	0.000000	0.696664	0.000000
4	6	0	-0.824813	-0.398622	0.000000
5	6	0	-2.210797	-0.054902	0.000000
6	6	0	-2.408294	1.300262	0.000000
7	16	0	-0.901414	2.179752	0.000000
8	6	0	1.473736	0.410963	0.000000
9	1	0	-3.023475	-0.774516	0.000000
10	6	0	1.768438	-0.460615	-1.255853
11	6	0	1.768438	-0.460615	1.255853
12	1	0	2.091294	1.314713	0.000000
13	1	0	1.606578	0.135888	-2.159551
14	6	0	0.850736	-1.720826	-1.254031

15	1	0	2.826714	-0.750103	-1.247243
16	1	0	1.452806	-2.637888	-1.246611
17	1	0	0.235147	-1.750111	-2.159158
18	6	0	-0.069373	-1.704614	0.000000
19	1	0	-0.735531	-2.574279	0.000000
20	6	0	0.850736	-1.720826	1.254031
21	1	0	1.606578	0.135888	2.159551
22	1	0	2.826714	-0.750103	1.247243
23	1	0	1.452806	-2.637888	1.246611

Hf = -786.469241728 hartree