Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Supporting Information

Orthogonal 4,10 and 6,12 Substitution of Dibenzo[def,mno]chrysene Polycyclic Aromatic Small Molecules

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MALDI-MS Characterization:

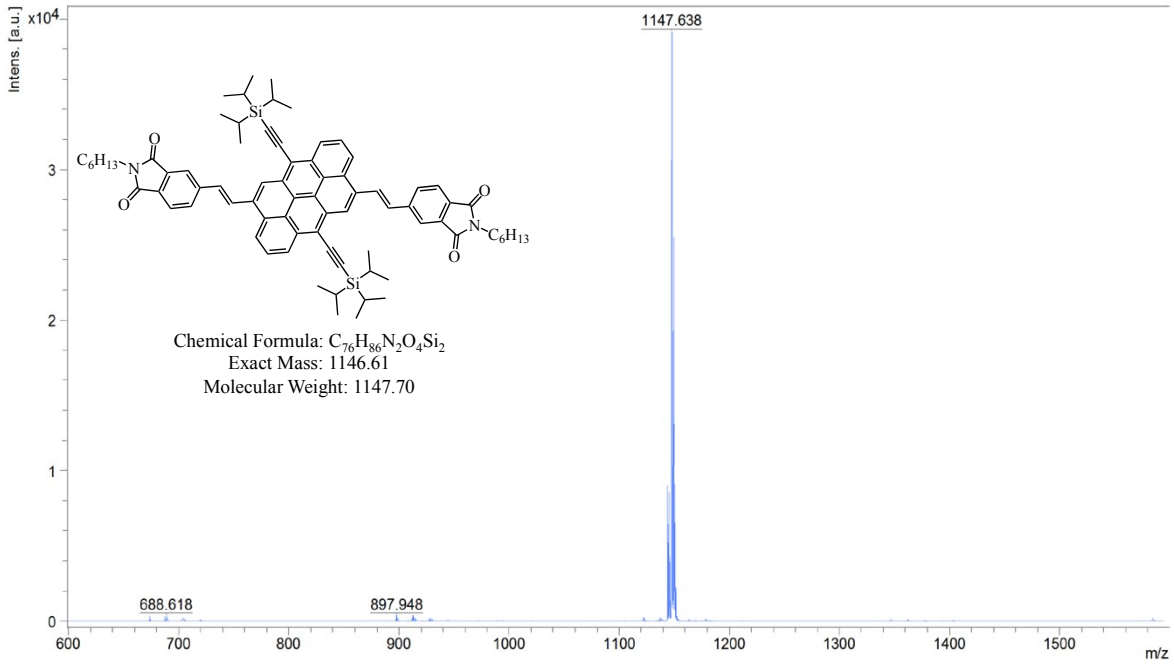


Figure S1. MALDI of **3.**

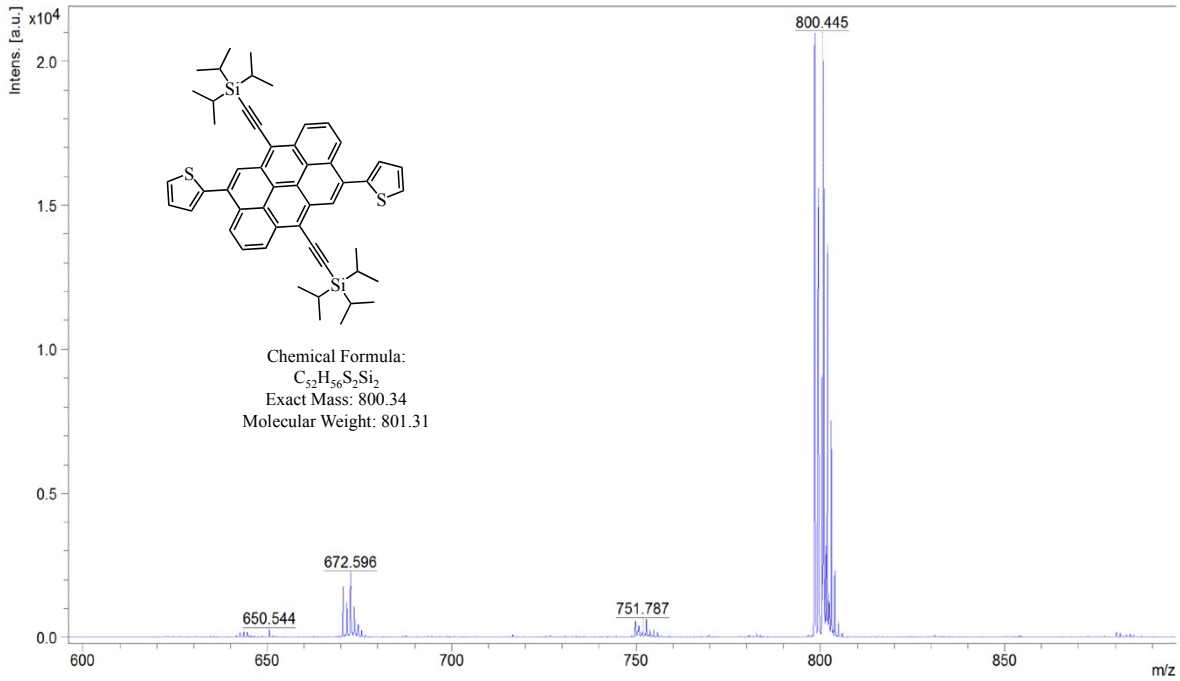


Figure S2. MALDI of **4.**

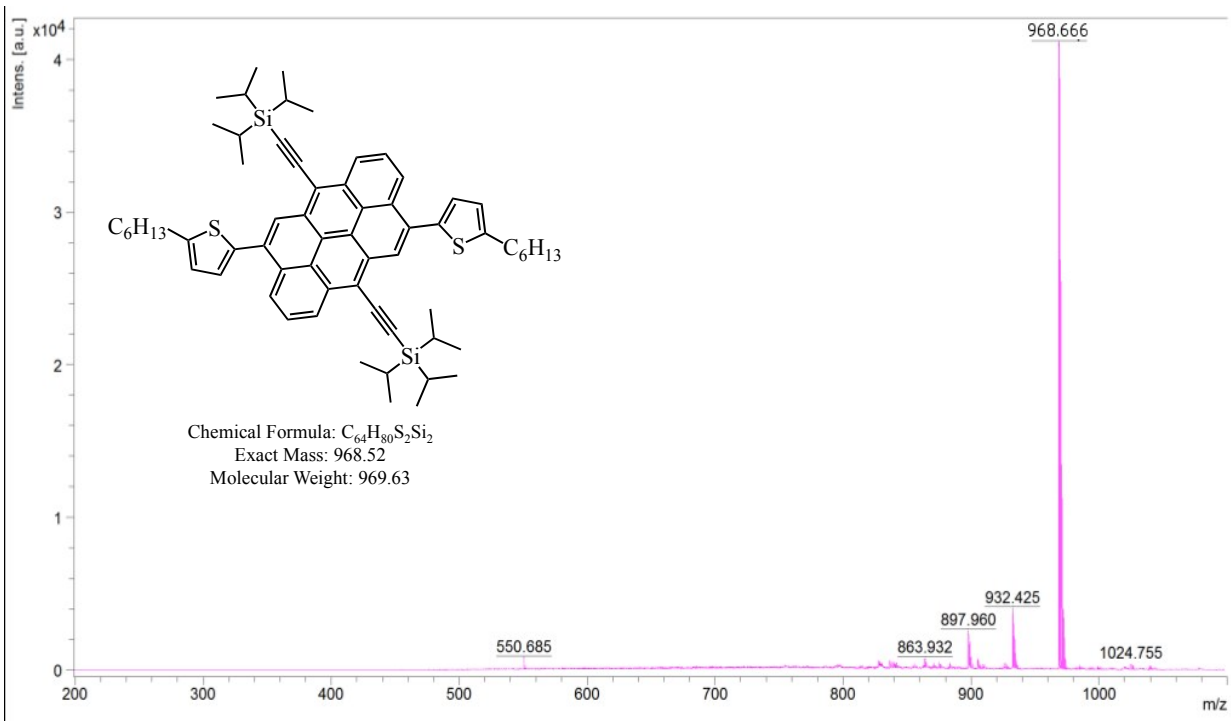


Figure S3. MALDI of **5.**

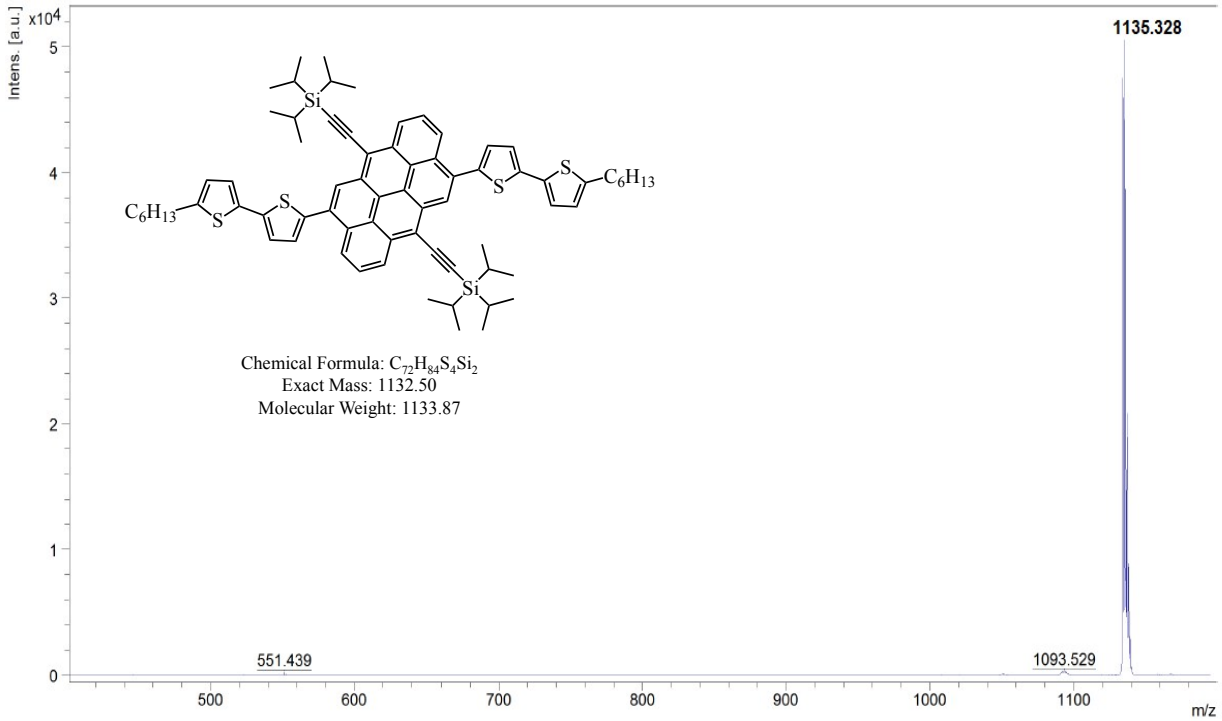


Figure S4. MALDI of **6.**

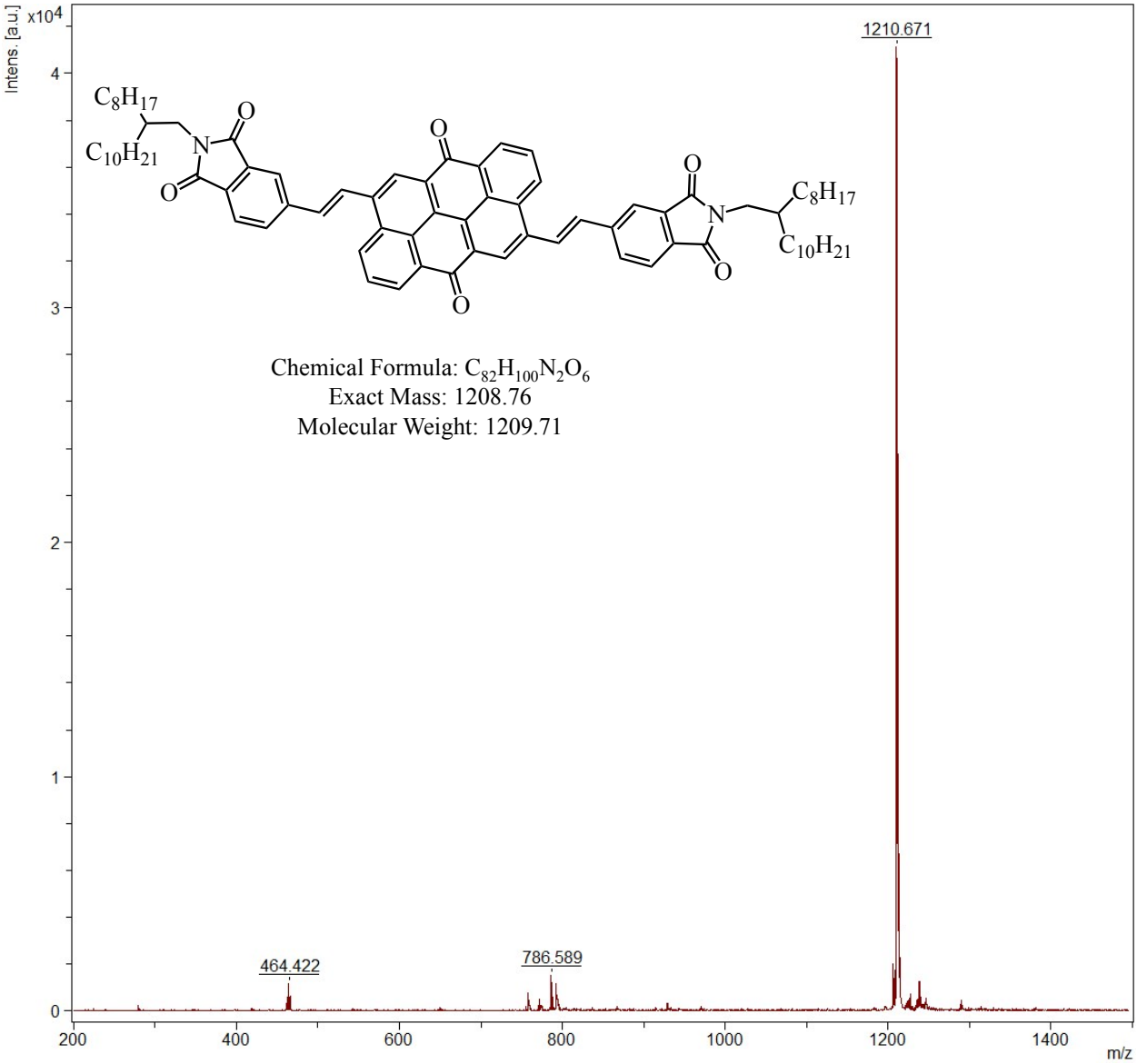


Figure S5. MALDI of **7.**

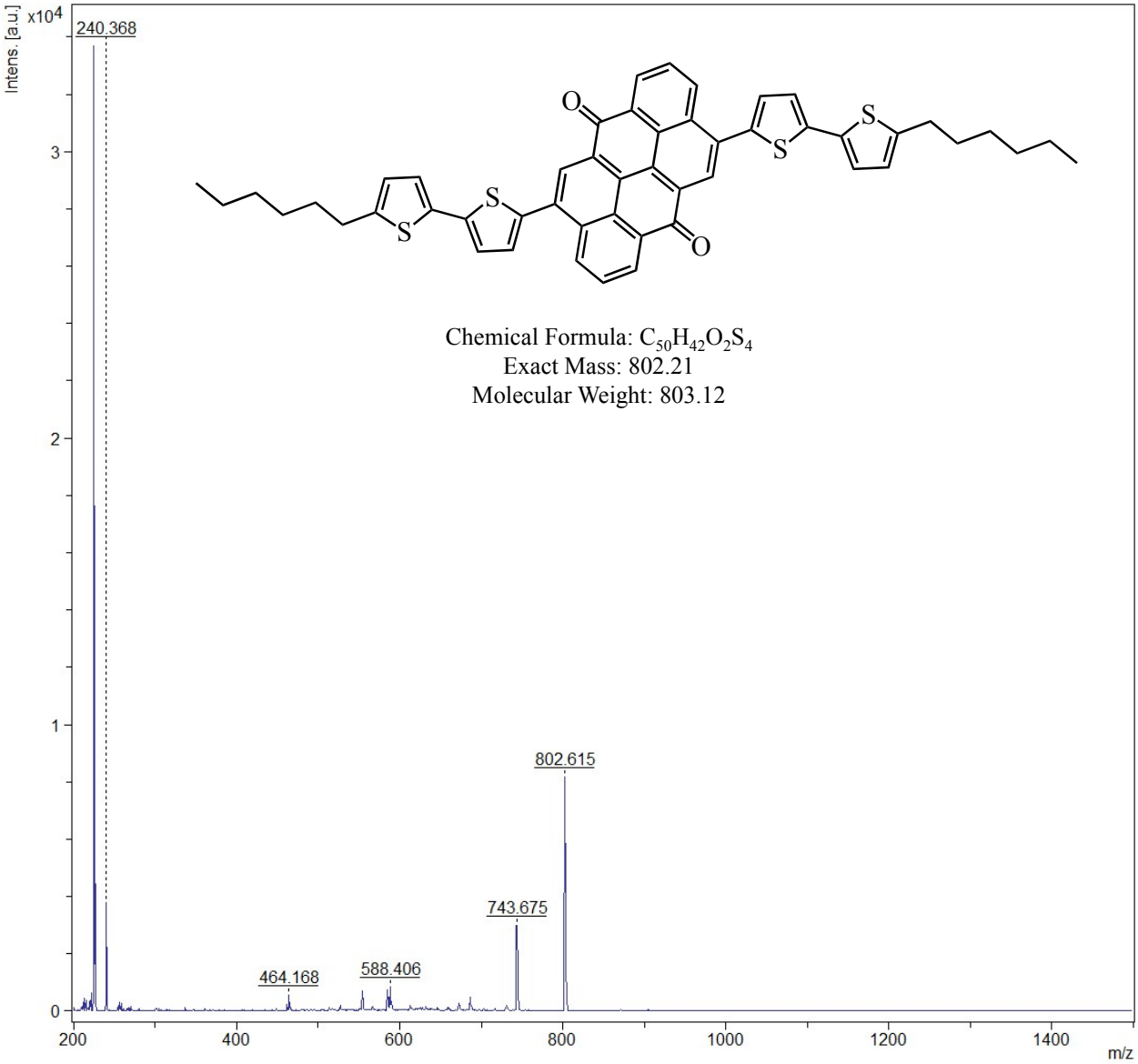


Figure S6. MALDI of **8.**

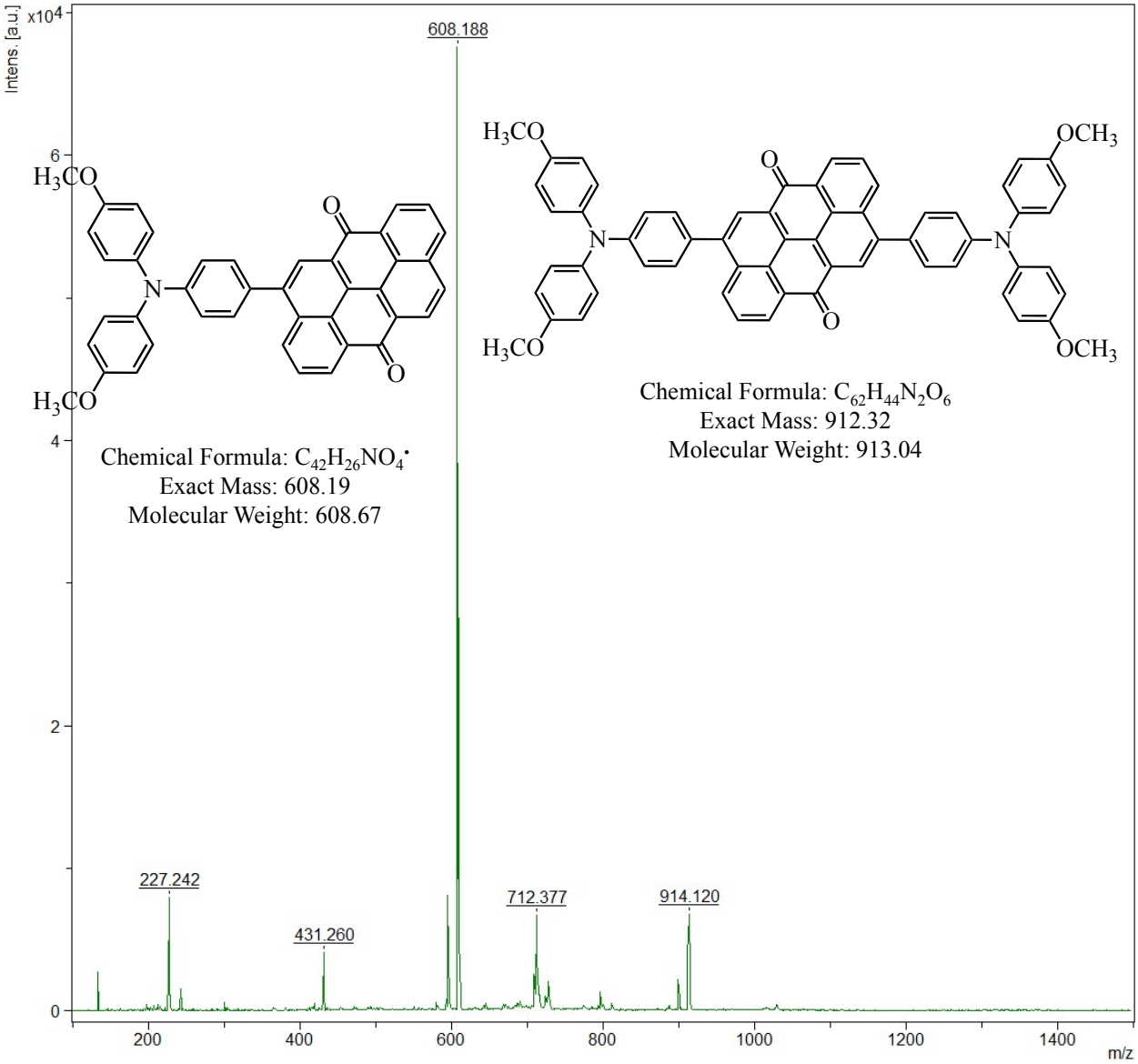


Figure S7. MALDI of **9.** Mass peak at 608amu is due to fragmentation during the MALDI experiment.

^{1}H NMR Spectra:

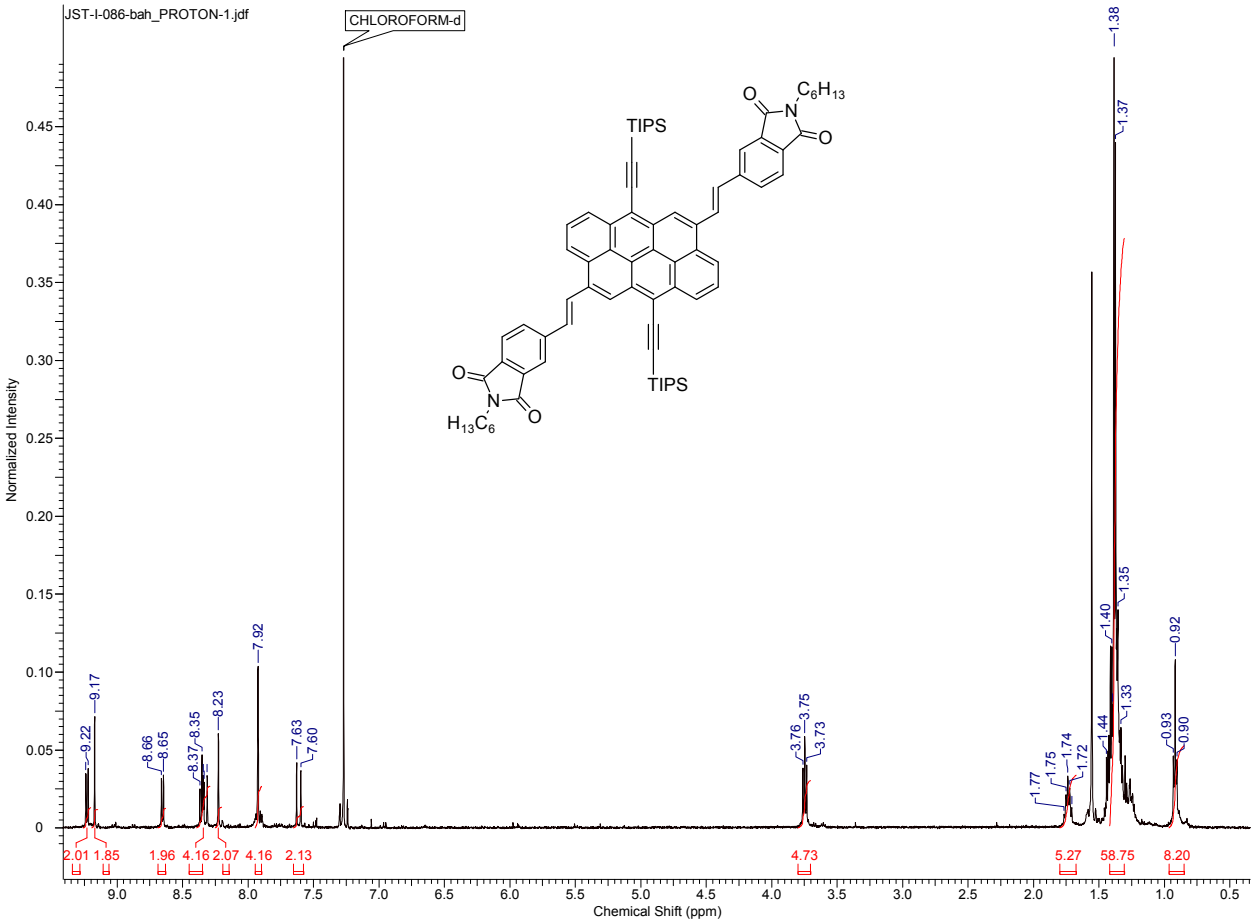


Figure S8. ^{1}H NMR ($CDCl_3$) of **3**.

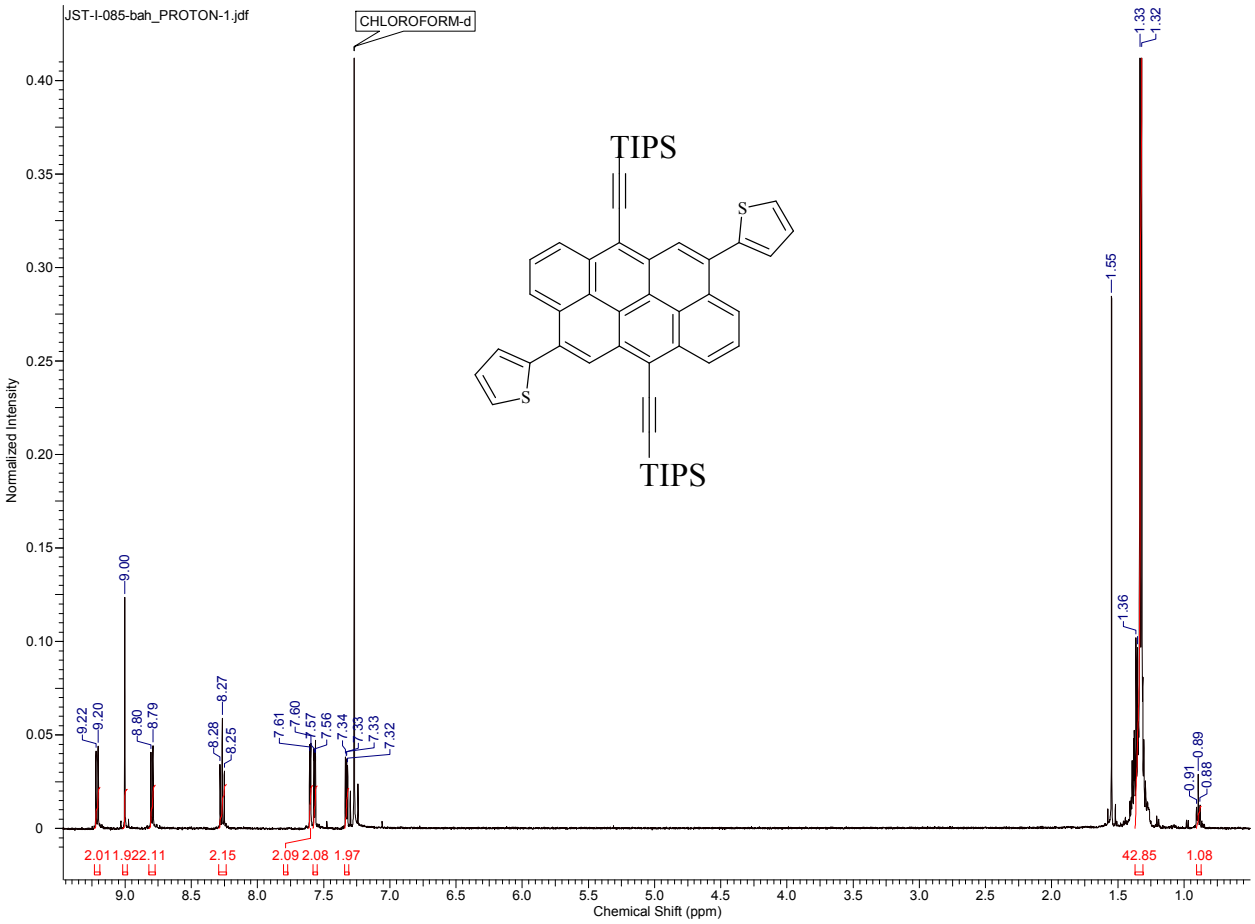


Figure S9. ^{1}H NMR ($CDCl_3$) of **4**.

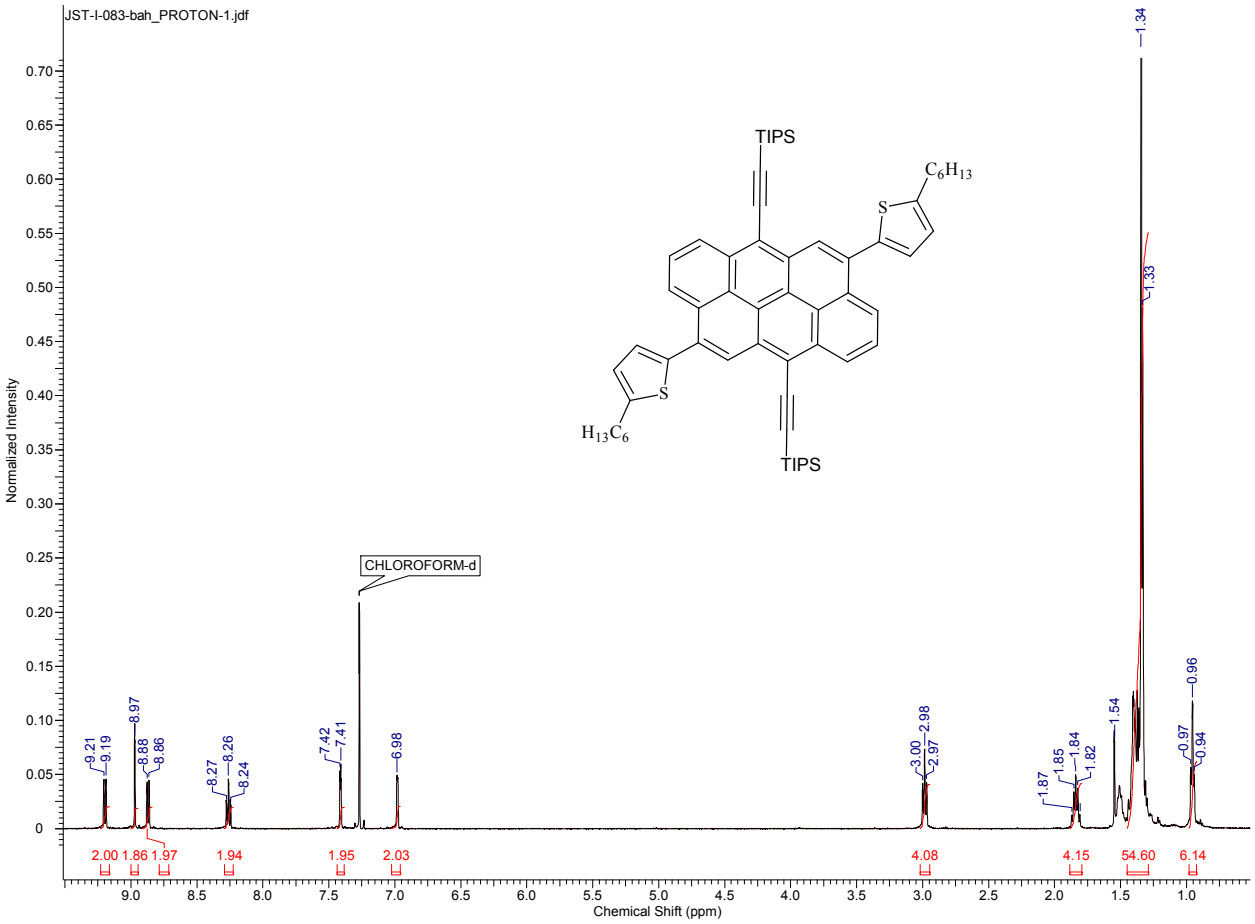


Figure S10. ^{1}H NMR ($CDCl_3$) of **5**.

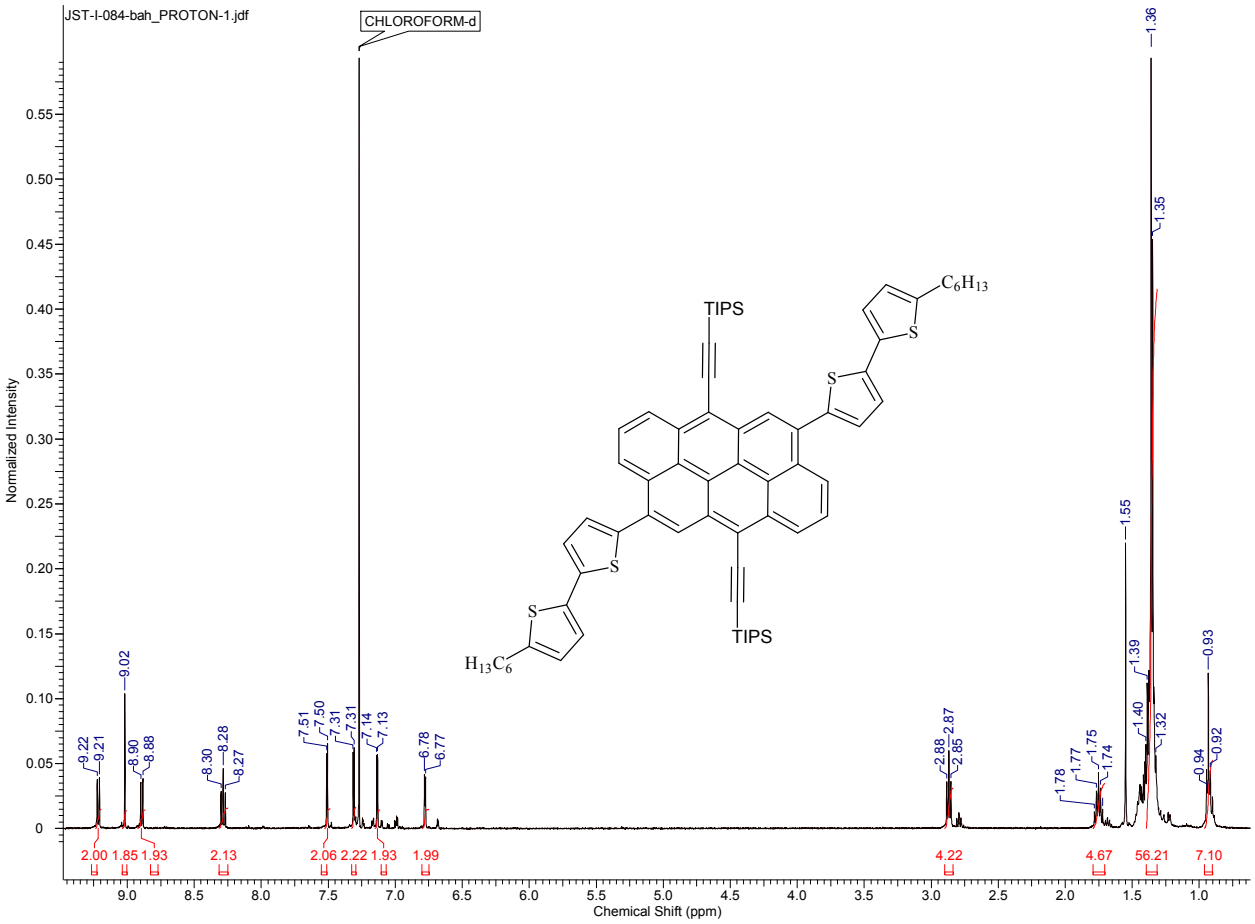


Figure S11. ^{1}H NMR ($CDCl_3$) of **6**.

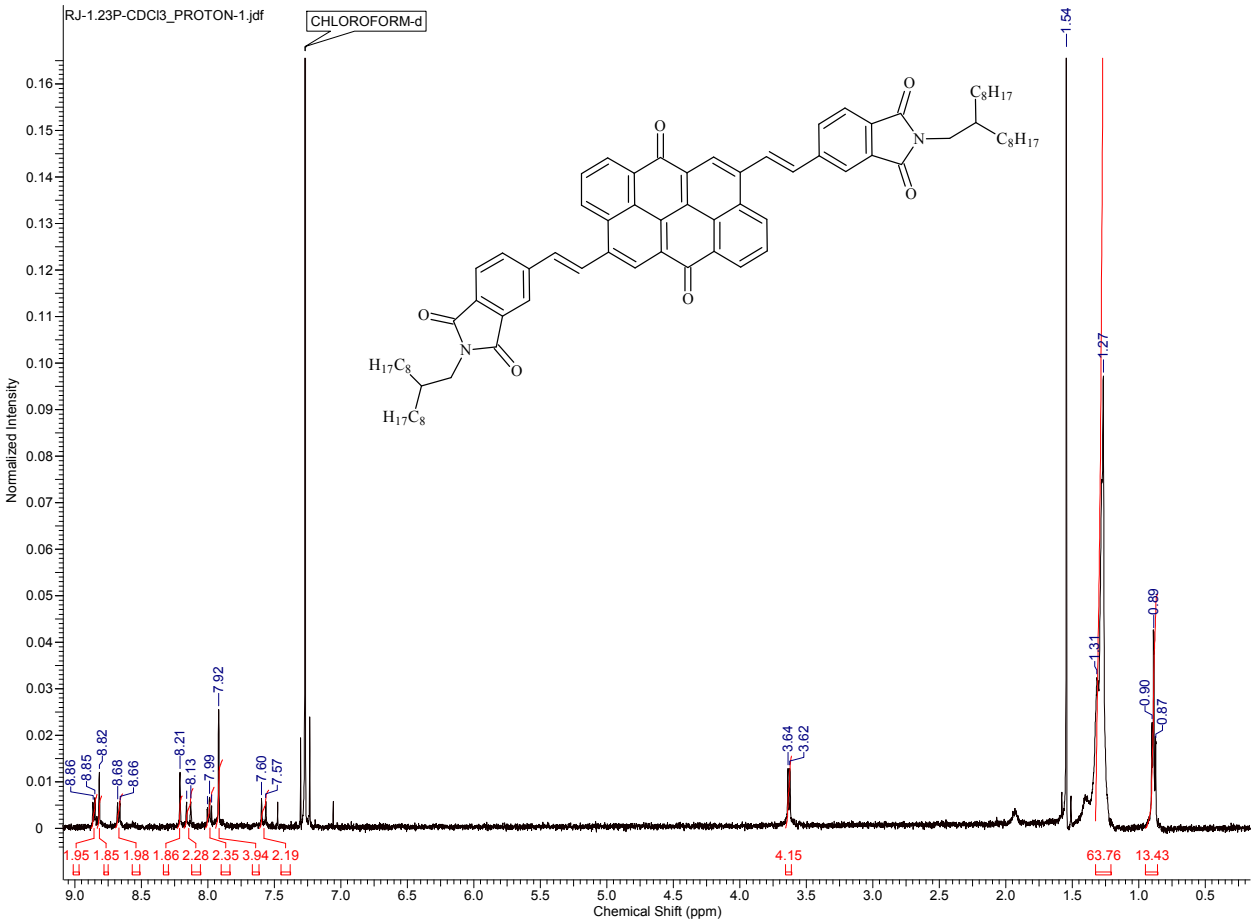


Figure S12. ^{1}H NMR ($CDCl_3$) of **7**.

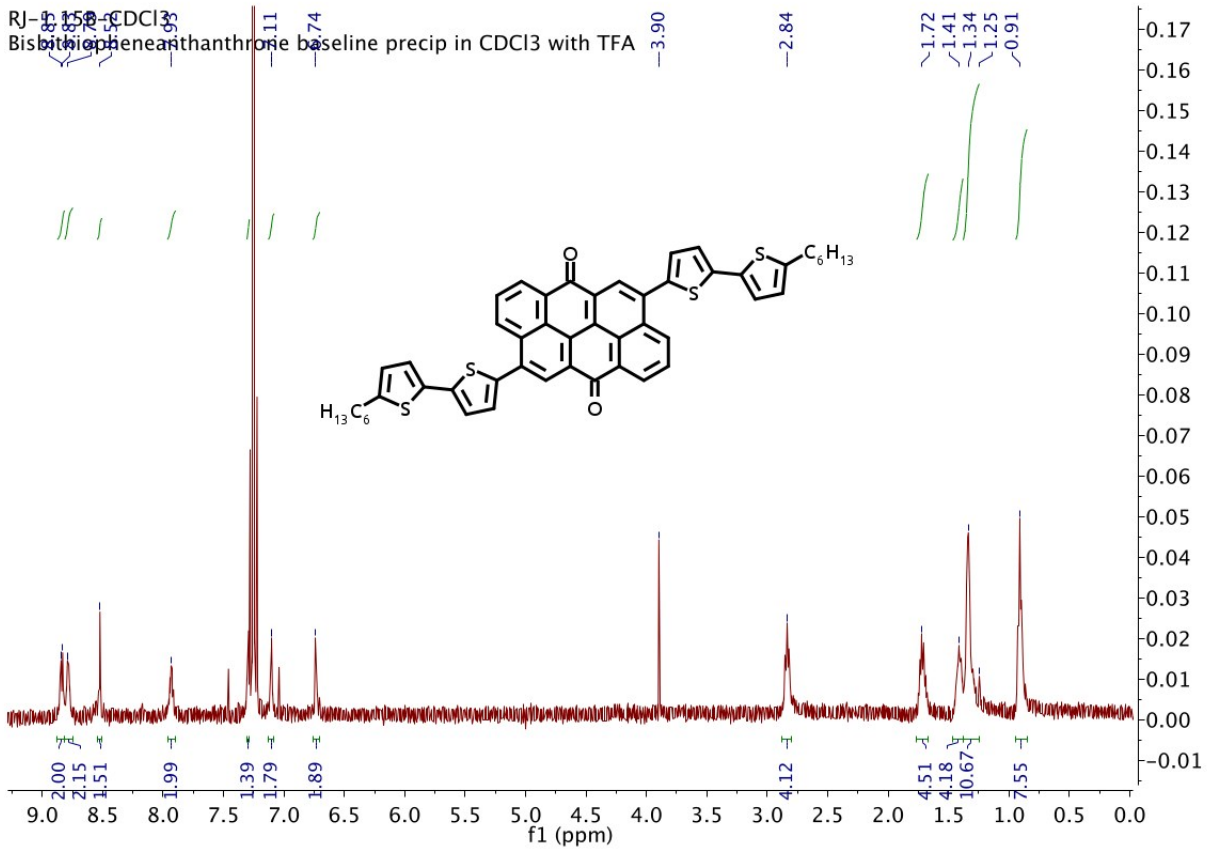


Figure S13. ^{1}H NMR ($CDCl_3$) of **8**.

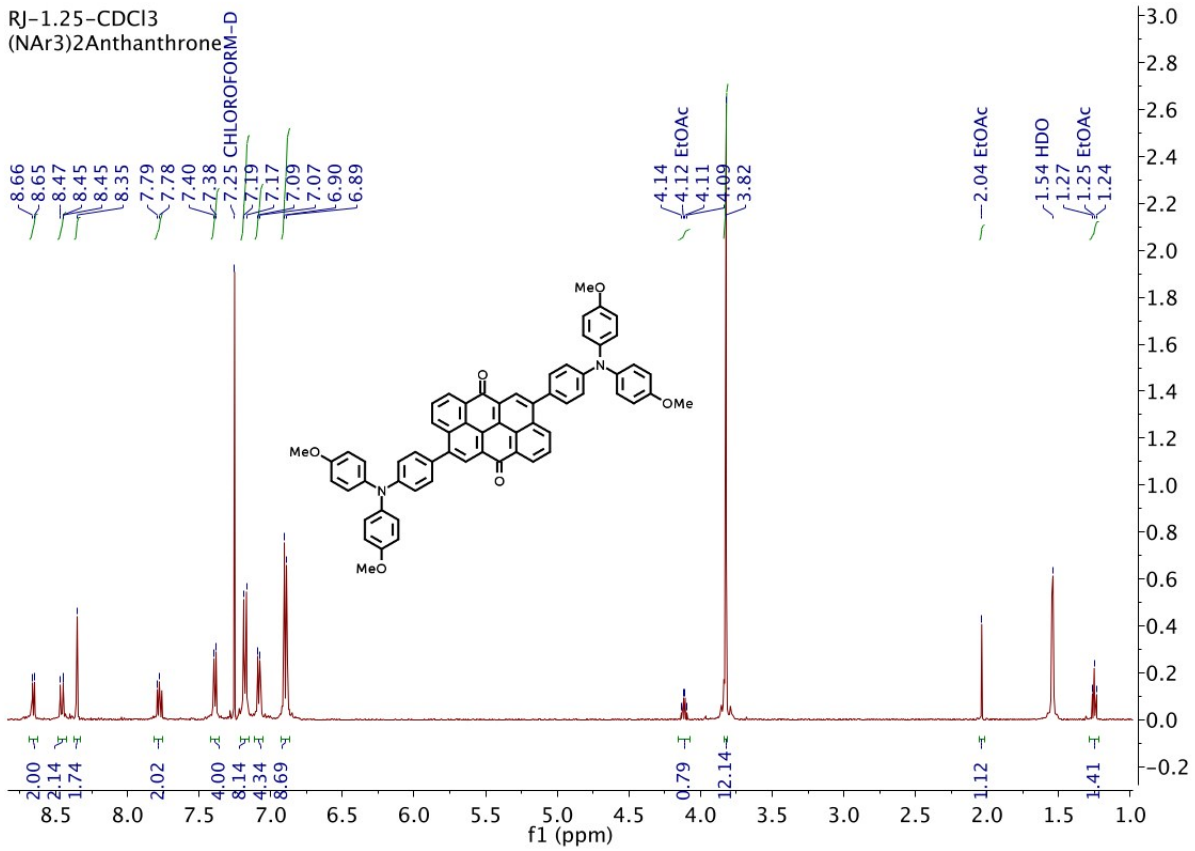


Figure S14. ^{1}H NMR ($CDCl_3$) of **9**.

Solution Phase Measurements:

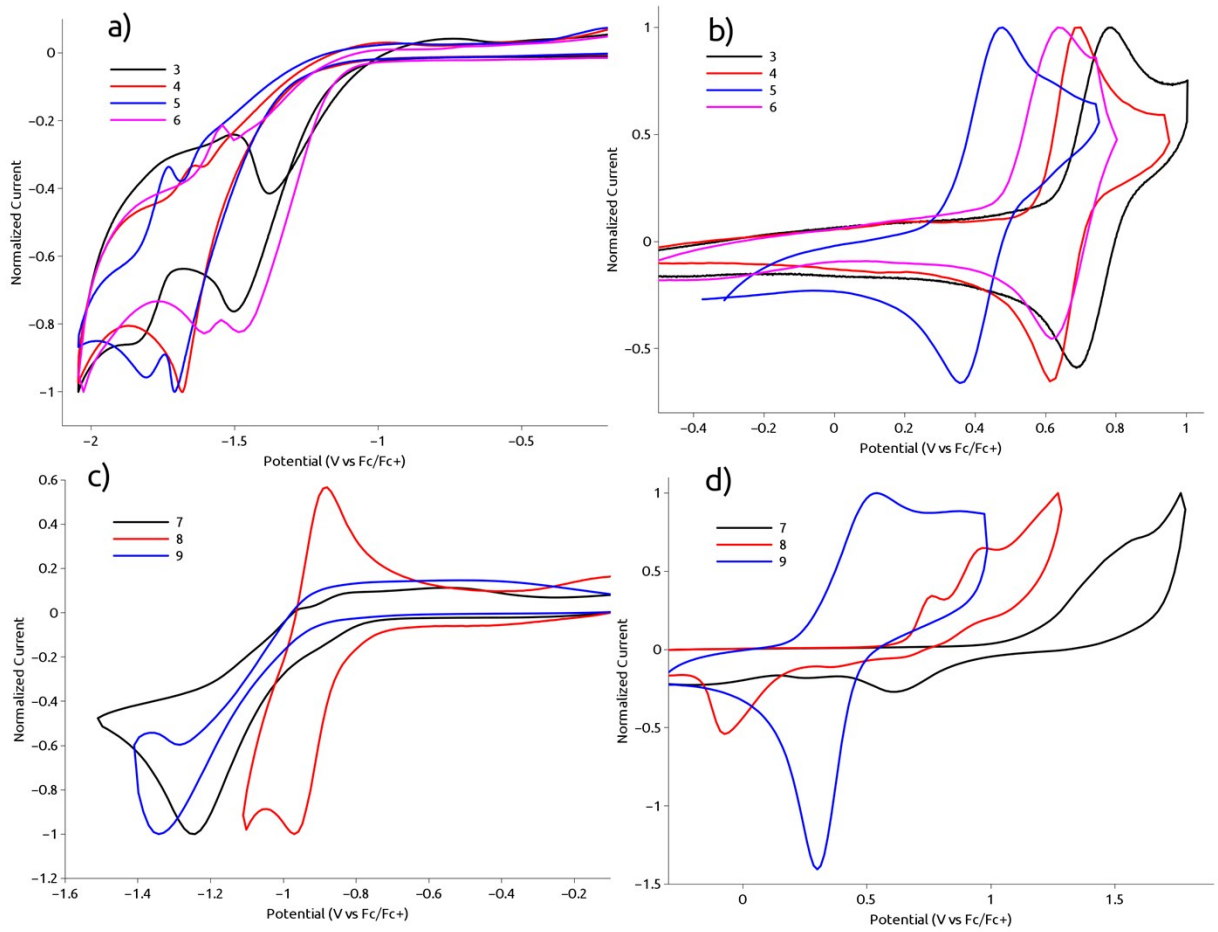


Figure S15. Solution phase CV: a) reduction and b) oxidation curves for **3-6**, c) reduction and d) oxidation curves for **7-9**.

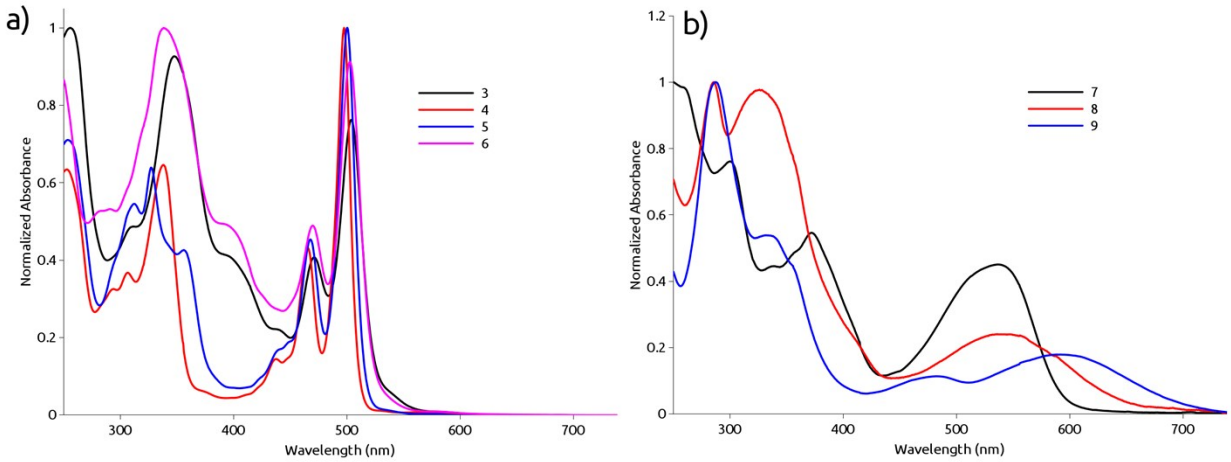


Figure S16. UV-Vis absorbance spectra for DCM solutions of a) **3-6**, and b) **7-9**.

DFT Computations:

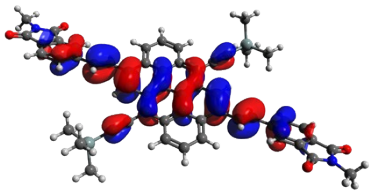
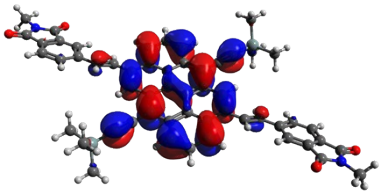
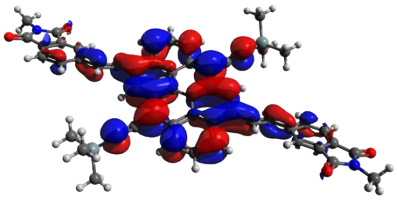
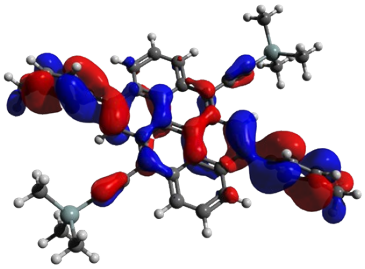
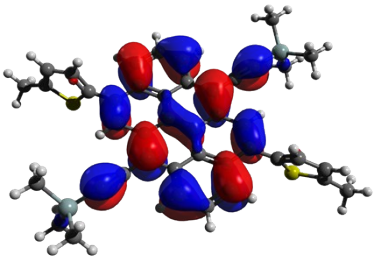
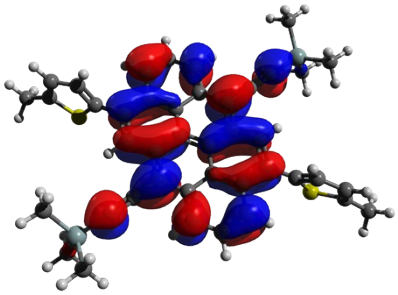
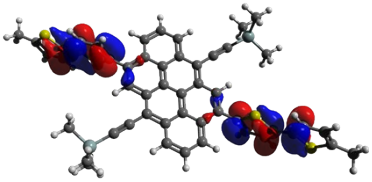
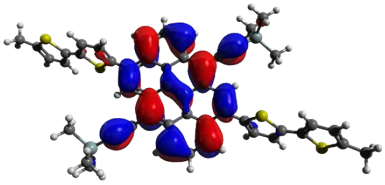
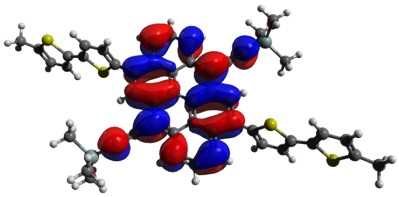
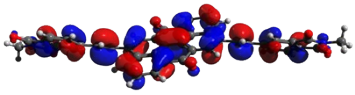
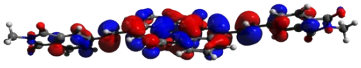
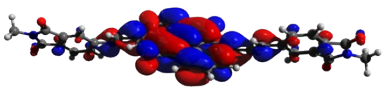
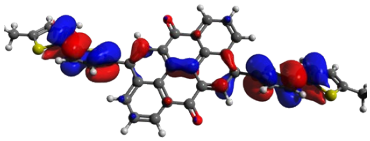
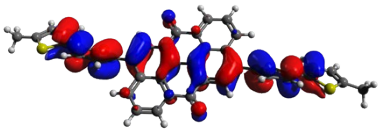
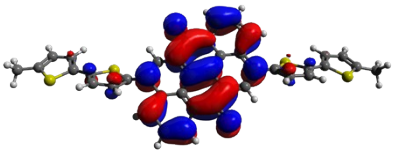
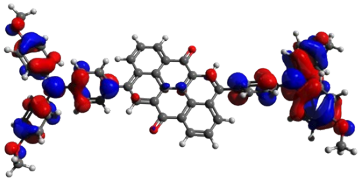
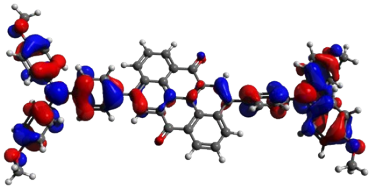
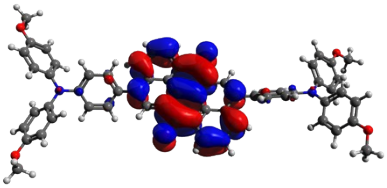
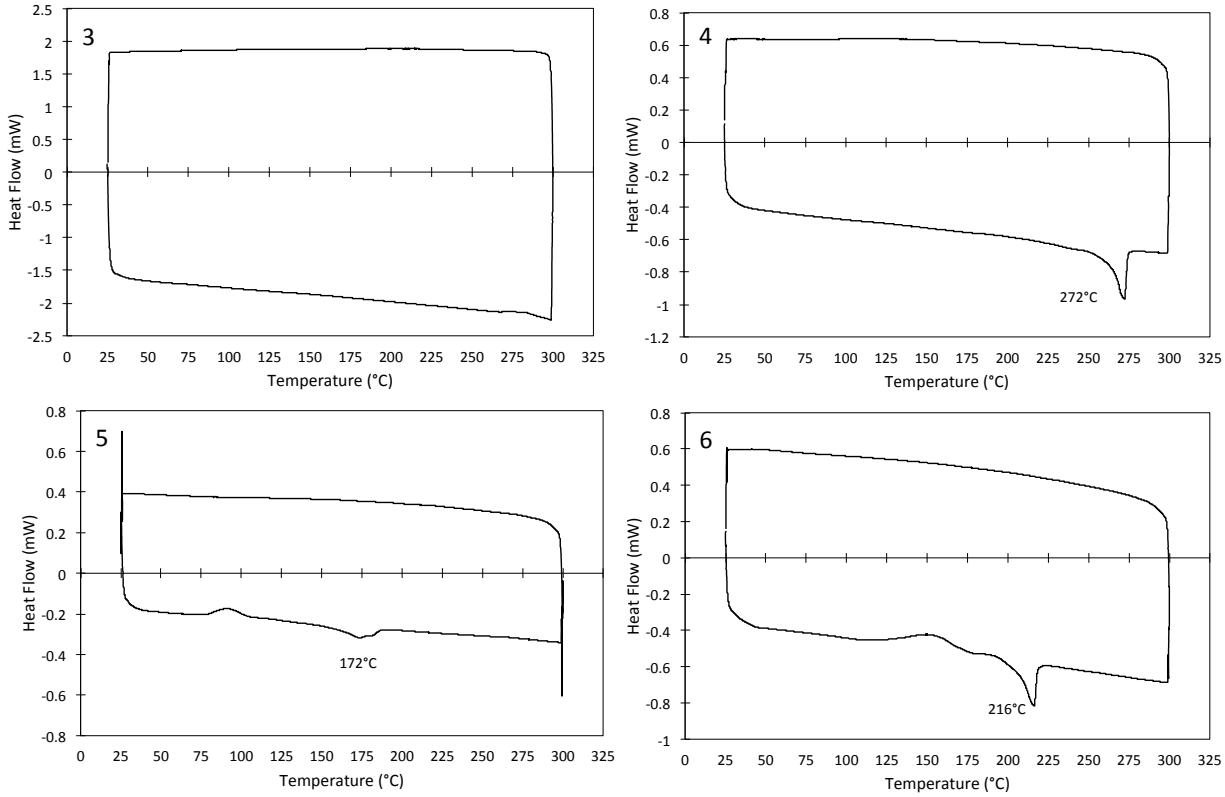
	HOMO-1	HOMO	LUMO
3			
5			
6			
7			
8			
9			

Figure S17. Molecular orbital densities for the model compounds.

Thermal Characterization:



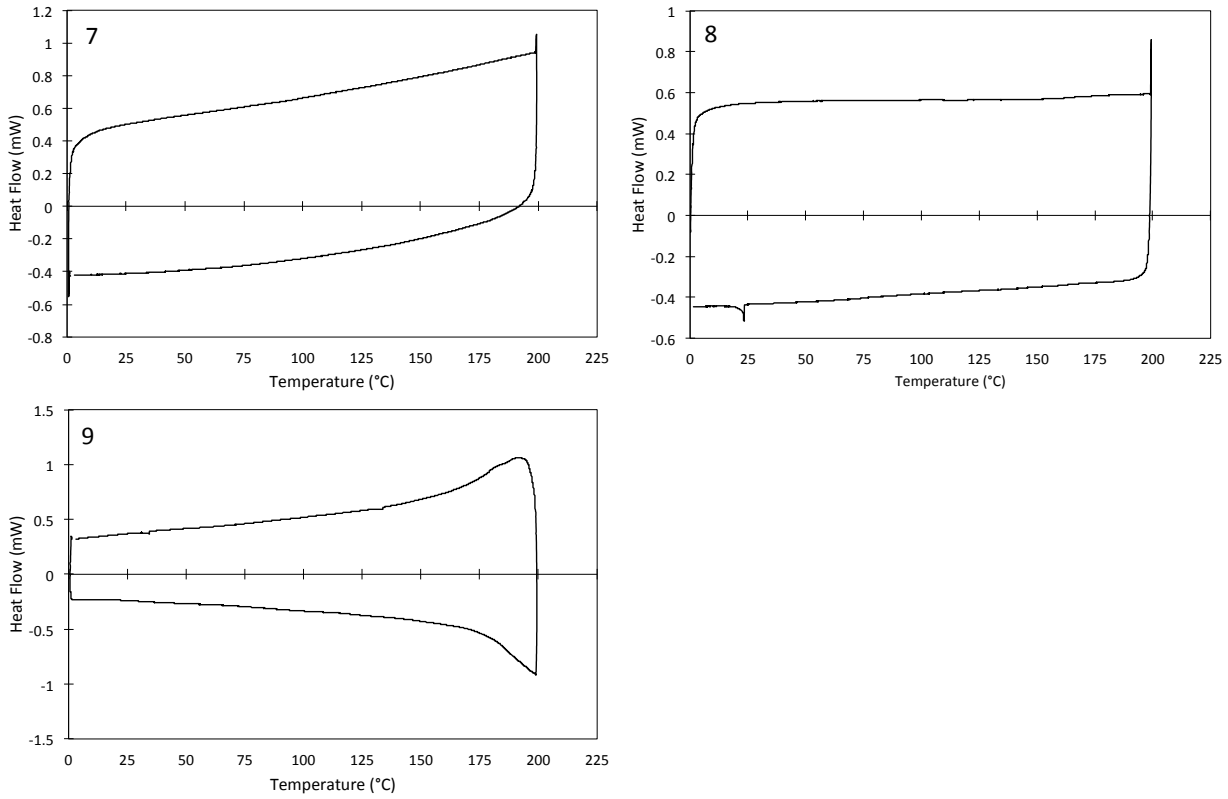


Figure S18. DSC traces for compounds **3-9**.

X-ray crystallography information:

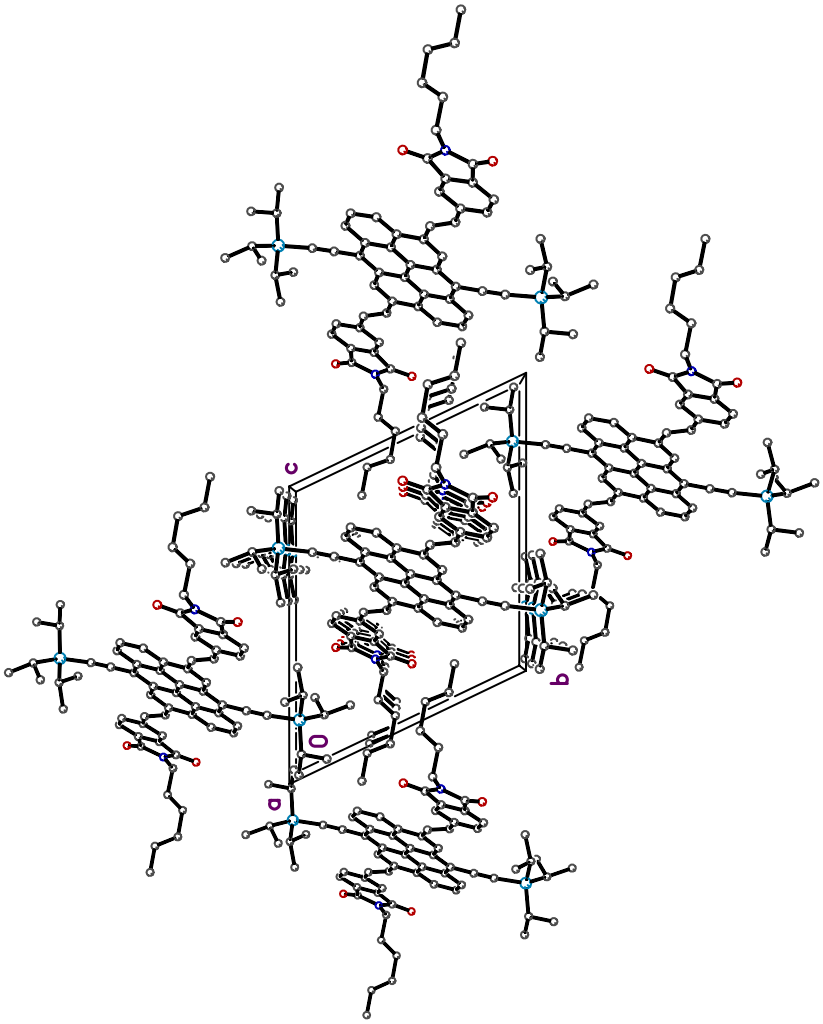


Figure S19. Ellipsoid plots of single crystals for **3**.

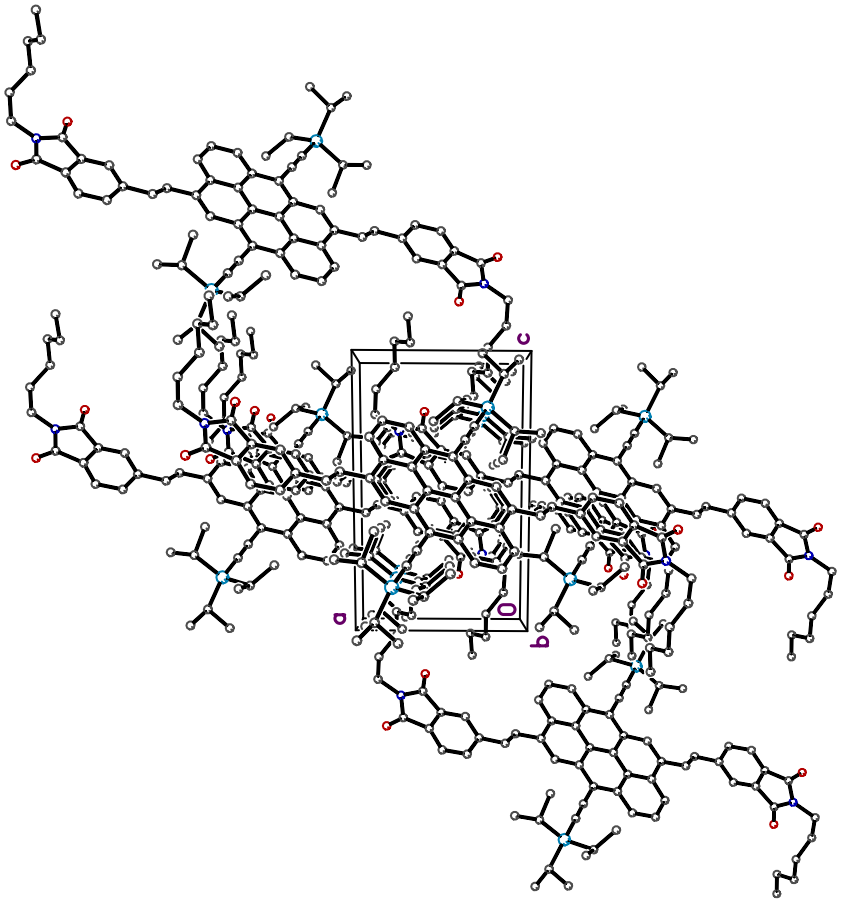


Figure S20. Ellipsoid plots of single crystals for **3**.

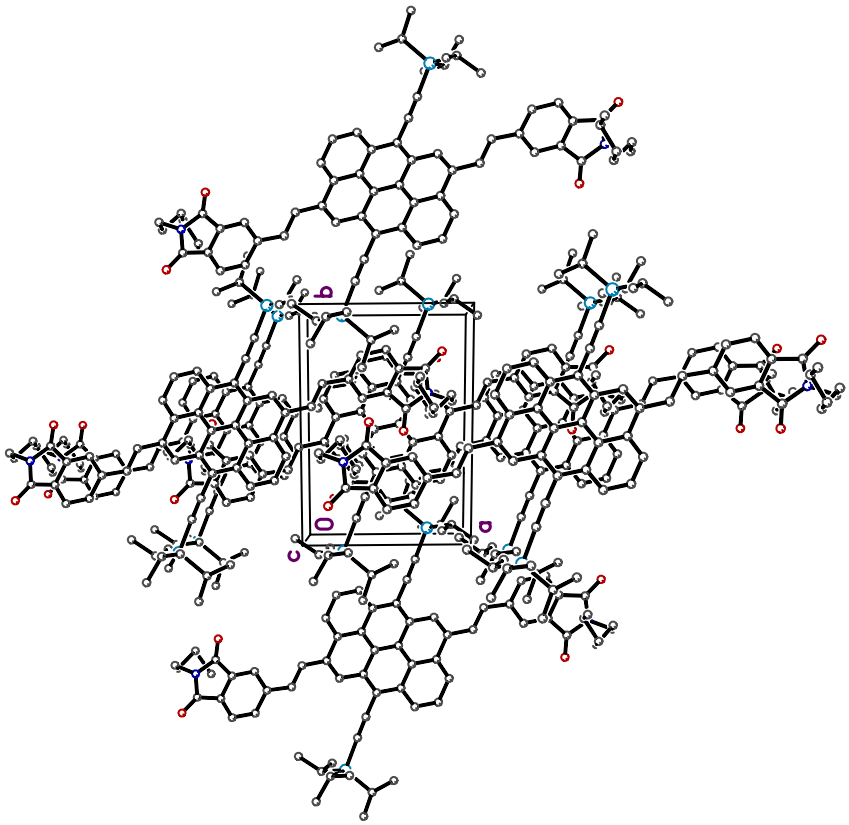


Figure S21. Ellipsoid plots of single crystals for **3**.

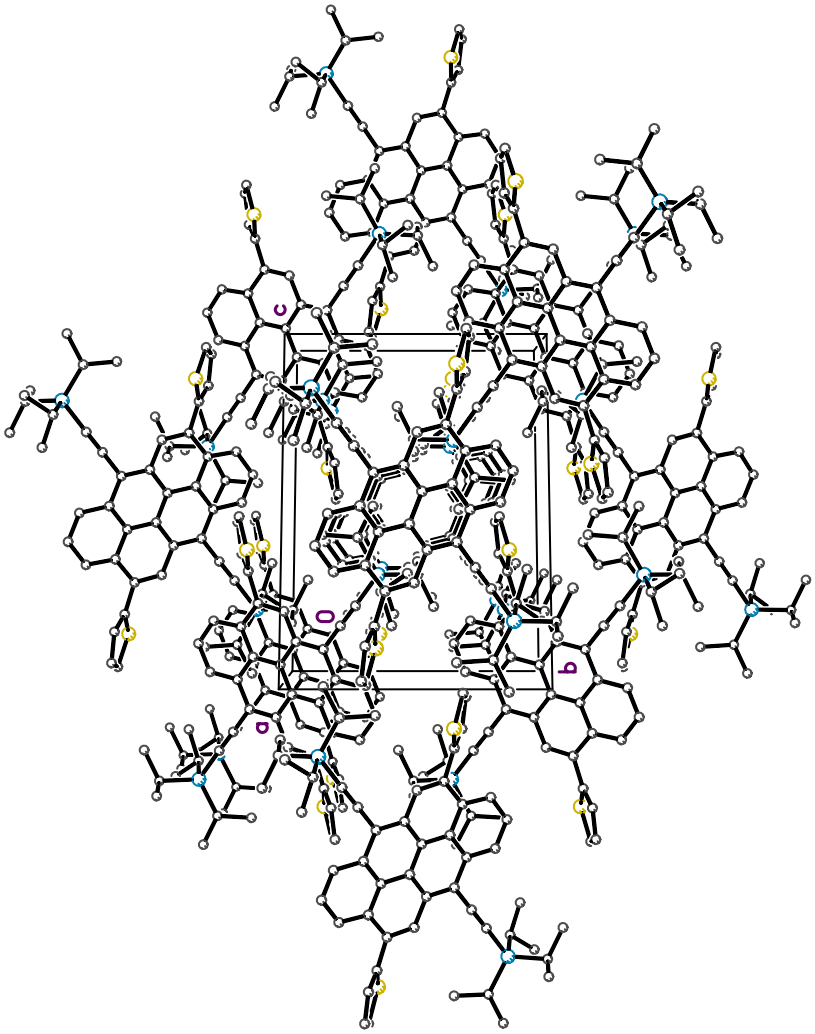


Figure S22. Ellipsoid plots of single crystals for **4**.

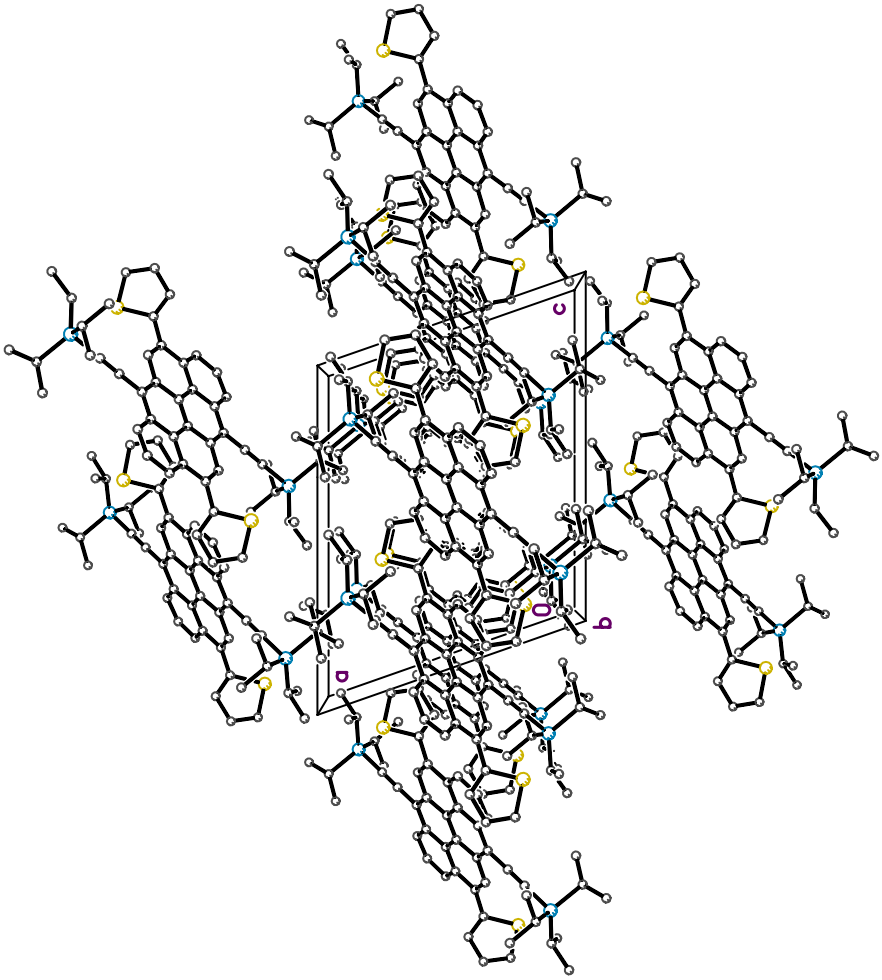


Figure S23. Ellipsoid plots of single crystals for **4**.

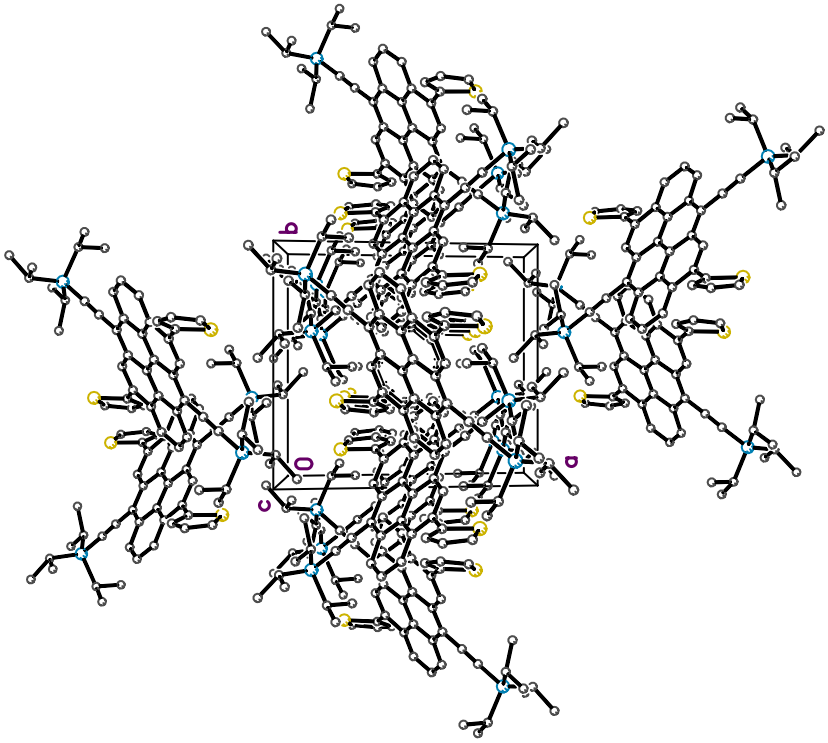


Figure S24. Ellipsoid plots of single crystals for **4**.

Table 1. Crystal data and structure refinement for compound **3**.

Identification code	x14415
Empirical formula	C76 H86 N2 O4 Si2
Formula weight	1147.64
Temperature	90.0(2) K
Wavelength	1.54178 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.5286(8) A alpha = 64.392(9) deg.
	b = 13.2963(16) A beta = 89.430(9) deg.
	c = 15.0772(19) A gamma = 89.359(8) deg.
Volume	1541.7(3) A^3
Z, Calculated density	1, 1.236 Mg/m^3
Absorption coefficient	0.933 mm^-1
F(000)	616
Crystal size	0.240 x 0.015 x 0.005 mm
Theta range for data collection	3.250 to 68.179 deg.
Limiting indices	-3<=h<=10, -15<=k<=16, -18<=l<=18
Reflections collected / unique	19592 / 5469 [R(int) = 0.0932]
Completeness to theta = 67.679	97.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.907 and 0.446
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5469 / 0 / 380
Goodness-of-fit on F^2	1.029

Final R indices [I>2sigma(I)]	R1 = 0.0620, wR2 = 0.1360
R indices (all data)	R1 = 0.1175, wR2 = 0.1619
Extinction coefficient	n/a
Largest diff. peak and hole	0.238 and -0.359 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **3.** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	7594(1)	10371(1)	1946(1)	37(1)
N(1)	17472(3)	6420(3)	7286(2)	38(1)
O(1)	18310(2)	8186(2)	6213(2)	45(1)
O(2)	16011(2)	4813(2)	8035(2)	42(1)
C(1)	5627(3)	6962(3)	3709(3)	31(1)
C(2)	6467(3)	6176(3)	4505(3)	31(1)
C(3)	8002(3)	6390(3)	4746(3)	32(1)
C(4)	8837(3)	5643(3)	5520(3)	32(1)
C(5)	8144(3)	4562(3)	6141(3)	34(1)
C(6)	8918(4)	3755(3)	6933(3)	37(1)
C(7)	8242(4)	2720(3)	7502(3)	38(1)
C(8)	6769(4)	2486(3)	7304(3)	36(1)
C(9)	5900(3)	3270(3)	6515(3)	32(1)
C(10)	6601(3)	4323(3)	5923(3)	32(1)
C(11)	5758(3)	5114(3)	5109(3)	31(1)
C(12)	6305(3)	8032(3)	3117(3)	34(1)
C(13)	6830(3)	8942(3)	2626(3)	36(1)
C(14)	5909(4)	11394(3)	1687(3)	42(1)
C(15)	4540(4)	10955(3)	2416(3)	51(1)
C(16)	6445(4)	12527(3)	1604(3)	51(1)
C(17)	8493(4)	10473(3)	769(3)	41(1)
C(18)	7287(4)	10328(3)	71(3)	47(1)
C(19)	9379(4)	11574(3)	222(3)	49(1)
C(20)	9134(4)	10551(3)	2757(3)	39(1)
C(21)	10581(4)	9836(3)	2836(3)	46(1)
C(22)	8486(4)	10312(4)	3774(3)	48(1)
C(23)	10433(3)	5889(3)	5725(3)	35(1)
C(24)	11104(4)	6873(3)	5426(3)	39(1)
C(25)	12710(4)	7053(3)	5660(3)	36(1)
C(26)	13449(4)	8076(3)	5099(3)	37(1)
C(27)	14963(4)	8301(3)	5287(3)	37(1)
C(28)	15746(4)	7478(3)	6060(3)	36(1)
C(29)	17320(4)	7464(3)	6483(3)	38(1)
C(30)	16153(4)	5754(3)	7408(3)	37(1)
C(31)	15038(3)	6455(3)	6619(3)	34(1)
C(32)	13547(3)	6226(3)	6437(3)	34(1)
C(33)	18880(4)	6063(3)	7894(3)	40(1)
C(34)	18800(4)	6313(3)	8788(3)	40(1)
C(35)	17716(4)	5543(3)	9611(3)	43(1)
C(36)	17723(4)	5766(3)	10518(3)	43(1)
C(37)	16799(4)	6777(3)	10428(3)	44(1)
C(38)	16913(4)	7015(3)	11322(3)	49(1)

Table 3. Bond lengths [A] and angles [deg] for compound **3.**

Si(1)-C(13)	1.848(4)
Si(1)-C(17)	1.876(4)
Si(1)-C(20)	1.889(4)
Si(1)-C(14)	1.891(4)
N(1)-C(29)	1.398(5)

N(1)-C(30)	1.400(4)
N(1)-C(33)	1.463(4)
O(1)-C(29)	1.215(4)
O(2)-C(30)	1.206(4)
C(1)-C(2)	1.401(5)
C(1)-C(9)#1	1.419(4)
C(1)-C(12)	1.437(5)
C(2)-C(3)	1.426(4)
C(2)-C(11)	1.445(4)
C(3)-C(4)	1.361(5)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.462(5)
C(4)-C(23)	1.470(4)
C(5)-C(6)	1.380(5)
C(5)-C(10)	1.431(4)
C(6)-C(7)	1.396(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.364(4)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.406(5)
C(8)-H(8A)	0.9500
C(9)-C(1)#1	1.419(4)
C(9)-C(10)	1.429(4)
C(10)-C(11)	1.419(5)
C(11)-C(11)#1	1.405(6)
C(12)-C(13)	1.202(5)
C(14)-C(16)	1.532(5)
C(14)-C(15)	1.533(5)
C(14)-H(14A)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(19)	1.537(5)
C(17)-C(18)	1.551(5)
C(17)-H(17A)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-C(21)	1.523(5)
C(20)-C(22)	1.524(5)
C(20)-H(20A)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.320(5)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.466(4)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.406(5)
C(25)-C(32)	1.406(5)
C(26)-C(27)	1.388(4)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.377(5)
C(27)-H(27A)	0.9500

C(28)-C(31)	1.394(5)
C(28)-C(29)	1.488(5)
C(30)-C(31)	1.494(5)
C(31)-C(32)	1.368(4)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.521(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.531(5)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.519(5)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900
C(36)-C(37)	1.506(5)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(38)	1.516(5)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800

C(13)-Si(1)-C(17)	107.78(16)
C(13)-Si(1)-C(20)	106.31(16)
C(17)-Si(1)-C(20)	110.66(15)
C(13)-Si(1)-C(14)	108.63(15)
C(17)-Si(1)-C(14)	110.74(18)
C(20)-Si(1)-C(14)	112.49(17)
C(29)-N(1)-C(30)	112.0(3)
C(29)-N(1)-C(33)	123.3(3)
C(30)-N(1)-C(33)	124.6(3)
C(2)-C(1)-C(9)#1	121.2(3)
C(2)-C(1)-C(12)	119.7(3)
C(9)#1-C(1)-C(12)	119.1(3)
C(1)-C(2)-C(3)	122.3(3)
C(1)-C(2)-C(11)	119.2(3)
C(3)-C(2)-C(11)	118.5(3)
C(4)-C(3)-C(2)	123.4(3)
C(4)-C(3)-H(3A)	118.3
C(2)-C(3)-H(3A)	118.3
C(3)-C(4)-C(5)	119.1(3)
C(3)-C(4)-C(23)	121.4(3)
C(5)-C(4)-C(23)	119.5(3)
C(6)-C(5)-C(10)	118.3(3)
C(6)-C(5)-C(4)	122.7(3)
C(10)-C(5)-C(4)	119.0(3)
C(5)-C(6)-C(7)	121.5(3)
C(5)-C(6)-H(6A)	119.2
C(7)-C(6)-H(6A)	119.2
C(8)-C(7)-C(6)	120.6(3)
C(8)-C(7)-H(7A)	119.7
C(6)-C(7)-H(7A)	119.7
C(7)-C(8)-C(9)	121.2(3)
C(7)-C(8)-H(8A)	119.4
C(9)-C(8)-H(8A)	119.4
C(8)-C(9)-C(1)#1	122.0(3)
C(8)-C(9)-C(10)	118.2(3)
C(1)#1-C(9)-C(10)	119.8(3)
C(11)-C(10)-C(9)	119.1(3)
C(11)-C(10)-C(5)	120.8(3)
C(9)-C(10)-C(5)	120.1(3)

C(11)#1-C(11)-C(10)	121.1(4)
C(11)#1-C(11)-C(2)	119.7(4)
C(10)-C(11)-C(2)	119.2(3)
C(13)-C(12)-C(1)	177.9(4)
C(12)-C(13)-Si(1)	175.8(3)
C(16)-C(14)-C(15)	110.4(3)
C(16)-C(14)-Si(1)	112.3(2)
C(15)-C(14)-Si(1)	114.0(3)
C(16)-C(14)-H(14A)	106.5
C(15)-C(14)-H(14A)	106.5
Si(1)-C(14)-H(14A)	106.5
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(19)-C(17)-C(18)	109.7(3)
C(19)-C(17)-Si(1)	111.7(3)
C(18)-C(17)-Si(1)	113.2(2)
C(19)-C(17)-H(17A)	107.3
C(18)-C(17)-H(17A)	107.3
Si(1)-C(17)-H(17A)	107.3
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(21)-C(20)-C(22)	110.8(3)
C(21)-C(20)-Si(1)	111.5(3)
C(22)-C(20)-Si(1)	111.8(2)
C(21)-C(20)-H(20A)	107.5
C(22)-C(20)-H(20A)	107.5
Si(1)-C(20)-H(20A)	107.5
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(4)	128.0(3)
C(24)-C(23)-H(23A)	116.0
C(4)-C(23)-H(23A)	116.0
C(23)-C(24)-C(25)	124.9(4)

C(23)-C(24)-H(24A)	117.5
C(25)-C(24)-H(24A)	117.5
C(26)-C(25)-C(32)	118.4(3)
C(26)-C(25)-C(24)	119.8(3)
C(32)-C(25)-C(24)	121.8(3)
C(27)-C(26)-C(25)	122.6(3)
C(27)-C(26)-H(26A)	118.7
C(25)-C(26)-H(26A)	118.7
C(28)-C(27)-C(26)	117.6(3)
C(28)-C(27)-H(27A)	121.2
C(26)-C(27)-H(27A)	121.2
C(27)-C(28)-C(31)	120.7(3)
C(27)-C(28)-C(29)	131.3(3)
C(31)-C(28)-C(29)	108.0(3)
O(1)-C(29)-N(1)	124.9(3)
O(1)-C(29)-C(28)	129.0(4)
N(1)-C(29)-C(28)	106.1(3)
O(2)-C(30)-N(1)	124.8(3)
O(2)-C(30)-C(31)	129.5(3)
N(1)-C(30)-C(31)	105.7(3)
C(32)-C(31)-C(28)	122.1(3)
C(32)-C(31)-C(30)	129.7(3)
C(28)-C(31)-C(30)	108.2(3)
C(31)-C(32)-C(25)	118.6(3)
C(31)-C(32)-H(32A)	120.7
C(25)-C(32)-H(32A)	120.7
N(1)-C(33)-C(34)	113.1(3)
N(1)-C(33)-H(33A)	109.0
C(34)-C(33)-H(33A)	109.0
N(1)-C(33)-H(33B)	109.0
C(34)-C(33)-H(33B)	109.0
H(33A)-C(33)-H(33B)	107.8
C(33)-C(34)-C(35)	114.4(3)
C(33)-C(34)-H(34A)	108.7
C(35)-C(34)-H(34A)	108.7
C(33)-C(34)-H(34B)	108.7
C(35)-C(34)-H(34B)	108.7
H(34A)-C(34)-H(34B)	107.6
C(36)-C(35)-C(34)	113.5(3)
C(36)-C(35)-H(35A)	108.9
C(34)-C(35)-H(35A)	108.9
C(36)-C(35)-H(35B)	108.9
C(34)-C(35)-H(35B)	108.9
H(35A)-C(35)-H(35B)	107.7
C(37)-C(36)-C(35)	115.1(3)
C(37)-C(36)-H(36A)	108.5
C(35)-C(36)-H(36A)	108.5
C(37)-C(36)-H(36B)	108.5
C(35)-C(36)-H(36B)	108.5
H(36A)-C(36)-H(36B)	107.5
C(36)-C(37)-C(38)	113.7(3)
C(36)-C(37)-H(37A)	108.8
C(38)-C(37)-H(37A)	108.8
C(36)-C(37)-H(37B)	108.8
C(38)-C(37)-H(37B)	108.8
H(37A)-C(37)-H(37B)	107.7
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound **3.** The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Si(1)	24(1)	36(1)	50(1)	-18(1)	2(1)	-3(1)
N(1)	20(1)	45(2)	48(2)	-21(2)	1(1)	-3(1)
O(1)	30(1)	47(2)	57(2)	-22(2)	2(1)	-11(1)
O(2)	32(1)	38(2)	53(2)	-17(1)	-2(1)	-2(1)
C(1)	26(2)	31(2)	38(2)	-16(2)	3(1)	-1(1)
C(2)	25(2)	30(2)	36(2)	-13(2)	1(1)	0(1)
C(3)	26(2)	32(2)	38(2)	-14(2)	3(1)	-4(1)
C(4)	25(2)	33(2)	43(2)	-20(2)	1(1)	-1(1)
C(5)	25(2)	36(2)	42(2)	-19(2)	1(1)	-2(1)
C(6)	27(2)	41(2)	42(2)	-19(2)	-2(2)	-3(2)
C(7)	33(2)	33(2)	45(3)	-13(2)	-4(2)	0(1)
C(8)	32(2)	33(2)	44(2)	-16(2)	1(2)	-1(1)
C(9)	25(2)	32(2)	39(2)	-14(2)	2(1)	-2(1)
C(10)	27(2)	33(2)	38(2)	-18(2)	0(1)	-1(1)
C(11)	23(2)	32(2)	37(2)	-16(2)	3(1)	-3(1)
C(12)	27(2)	35(2)	40(2)	-17(2)	-3(1)	1(1)
C(13)	22(2)	40(2)	45(2)	-19(2)	1(1)	0(1)
C(14)	30(2)	45(2)	48(3)	-18(2)	1(2)	-2(2)
C(15)	31(2)	48(2)	73(3)	-26(2)	6(2)	3(2)
C(16)	42(2)	41(2)	66(3)	-21(2)	5(2)	-2(2)
C(17)	28(2)	39(2)	52(3)	-17(2)	0(2)	-1(1)
C(18)	41(2)	48(2)	53(3)	-22(2)	4(2)	-10(2)
C(19)	45(2)	51(3)	50(3)	-22(2)	8(2)	-13(2)
C(20)	30(2)	37(2)	48(3)	-17(2)	3(2)	-6(2)
C(21)	32(2)	53(2)	52(3)	-21(2)	-2(2)	1(2)
C(22)	34(2)	59(3)	51(3)	-25(2)	0(2)	-7(2)
C(23)	24(2)	38(2)	45(2)	-18(2)	0(1)	1(1)
C(24)	27(2)	41(2)	46(3)	-17(2)	-2(2)	-2(2)
C(25)	27(2)	40(2)	45(2)	-22(2)	2(2)	-5(2)
C(26)	28(2)	39(2)	44(2)	-18(2)	-2(2)	0(1)
C(27)	31(2)	39(2)	46(2)	-22(2)	5(2)	-6(2)
C(28)	25(2)	41(2)	44(2)	-21(2)	0(2)	-4(1)
C(29)	24(2)	44(2)	51(3)	-26(2)	1(2)	-4(2)
C(30)	28(2)	38(2)	46(3)	-20(2)	3(2)	0(1)
C(31)	27(2)	38(2)	40(2)	-19(2)	0(1)	-1(1)
C(32)	27(2)	37(2)	41(2)	-19(2)	3(2)	-4(1)
C(33)	24(2)	48(2)	49(3)	-21(2)	-1(2)	2(2)
C(34)	27(2)	46(2)	51(3)	-24(2)	-3(2)	-1(2)
C(35)	32(2)	42(2)	51(3)	-17(2)	-1(2)	-4(2)
C(36)	40(2)	43(2)	44(3)	-18(2)	2(2)	0(2)
C(37)	33(2)	46(2)	51(3)	-20(2)	4(2)	1(2)
C(38)	44(2)	45(2)	55(3)	-19(2)	9(2)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **3.**

	x	y	z	U(eq)
H(3A)	8465	7089	4347	39
H(6A)	9935	3907	7094	44
H(7A)	8813	2173	8032	46
H(8A)	6322	1782	7705	44
H(14A)	5490	11529	1028	50
H(15A)	4211	10230	2462	77
H(15B)	4874	10869	3066	77

H(15C)	3660	11484	2189	77
H(16A)	7319	12797	1136	76
H(16B)	5571	13062	1374	76
H(16C)	6785	12448	2250	76
H(17A)	9278	9853	947	49
H(18A)	6725	9626	423	70
H(18B)	6538	10952	-153	70
H(18C)	7837	10315	-498	70
H(19A)	10140	11662	666	73
H(19B)	9931	11562	-347	73
H(19C)	8632	12199	-3	73
H(20A)	9467	11349	2440	47
H(21A)	10978	10003	2175	70
H(21B)	11392	10000	3209	70
H(21C)	10303	9046	3174	70
H(22A)	7557	10779	3707	72
H(22B)	8197	9524	4117	72
H(22C)	9287	10478	4152	72
H(23A)	11060	5262	6122	43
H(24A)	10500	7512	5029	47
H(26A)	12890	8635	4571	45
H(27A)	15442	8997	4898	45
H(32A)	13087	5523	6828	41
H(33A)	19801	6444	7488	48
H(33B)	19031	5251	8118	48
H(34A)	18437	7092	8574	48
H(34B)	19870	6253	9055	48
H(35A)	16632	5634	9357	52
H(35B)	18041	4759	9803	52
H(36A)	17297	5104	11080	52
H(36B)	18823	5854	10674	52
H(37A)	15683	6669	10318	52
H(37B)	17179	7435	9844	52
H(38A)	16320	7696	11205	73
H(38B)	18015	7114	11442	73
H(38C)	16477	6387	11897	73

Table 6. Torsion angles [deg] for compound **3**.

C(9)#1-C(1)-C(2)-C(3)	-179.9(3)
C(12)-C(1)-C(2)-C(3)	-1.0(5)
C(9)#1-C(1)-C(2)-C(11)	-0.3(5)
C(12)-C(1)-C(2)-C(11)	178.5(3)
C(1)-C(2)-C(3)-C(4)	179.5(3)
C(11)-C(2)-C(3)-C(4)	-0.1(5)
C(2)-C(3)-C(4)-C(5)	0.2(5)
C(2)-C(3)-C(4)-C(23)	178.3(3)
C(3)-C(4)-C(5)-C(6)	179.3(3)
C(23)-C(4)-C(5)-C(6)	1.2(5)
C(3)-C(4)-C(5)-C(10)	-0.6(5)
C(23)-C(4)-C(5)-C(10)	-178.8(3)
C(10)-C(5)-C(6)-C(7)	1.3(5)
C(4)-C(5)-C(6)-C(7)	-178.7(3)
C(5)-C(6)-C(7)-C(8)	-1.6(6)
C(6)-C(7)-C(8)-C(9)	1.0(6)
C(7)-C(8)-C(9)-C(1)#1	179.3(3)
C(7)-C(8)-C(9)-C(10)	0.0(5)
C(8)-C(9)-C(10)-C(11)	178.4(3)
C(1)#1-C(9)-C(10)-C(11)	-0.9(5)
C(8)-C(9)-C(10)-C(5)	-0.4(5)
C(1)#1-C(9)-C(10)-C(5)	-179.6(3)
C(6)-C(5)-C(10)-C(11)	-179.0(3)
C(4)-C(5)-C(10)-C(11)	0.9(5)

C(6)-C(5)-C(10)-C(9)	-0.3(5)
C(4)-C(5)-C(10)-C(9)	179.7(3)
C(9)-C(10)-C(11)-C(11)#1	1.3(6)
C(5)-C(10)-C(11)-C(11)#1	-180.0(4)
C(9)-C(10)-C(11)-C(2)	-179.6(3)
C(5)-C(10)-C(11)-C(2)	-0.8(5)
C(1)-C(2)-C(11)-C(11)#1	-0.1(6)
C(3)-C(2)-C(11)-C(11)#1	179.5(4)
C(1)-C(2)-C(11)-C(10)	-179.2(3)
C(3)-C(2)-C(11)-C(10)	0.4(5)
C(13)-Si(1)-C(14)-C(16)	151.9(3)
C(17)-Si(1)-C(14)-C(16)	-89.9(3)
C(20)-Si(1)-C(14)-C(16)	34.5(3)
C(13)-Si(1)-C(14)-C(15)	25.4(3)
C(17)-Si(1)-C(14)-C(15)	143.6(3)
C(20)-Si(1)-C(14)-C(15)	-92.0(3)
C(13)-Si(1)-C(17)-C(19)	-171.5(2)
C(20)-Si(1)-C(17)-C(19)	-55.7(3)
C(14)-Si(1)-C(17)-C(19)	69.8(3)
C(13)-Si(1)-C(17)-C(18)	64.0(3)
C(20)-Si(1)-C(17)-C(18)	179.8(3)
C(14)-Si(1)-C(17)-C(18)	-54.7(3)
C(13)-Si(1)-C(20)-C(21)	69.4(3)
C(17)-Si(1)-C(20)-C(21)	-47.4(3)
C(14)-Si(1)-C(20)-C(21)	-171.9(2)
C(13)-Si(1)-C(20)-C(22)	-55.3(3)
C(17)-Si(1)-C(20)-C(22)	-172.0(3)
C(14)-Si(1)-C(20)-C(22)	63.5(3)
C(3)-C(4)-C(23)-C(24)	20.3(6)
C(5)-C(4)-C(23)-C(24)	-161.6(4)
C(4)-C(23)-C(24)-C(25)	-179.9(3)
C(23)-C(24)-C(25)-C(26)	162.6(4)
C(23)-C(24)-C(25)-C(32)	-17.5(6)
C(32)-C(25)-C(26)-C(27)	-0.4(6)
C(24)-C(25)-C(26)-C(27)	179.6(3)
C(25)-C(26)-C(27)-C(28)	-0.3(6)
C(26)-C(27)-C(28)-C(31)	0.8(5)
C(26)-C(27)-C(28)-C(29)	-176.7(4)
C(30)-N(1)-C(29)-O(1)	-178.8(3)
C(33)-N(1)-C(29)-O(1)	-1.1(6)
C(30)-N(1)-C(29)-C(28)	1.0(4)
C(33)-N(1)-C(29)-C(28)	178.7(3)
C(27)-C(28)-C(29)-O(1)	-2.6(7)
C(31)-C(28)-C(29)-O(1)	179.6(4)
C(27)-C(28)-C(29)-N(1)	177.6(4)
C(31)-C(28)-C(29)-N(1)	-0.2(4)
C(29)-N(1)-C(30)-O(2)	178.5(4)
C(33)-N(1)-C(30)-O(2)	0.8(6)
C(29)-N(1)-C(30)-C(31)	-1.4(4)
C(33)-N(1)-C(30)-C(31)	-179.1(3)
C(27)-C(28)-C(31)-C(32)	-0.7(6)
C(29)-C(28)-C(31)-C(32)	177.3(3)
C(27)-C(28)-C(31)-C(30)	-178.7(3)
C(29)-C(28)-C(31)-C(30)	-0.7(4)
O(2)-C(30)-C(31)-C(32)	3.6(7)
N(1)-C(30)-C(31)-C(32)	-176.5(4)
O(2)-C(30)-C(31)-C(28)	-178.6(4)
N(1)-C(30)-C(31)-C(28)	1.2(4)
C(28)-C(31)-C(32)-C(25)	0.1(5)
C(30)-C(31)-C(32)-C(25)	177.6(4)
C(26)-C(25)-C(32)-C(31)	0.5(5)
C(24)-C(25)-C(32)-C(31)	-179.5(3)
C(29)-N(1)-C(33)-C(34)	92.5(4)

C(30)-N(1)-C(33)-C(34)	-90.1(4)
N(1)-C(33)-C(34)-C(35)	74.2(4)
C(33)-C(34)-C(35)-C(36)	176.8(3)
C(34)-C(35)-C(36)-C(37)	76.7(4)
C(35)-C(36)-C(37)-C(38)	-176.4(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table 1. Crystal data and structure refinement for compound **4**.

Identification code	s15002
Empirical formula	C52 H56 S2 Si2
Formula weight	801.26
Temperature	100(2) K
Wavelength	0.8857 A [ALS synchrotron beamline 11.3.1]
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.9931(5) A alpha = 90 deg.
	b = 11.3571(4) A beta = 109.323(2) deg.
	c = 15.9701(6) A gamma = 90 deg.
Volume	2223.86(15) A^3
Z, Calculated density	2, 1.197 Mg/m^3
Absorption coefficient	0.373 mm^-1
F(000)	856
Crystal size	0.038 x 0.028 x 0.009 mm
Theta range for data collection	2.799 to 32.358 deg.
Limiting indices	-15<=h<=15, -13<=k<=13, -19<=l<=19
Reflections collected / unique	23319 / 4102 [R(int) = 0.0595]
Completeness to theta = 32.101	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.994 and 0.924
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4102 / 176 / 306
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1194
R indices (all data)	R1 = 0.0871, wR2 = 0.1375
Extinction coefficient	n/a
Largest diff. peak and hole	0.236 and -0.288 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compound **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	8734(1)	1420(1)	8102(1)	50(1)
C(1)	6384(2)	3524(2)	5927(2)	35(1)
C(2)	5983(2)	4588(2)	6124(2)	34(1)
C(3)	6314(2)	5055(2)	7005(2)	36(1)
C(4)	5926(2)	6078(2)	7218(2)	35(1)
C(5)	5147(2)	6772(2)	6525(2)	36(1)
C(6)	4764(2)	7866(2)	6681(2)	43(1)
C(7)	4020(2)	8497(2)	5997(2)	47(1)
C(8)	3627(2)	8051(2)	5156(2)	43(1)
C(9)	3987(2)	6945(2)	4952(2)	36(1)
C(10)	4770(2)	6302(2)	5638(2)	33(1)
C(11)	5183(2)	5225(2)	5436(1)	33(1)
C(12)	7148(2)	2854(2)	6621(2)	40(1)
C(13)	7772(2)	2273(2)	7204(2)	45(1)
C(14)	8135(2)	-82(2)	8098(2)	48(1)
C(15)	7170(3)	-69(3)	8449(3)	77(1)
C(16)	7774(4)	-680(3)	7185(2)	90(1)
C(17)	9943(9)	1285(13)	7658(9)	64(2)
C(18)	10781(11)	302(12)	8177(9)	85(3)
C(19)	9676(8)	886(10)	6715(7)	84(2)
C(17')	10166(7)	1683(10)	8090(7)	64(2)
C(18')	11050(16)	743(16)	8473(10)	85(3)
C(19')	10116(9)	1599(11)	7121(7)	84(2)
C(17")	10032(12)	1180(20)	7810(13)	64(2)
C(18")	10923(19)	830(20)	8731(13)	85(3)
C(19")	10510(12)	2337(14)	7679(12)	84(2)
C(20)	8800(30)	2186(14)	9157(10)	77(2)

C(21)	9056(13)	3510(10)	9236(9)	76(3)
C(22)	9440(30)	1600(20)	10041(19)	130(10)
C(20')	8920(40)	2330(20)	9126(16)	77(2)
C(21')	9424(18)	3522(18)	9003(15)	76(3)
C(22')	9740(60)	1700(40)	9910(30)	130(10)
C(23)	6256(18)	6460(70)	8161(10)	37(1)
C(24)	5667(9)	6764(14)	8655(9)	48(1)
C(25)	6259(9)	6910(20)	9584(7)	53(2)
C(26)	7334(10)	6781(16)	9745(7)	52(2)
S(1)	7629(1)	6431(2)	8789(1)	47(1)
C(23')	6320(30)	6450(140)	8160(20)	37(1)
C(24')	7335(12)	6390(20)	8713(11)	47(1)
C(25')	7450(20)	6600(30)	9625(15)	52(2)
C(26')	6479(19)	6860(50)	9707(15)	53(2)
S(1')	5420(4)	6761(7)	8722(4)	48(1)

Table 3. Bond lengths [A] and angles [deg] for compound **4**.

Si(1)-C(13)	1.836(3)
Si(1)-C(20)	1.874(9)
Si(1)-C(14)	1.875(3)
Si(1)-C(20')	1.883(13)
Si(1)-C(17')	1.890(9)
Si(1)-C(17")	1.912(13)
Si(1)-C(17)	1.931(10)
C(1)-C(2)	1.392(3)
C(1)-C(9)#1	1.428(3)
C(1)-C(12)	1.437(3)
C(2)-C(3)	1.430(3)
C(2)-C(11)	1.434(3)
C(3)-C(4)	1.354(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.460(3)
C(4)-C(23')	1.48(3)
C(4)-C(23)	1.486(14)
C(5)-C(6)	1.391(3)
C(5)-C(10)	1.440(3)
C(6)-C(7)	1.394(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.366(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.415(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.426(3)
C(9)-C(1)#1	1.428(3)
C(10)-C(11)	1.415(3)
C(11)-C(11)#1	1.410(4)
C(12)-C(13)	1.208(3)
C(14)-C(15)	1.533(4)
C(14)-C(16)	1.535(4)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(19)	1.499(13)
C(17)-C(18)	1.588(11)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800

C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(17')-C(19')	1.531(12)
C(17')-C(18')	1.539(11)
C(17')-H(17')	1.0000
C(18')-H(18D)	0.9800
C(18')-H(18E)	0.9800
C(18')-H(18F)	0.9800
C(19')-H(19D)	0.9800
C(19')-H(19E)	0.9800
C(19')-H(19F)	0.9800
C(17")-C(19")	1.500(15)
C(17")-C(18")	1.591(14)
C(17")-H(17")	1.0000
C(18")-H(18G)	0.9800
C(18")-H(18H)	0.9800
C(18")-H(18I)	0.9800
C(19")-H(19G)	0.9800
C(19")-H(19H)	0.9800
C(19")-H(19I)	0.9800
C(20)-C(22)	1.533(10)
C(20)-C(21)	1.536(9)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(20')-C(22')	1.530(14)
C(20')-C(21')	1.542(14)
C(20')-H(20')	1.0000
C(21')-H(21D)	0.9800
C(21')-H(21E)	0.9800
C(21')-H(21F)	0.9800
C(22')-H(22D)	0.9800
C(22')-H(22E)	0.9800
C(22')-H(22F)	0.9800
C(23)-C(24)	1.31(2)
C(23)-S(1)	1.733(19)
C(24)-C(25)	1.438(15)
C(24)-H(24)	0.9500
C(25)-C(26)	1.341(8)
C(25)-H(25)	0.9500
C(26)-S(1)	1.739(8)
C(26)-H(26)	0.9500
C(23')-C(24')	1.32(3)
C(23')-S(1')	1.74(3)
C(24')-C(25')	1.43(2)
C(24')-H(24')	0.9500
C(25')-C(26')	1.344(14)
C(25')-H(25')	0.9500
C(26')-S(1')	1.717(19)
C(26')-H(26')	0.9500

C(13)-Si(1)-C(20)	105.8(9)
C(13)-Si(1)-C(14)	107.63(13)
C(20)-Si(1)-C(14)	108.6(5)
C(13)-Si(1)-C(20')	104.2(14)
C(14)-Si(1)-C(20')	115.9(8)
C(13)-Si(1)-C(17')	109.1(3)

C(14)-Si(1)-C(17')	123.5(3)
C(20')-Si(1)-C(17')	94.5(14)
C(13)-Si(1)-C(17")	108.3(5)
C(14)-Si(1)-C(17")	105.5(7)
C(13)-Si(1)-C(17)	100.5(4)
C(20)-Si(1)-C(17)	124.6(10)
C(14)-Si(1)-C(17)	108.3(4)
C(2)-C(1)-C(9)#1	121.1(2)
C(2)-C(1)-C(12)	120.0(2)
C(9)#1-C(1)-C(12)	118.8(2)
C(1)-C(2)-C(3)	122.1(2)
C(1)-C(2)-C(11)	119.7(2)
C(3)-C(2)-C(11)	118.2(2)
C(4)-C(3)-C(2)	123.4(2)
C(4)-C(3)-H(3)	118.3
C(2)-C(3)-H(3)	118.3
C(3)-C(4)-C(5)	119.7(2)
C(3)-C(4)-C(23')	118(5)
C(5)-C(4)-C(23')	123(5)
C(3)-C(4)-C(23)	120(2)
C(5)-C(4)-C(23)	120(2)
C(6)-C(5)-C(10)	118.8(2)
C(6)-C(5)-C(4)	123.1(2)
C(10)-C(5)-C(4)	118.1(2)
C(5)-C(6)-C(7)	121.0(2)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(8)-C(7)-C(6)	121.1(2)
C(8)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
C(7)-C(8)-C(9)	120.8(2)
C(7)-C(8)-H(8)	119.6
C(9)-C(8)-H(8)	119.6
C(8)-C(9)-C(10)	118.9(2)
C(8)-C(9)-C(1)#1	121.9(2)
C(10)-C(9)-C(1)#1	119.1(2)
C(11)-C(10)-C(9)	119.7(2)
C(11)-C(10)-C(5)	120.9(2)
C(9)-C(10)-C(5)	119.3(2)
C(11)#1-C(11)-C(10)	120.6(3)
C(11)#1-C(11)-C(2)	119.7(3)
C(10)-C(11)-C(2)	119.7(2)
C(13)-C(12)-C(1)	178.5(3)
C(12)-C(13)-Si(1)	178.8(3)
C(15)-C(14)-C(16)	108.8(3)
C(15)-C(14)-Si(1)	112.3(2)
C(16)-C(14)-Si(1)	113.7(2)
C(15)-C(14)-H(14)	107.3
C(16)-C(14)-H(14)	107.3
Si(1)-C(14)-H(14)	107.3
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(19)-C(17)-C(18)	101.7(9)

C(19)-C(17)-Si(1)	116.5(8)
C(18)-C(17)-Si(1)	111.4(9)
C(19)-C(17)-H(17)	108.9
C(18)-C(17)-H(17)	108.9
Si(1)-C(17)-H(17)	108.9
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(19')-C(17')-C(18')	97.7(9)
C(19')-C(17')-Si(1)	106.8(7)
C(18')-C(17')-Si(1)	119.6(11)
C(19')-C(17')-H(17')	110.6
C(18')-C(17')-H(17')	110.6
Si(1)-C(17')-H(17')	110.6
C(17')-C(18')-H(18D)	109.5
C(17')-C(18')-H(18E)	109.5
H(18D)-C(18')-H(18E)	109.5
C(17')-C(18')-H(18F)	109.5
H(18D)-C(18')-H(18F)	109.5
H(18E)-C(18')-H(18F)	109.5
C(17')-C(19')-H(19D)	109.5
C(17')-C(19')-H(19E)	109.5
H(19D)-C(19')-H(19E)	109.5
C(17')-C(19')-H(19F)	109.5
H(19D)-C(19')-H(19F)	109.5
H(19E)-C(19')-H(19F)	109.5
C(19")-C(17")-C(18")	97.9(15)
C(19")-C(17")-Si(1)	110.3(12)
C(18")-C(17")-Si(1)	104.0(12)
C(19")-C(17")-H(17")	114.4
C(18")-C(17")-H(17")	114.4
Si(1)-C(17")-H(17")	114.4
C(17")-C(18")-H(18G)	109.5
C(17")-C(18")-H(18H)	109.5
H(18G)-C(18")-H(18H)	109.5
C(17")-C(18")-H(18I)	109.5
H(18G)-C(18")-H(18I)	109.5
H(18H)-C(18")-H(18I)	109.5
C(17")-C(19")-H(19G)	109.5
C(17")-C(19")-H(19H)	109.5
H(19G)-C(19")-H(19H)	109.5
C(17")-C(19")-H(19I)	109.5
H(19G)-C(19")-H(19I)	109.5
H(19H)-C(19")-H(19I)	109.5
C(22)-C(20)-C(21)	108.0(11)
C(22)-C(20)-Si(1)	118.5(19)
C(21)-C(20)-Si(1)	118.1(10)
C(22)-C(20)-H(20)	103.3
C(21)-C(20)-H(20)	103.3
Si(1)-C(20)-H(20)	103.3
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5

H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(22')-C(20')-C(21')	107.6(17)
C(22')-C(20')-Si(1)	108(3)
C(21')-C(20')-Si(1)	108.0(15)
C(22')-C(20')-H(20')	111.1
C(21')-C(20')-H(20')	111.1
Si(1)-C(20')-H(20')	111.1
C(20')-C(21')-H(21D)	109.5
C(20')-C(21')-H(21E)	109.5
H(21D)-C(21')-H(21E)	109.5
C(20')-C(21')-H(21F)	109.5
H(21D)-C(21')-H(21F)	109.5
H(21E)-C(21')-H(21F)	109.5
C(20')-C(22')-H(22D)	109.5
C(20')-C(22')-H(22E)	109.5
H(22D)-C(22')-H(22E)	109.5
C(20')-C(22')-H(22F)	109.5
H(22D)-C(22')-H(22F)	109.5
H(22E)-C(22')-H(22F)	109.5
C(24)-C(23)-C(4)	130.8(16)
C(24)-C(23)-S(1)	110.5(8)
C(4)-C(23)-S(1)	118.5(12)
C(23)-C(24)-C(25)	115.5(12)
C(23)-C(24)-H(24)	122.2
C(25)-C(24)-H(24)	122.2
C(26)-C(25)-C(24)	110.6(12)
C(26)-C(25)-H(25)	124.7
C(24)-C(25)-H(25)	124.7
C(25)-C(26)-S(1)	112(1)
C(25)-C(26)-H(26)	124.0
S(1)-C(26)-H(26)	124.0
C(23)-S(1)-C(26)	91.1(6)
C(24')-C(23')-C(4)	127(3)
C(24')-C(23')-S(1')	110.9(12)
C(4)-C(23')-S(1')	121(3)
C(23')-C(24')-C(25')	114.7(18)
C(23')-C(24')-H(24')	122.7
C(25')-C(24')-H(24')	122.7
C(26')-C(25')-C(24')	111(2)
C(26')-C(25')-H(25')	124.7
C(24')-C(25')-H(25')	124.7
C(25')-C(26')-S(1')	113(2)
C(25')-C(26')-H(26')	123.6
S(1')-C(26')-H(26')	123.6
C(26')-S(1')-C(23')	90.8(12)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for compound **4.**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Si(1)	42(1)	52(1)	48(1)	19(1)	4(1)	11(1)

C(1)	39(1)	35(1)	31(1)	9(1)	11(1)	6(1)
C(2)	36(1)	35(1)	30(1)	8(1)	10(1)	3(1)
C(3)	36(1)	40(1)	30(1)	7(1)	10(1)	3(1)
C(4)	37(1)	38(1)	30(1)	5(1)	9(1)	-2(1)
C(5)	40(1)	36(1)	33(1)	5(1)	12(1)	2(1)
C(6)	53(2)	39(2)	36(1)	-1(1)	13(1)	2(1)
C(7)	58(2)	37(2)	44(2)	3(1)	16(1)	15(1)
C(8)	51(2)	42(2)	35(1)	9(1)	12(1)	14(1)
C(9)	41(1)	36(1)	33(1)	8(1)	13(1)	5(1)
C(10)	36(1)	35(1)	28(1)	5(1)	10(1)	2(1)
C(11)	38(1)	32(1)	29(1)	6(1)	12(1)	2(1)
C(12)	42(2)	41(2)	36(1)	4(1)	13(1)	6(1)
C(13)	46(2)	46(2)	41(2)	12(1)	12(1)	9(1)
C(14)	50(2)	49(2)	42(2)	12(1)	10(1)	17(1)
C(15)	78(2)	59(2)	108(3)	16(2)	51(2)	9(2)
C(16)	126(3)	78(3)	55(2)	-7(2)	15(2)	-1(2)
C(17)	39(3)	51(4)	93(6)	18(3)	8(4)	1(3)
C(18)	40(5)	95(7)	115(8)	10(6)	20(4)	20(4)
C(19)	64(5)	91(6)	107(6)	2(4)	41(4)	3(4)
C(17')	39(3)	51(4)	93(6)	18(3)	8(4)	1(3)
C(18')	40(5)	95(7)	115(8)	10(6)	20(4)	20(4)
C(19')	64(5)	91(6)	107(6)	2(4)	41(4)	3(4)
C(17")	39(3)	51(4)	93(6)	18(3)	8(4)	1(3)
C(18")	40(5)	95(7)	115(8)	10(6)	20(4)	20(4)
C(19")	64(5)	91(6)	107(6)	2(4)	41(4)	3(4)
C(20)	103(6)	50(4)	47(2)	8(3)	-16(2)	5(3)
C(21)	73(8)	54(2)	77(6)	1(4)	-9(4)	12(5)
C(22)	220(20)	66(4)	51(8)	6(3)	-27(9)	31(8)
C(20')	103(6)	50(4)	47(2)	8(3)	-16(2)	5(3)
C(21')	73(8)	54(2)	77(6)	1(4)	-9(4)	12(5)
C(22')	220(20)	66(4)	51(8)	6(3)	-27(9)	31(8)
C(23)	41(3)	36(2)	30(1)	3(1)	8(1)	1(4)
C(24)	50(3)	60(1)	35(1)	-3(1)	13(1)	6(2)
C(25)	52(5)	65(3)	36(3)	-11(4)	9(3)	2(5)
C(26)	54(3)	67(6)	28(3)	-9(3)	7(2)	0(3)
S(1)	40(1)	60(1)	35(1)	-1(1)	4(1)	-1(1)
C(23')	41(3)	36(2)	30(1)	3(1)	8(1)	1(4)
C(24')	40(1)	60(1)	35(1)	-1(1)	4(1)	-1(1)
C(25')	54(3)	67(6)	28(3)	-9(3)	7(2)	0(3)
C(26')	52(5)	65(3)	36(3)	-11(4)	9(3)	2(5)
S(1')	50(3)	60(1)	35(1)	-3(1)	13(1)	6(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for compound **4.**

	x	y	z	U(eq)
H(3)	6832	4625	7465	43
H(6)	5014	8188	7263	52
H(7)	3782	9249	6118	56
H(8)	3108	8488	4703	52
H(14)	8716	-586	8509	58
H(15A)	6581	415	8058	115
H(15B)	7405	261	9049	115
H(15C)	6906	-875	8462	115
H(16A)	7497	-1470	7234	135
H(16B)	8398	-740	6971	135
H(16C)	7198	-212	6765	135
H(17)	10330	2059	7732	77
H(18A)	11021	470	8815	127
H(18B)	10426	-470	8064	127
H(18C)	11414	301	7973	127

H(19A)	9154	1434	6321	126
H(19B)	10344	867	6558	126
H(19C)	9356	96	6649	126
H(17')	10433	2476	8339	77
H(18D)	11195	672	9113	127
H(18E)	10797	-16	8187	127
H(18F)	11720	975	8363	127
H(19D)	9574	2157	6761	126
H(19E)	10834	1788	7079	126
H(19F)	9910	797	6902	126
H(17")	9952	596	7322	77
H(18G)	10736	67	8927	127
H(18H)	11641	781	8657	127
H(18I)	10940	1431	9176	127
H(19G)	10051	2693	7122	126
H(19H)	10546	2863	8174	126
H(19I)	11246	2212	7655	126
H(20)	8027	2152	9153	92
H(21A)	8927	3826	9763	114
H(21B)	8585	3916	8706	114
H(21C)	9822	3631	9288	114
H(22A)	10204	1508	10075	196
H(22B)	9126	831	10081	196
H(22C)	9407	2101	10533	196
H(20')	8210	2449	9232	92
H(21D)	9523	4015	9528	114
H(21E)	8938	3921	8477	114
H(21F)	10133	3385	8928	114
H(22D)	10424	1577	9780	196
H(22E)	9446	935	9999	196
H(22F)	9890	2178	10445	196
H(24)	4901	6880	8413	58
H(25)	5934	7071	10024	63
H(26)	7870	6873	10313	62
H(24')	7940	6222	8522	56
H(25')	8117	6553	10104	62
H(26')	6389	7081	10253	63

Table 6. Torsion angles [deg] for compound **4**.

C(9)#1-C(1)-C(2)-C(3)	177.8(2)
C(12)-C(1)-C(2)-C(3)	0.5(4)
C(9)#1-C(1)-C(2)-C(11)	0.1(4)
C(12)-C(1)-C(2)-C(11)	-177.2(2)
C(1)-C(2)-C(3)-C(4)	-179.0(2)
C(11)-C(2)-C(3)-C(4)	-1.3(4)
C(2)-C(3)-C(4)-C(5)	-1.4(4)
C(2)-C(3)-C(4)-C(23')	179(5)
C(2)-C(3)-C(4)-C(23)	176(2)
C(3)-C(4)-C(5)-C(6)	-175.8(2)
C(23')-C(4)-C(5)-C(6)	4(5)
C(23)-C(4)-C(5)-C(6)	7(3)
C(3)-C(4)-C(5)-C(10)	3.5(4)
C(23')-C(4)-C(5)-C(10)	-177(5)
C(23)-C(4)-C(5)-C(10)	-174(3)
C(10)-C(5)-C(6)-C(7)	0.7(4)
C(4)-C(5)-C(6)-C(7)	-180.0(2)
C(5)-C(6)-C(7)-C(8)	1.2(4)
C(6)-C(7)-C(8)-C(9)	-1.5(4)
C(7)-C(8)-C(9)-C(10)	-0.2(4)
C(7)-C(8)-C(9)-C(1)#1	-178.0(3)
C(8)-C(9)-C(10)-C(11)	-176.6(2)

C(1)#1-C(9)-C(10)-C(11)	1.2(3)
C(8)-C(9)-C(10)-C(5)	2.1(4)
C(1)#1-C(9)-C(10)-C(5)	179.9(2)
C(6)-C(5)-C(10)-C(11)	176.3(2)
C(4)-C(5)-C(10)-C(11)	-3.0(3)
C(6)-C(5)-C(10)-C(9)	-2.4(4)
C(4)-C(5)-C(10)-C(9)	178.3(2)
C(9)-C(10)-C(11)-C(11)#1	-0.7(4)
C(5)-C(10)-C(11)-C(11)#1	-179.4(3)
C(9)-C(10)-C(11)-C(2)	179.1(2)
C(5)-C(10)-C(11)-C(2)	0.4(3)
C(1)-C(2)-C(11)-C(11)#1	-0.6(4)
C(3)-C(2)-C(11)-C(11)#1	-178.4(3)
C(1)-C(2)-C(11)-C(10)	179.6(2)
C(3)-C(2)-C(11)-C(10)	1.8(3)
C(13)-Si(1)-C(14)-C(15)	-72.6(2)
C(20)-Si(1)-C(14)-C(15)	41.5(10)
C(20')-Si(1)-C(14)-C(15)	43.5(17)
C(17')-Si(1)-C(14)-C(15)	158.8(4)
C(17")-Si(1)-C(14)-C(15)	171.9(6)
C(17)-Si(1)-C(14)-C(15)	179.5(4)
C(13)-Si(1)-C(14)-C(16)	51.4(3)
C(20)-Si(1)-C(14)-C(16)	165.6(10)
C(20')-Si(1)-C(14)-C(16)	167.6(17)
C(17')-Si(1)-C(14)-C(16)	-77.2(5)
C(17")-Si(1)-C(14)-C(16)	-64.1(6)
C(17)-Si(1)-C(14)-C(16)	-56.5(5)
C(13)-Si(1)-C(17')-C(19')	-44.9(8)
C(14)-Si(1)-C(17')-C(19')	83.0(8)
C(20')-Si(1)-C(17')-C(19')	-151.7(13)
C(13)-Si(1)-C(17')-C(18')	-154.4(9)
C(14)-Si(1)-C(17')-C(18')	-26.5(11)
C(20')-Si(1)-C(17')-C(18')	98.8(15)
C(13)-Si(1)-C(20)-C(22)	173.3(14)
C(14)-Si(1)-C(20)-C(22)	57.9(15)
C(17)-Si(1)-C(20)-C(22)	-71.5(16)
C(13)-Si(1)-C(20)-C(21)	-53(2)
C(14)-Si(1)-C(20)-C(21)	-168.7(16)
C(17)-Si(1)-C(20)-C(21)	62(2)
C(13)-Si(1)-C(20')-C(22')	-178(2)
C(14)-Si(1)-C(20')-C(22')	64(2)
C(17')-Si(1)-C(20')-C(22')	-67(2)
C(13)-Si(1)-C(20')-C(21')	-62(3)
C(14)-Si(1)-C(20')-C(21')	179.6(18)
C(17')-Si(1)-C(20')-C(21')	49(3)
C(3)-C(4)-C(23)-C(24)	-126(6)
C(5)-C(4)-C(23)-C(24)	51(9)
C(3)-C(4)-C(23)-S(1)	48(6)
C(5)-C(4)-C(23)-S(1)	-134(4)
C(4)-C(23)-C(24)-C(25)	171(6)
S(1)-C(23)-C(24)-C(25)	-5(6)
C(23)-C(24)-C(25)-C(26)	5(5)
C(24)-C(25)-C(26)-S(1)	-2(2)
C(24)-C(23)-S(1)-C(26)	3(5)
C(4)-C(23)-S(1)-C(26)	-173(5)
C(25)-C(26)-S(1)-C(23)	0(3)
C(3)-C(4)-C(23')-C(24')	42(15)
C(5)-C(4)-C(23')-C(24')	-138(11)
C(3)-C(4)-C(23')-S(1')	-125(8)
C(5)-C(4)-C(23')-S(1')	55(12)
C(4)-C(23')-C(24')-C(25')	-169(10)
S(1')-C(23')-C(24')-C(25')	0(12)
C(23')-C(24')-C(25')-C(26')	-3(9)

C(24')-C(25')-C(26')-S(1')	4(5)
C(25')-C(26')-S(1')-C(23')	-4(6)
C(24')-C(23')-S(1')-C(26')	2(10)
C(4)-C(23')-S(1')-C(26')	172(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1