Supporting Information for

Diacenaphthylene-Fused Benzo[1,2-b:4,5-b']dithiophenes: Polycyclic Heteroacenes Containing Full-Carbon Five-Membered Aromatic Rings

Experimental Section

Synthesis of Compound M1

M1. 1,8-Dibromonaphthalene (171.5 mg, 0.6 mmol), potassiumcarbonate (276 mg, 2 mmol), benzo[b]thiophene (67.1 mg, 0.5 mmol), $Pd(OAc)_2$ (5 mg, 0.02 mmol) and di-*t*-butylmethylphosphoniumtetrafluoroborate (10 mg, 0.04 mmol) were added in a 100mL three-necked flask. The flask was flushed with nitrogen 3 times. Then, degassed DMA (20 mL) was added. The mixture was heated to100 °C for 20 h. After cooling to room temperature, the reaction was quenched with water. The organic product was extracted with dichloromethane (3×40 mL). The combined organic layers were washed with water (3×40 mL) and then dried over anhydrous $MgSO_4$. After removing solvent under vacuum, the residue was purified by column chromatography on silica gel (hexane as eluent) to give **M1** as yellow solid**.** ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 6.9 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.85 – 7.71 (m, 3H), 7.58 (dd, *J* = 14.2, 7.2 Hz, 2H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.55, 141.92, 138.99, 134.23, 134.10, 133.61, 133.44, 133.32, 129.06, 127.78, 127.71, 126.33, 125.13, 124.01, 121.97, 121.15. EI-MS: *m*/*z* 258 $[M]^+$. HRMS (EI): calcd. for $C_{18}H_{10}S$ $[M]^+$: 258.0503; found: 258.0510. Anal. calcd. for $C_{18}H_{10}S$: C, 83.69; H, 3.90; Found: C, 83.45; H, 3.90.

Syntheses of Compounds M2-M5

Compounds **M2-M5** were synthesized by the same procedure as compound **M1**.

M2. Yield: 55.5%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 6.9 Hz, 1H), 7.86 – 7.72 (m, 3H), 7.59 (dt, *J* = 22.4, 7.4 Hz, 2H), 4.36 (t, *J* = 6.8 Hz, 2H), 2.17 – 1.99 (m,

2H), 1.71 – 1.59 (m, 2H), 1.50 – 1.21 (m, 8H), 0.91 (t, *J* = 6.8 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 145.13, 141.53, 137.40, 136.27, 134.10, 133.22, 128.96, 128.10, 127.78, 127.46, 126.37, 126.07, 123.98, 121.69, 74.76, 31.86, 30.61, 29.56, 29.43, 26.09, 22.69, 14.13.MS (MALDI-TOF) *m/z*: 694.3[M]+. HRMS (MALDI) *m/z*: calcd for $C_{46}H_{46}O_2S_2$[M]$^+$: 694.2934; found: 694.2938. Anal. calcd. for $C_{46}H_{46}O_2S_2$: C, 79.50; H, 6.67; Found: C,79.27; H,6.71.

M3. Yield: 71.9 %. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 6.6 Hz, 2H), 7.83 (d, *J* = 7.1 Hz, 4H), 7.77 (d, *J* = 8.2 Hz, 2H), 7.60 (m, *J* = 13.8, 7.0 Hz, 4H), 4.20 (d, *J* = 6.9 Hz, 4H), 2.26 (m, *J* = 12.5, 6.3 Hz, 2H), 1.92 – 1.56 (m, 8H), 1.41 (d, *J* = 6.5 Hz, 8H), 1.05 (t, *J* = 7.4 Hz, 6H), 0.93 (t, *J* = 6.5 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.46, 141.62, 137.32, 136.45, 134.04, 133.23, 128.97, 128.04, 127.80, 127.47, 126.42, 126.08, 124.08, 121.76, 78.46, 40.78, 30.29, 29.05, 23.78, 23.16, 14.11, 11.26. MS (MALDI-TOF) *m/z*: 694.3[M]$^+$. HRMS (MALDI) *m/z*: calcd for $C_{46}H_{46}O_2S_2$ [M]$^+$: 694.2934, found: 694.2934. Anal. Calcd. for $C_{46}H_{46}O_2S_2$: C, 79.50; H, 6.67; Found: C, 79.70; H, 6.88.

M4. Yield: 25.8 %. ^{1}H NMR (400 MHz, $CD_2Cl_2CD_2Cl_2$) δ 8.00 (d, *J* = 7.1 Hz, 2H), 7.80 – 7.73 (m, 4H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.53 (dd, *J* = 15.1, 7.5 Hz, 4H), 3.71 – 3.44 (m, 4H), 1.98 (s, 4H), 1.71 – 1.55 (m, 4H), 1.23 (d, *J* = 24.0 Hz, 28H), 0.79 (d, *J* = 7.0 Hz, 6H). Due to the poor solubility, ^{13}C NMR cannot be acquired, MS (MALDI-TOF) *m/z*: 746.4[M]$^+$. HRMS (MALDI) *m/z*: calcd for $C_{52}H_{58}S_2$ [M]$^+$: 746.3974, found: 746.3972. Anal. Calcd. for $C_{52}H_{58}S_2$: C, 83.59; H, 7.82; Found: C, 83.27; H, 7.79.

M5. Yield: 90%. MS (MALDI-TOF) *m/z*: 467.9 (M$^+$). HRMS (MALDI) *m/z*: calcd for $C_{30}H_{13}O_2S_2$ [M + H]$^+$: 469.0351, found: 469.0344

Synthesis of Compound M6

A dry 100 mL three-neck flask was flushed with nitrogen, 5-ethynyl-1,3-di(*t*-butyl)benzene(0.64 g, 3 mmol) in dry THF (25 mL) was added and cooled to -78 ℃. *n*-BuLi (3 mmol, 2.5 M in THF) was added slowly, the reaction solution was retained at -78 °C for 1h. The reaction mixture was warmed to room temperature and stirred

for another 1h. Compounds **M5** (0.468 g, 1 mmol) was added quickly, and the mixture was stirred overnight. Stannous chloride Dihydrate (0.68 g, 3mmol) in 10% HCl (2 mL) was added. The reaction mixture was stirred for 2 h at 50 °C and was extracted with dichloromethane. The organic layer was washed with saturated brine solution, dried over anhydrous $MgSO_4$ and filtered. Dichloromethane was removed and the crude products were purified by column chromatography on silica gel (CH_2Cl_2 / hexane = 1:2), affording **M6** as red solid (190 mg, 22.1%). ^{1}H NMR (400 MHz, $C_2D_2Cl_4$) δ 9.02 (d, 2H), 7.86 (s, 2H), 7.81 (d, 2H), 7.72 (d, 2H), 7.67 (s,2H), 7.60 – 7.44 (m, 6H), 1.34 (s, 36H). Due to the poor solubility, ^{13}C NMR cannot be acquired. MS (MALDI-TOF) *m/z*: 862.4[M]$^+$. HRMS (MALDI) *m/z*: calcd for $C_{62}H_{54}S_2$ [M]$^+$: 862.3661, found: 862.3671.

Spectroelectrochemical Studies

The UV-vis spectroelectrochemical study was conducted at room temperature (293 K) in argon-saturated dichloromethane freshly distilled from CaH_2 and containing 10^{-1} M Bu_4NPF_6 (TBAH) recrystallized twice from absolute ethanol and dried overnight under vacuum at 353 K. The concentration of **M4** was close to saturation of the electrolyte used. The solution was filtered prior filling the spectroelectrochemical cell. For the10^{-5} M solution the absorbance changes upon oxidation were not perceptible.

The UV-vis absorption spectra were recorded with a Scinco S3100 diode array UV-vis spectrophotometer operating in the 'fast' mode. The potential control during the electrolyses within an OTTLE cell [1] was achieved with an EmStat3 potentiostat (PalmSense, the Netherlands). A thin-layer cyclic voltammogram was recoderd at v= 2 mVs^{-1} in the course of each spectroelectrochemical monitoring for comparative purposes. Each forward anodic or cathodic step was followed by the corresponding reverse reduction or reoxidation, respectively, to probe the chemical stability of the redox products, especially for the steps localized near the potential window limits of the organic electrolyte.

Transistor fabrication and characterization

The micro-sized transistor was a bottom-gate top-contact structure. n-Doped Si was used as the gate electrode and 300 nm SiO_2 was the dielectric layer. The OTS

modification was done according to the previously reported procedure.[2] The Au source and drain electrodes were fabricated through the "Au stripe mask". [2] The channel width (W) and length (L) of the devices were measured through optical microscope and AFM images. The transistors were characterized in air by using a Keithley 4200-SCS semiconductor analyzer and the mobility was calculated from saturation region.

References

[1] M. Krejčík, M. Daněk and F. Hartl, *J. Electroanal .Chem. Interfacial Electrochem.* **1991**, 317, 179

[2] M. Wang, J. Li, G. Zhao, Q. Wu, Y. Huang, W. Hu, X. Gao, H. Li, D. Zhu, *Adv. Mater.* **2013,** *25*, 2229

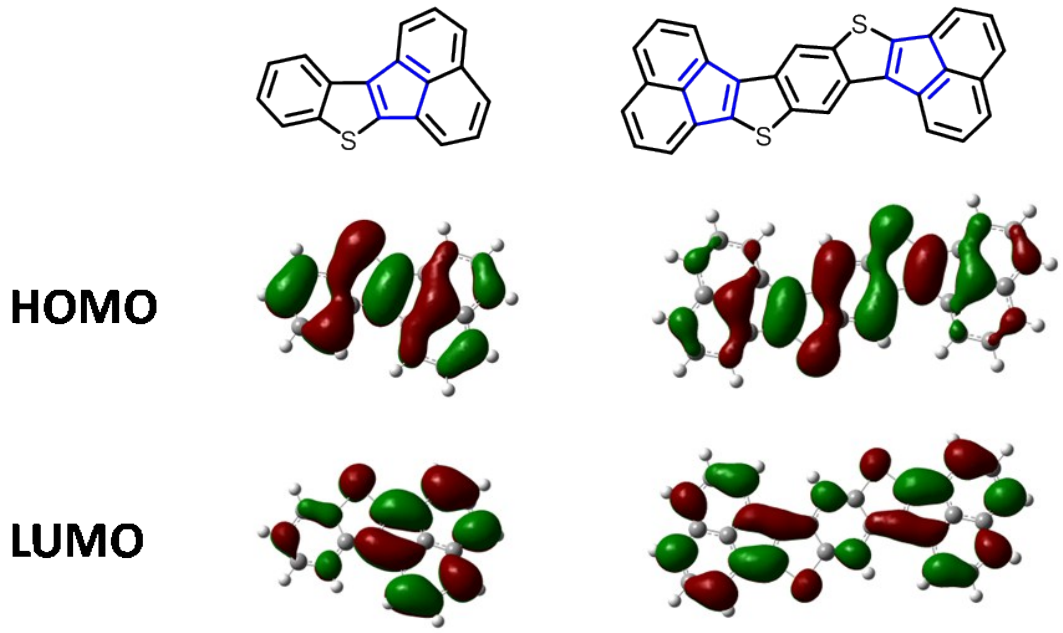

Figure S1. Frontier molecular orbitals of the unsubstituted CF-PAC models of **M1** (left) and **M2**-**M4** (right) calculated with Gaussian 09 package at B3LYP/6-31G(d,p) level of theory

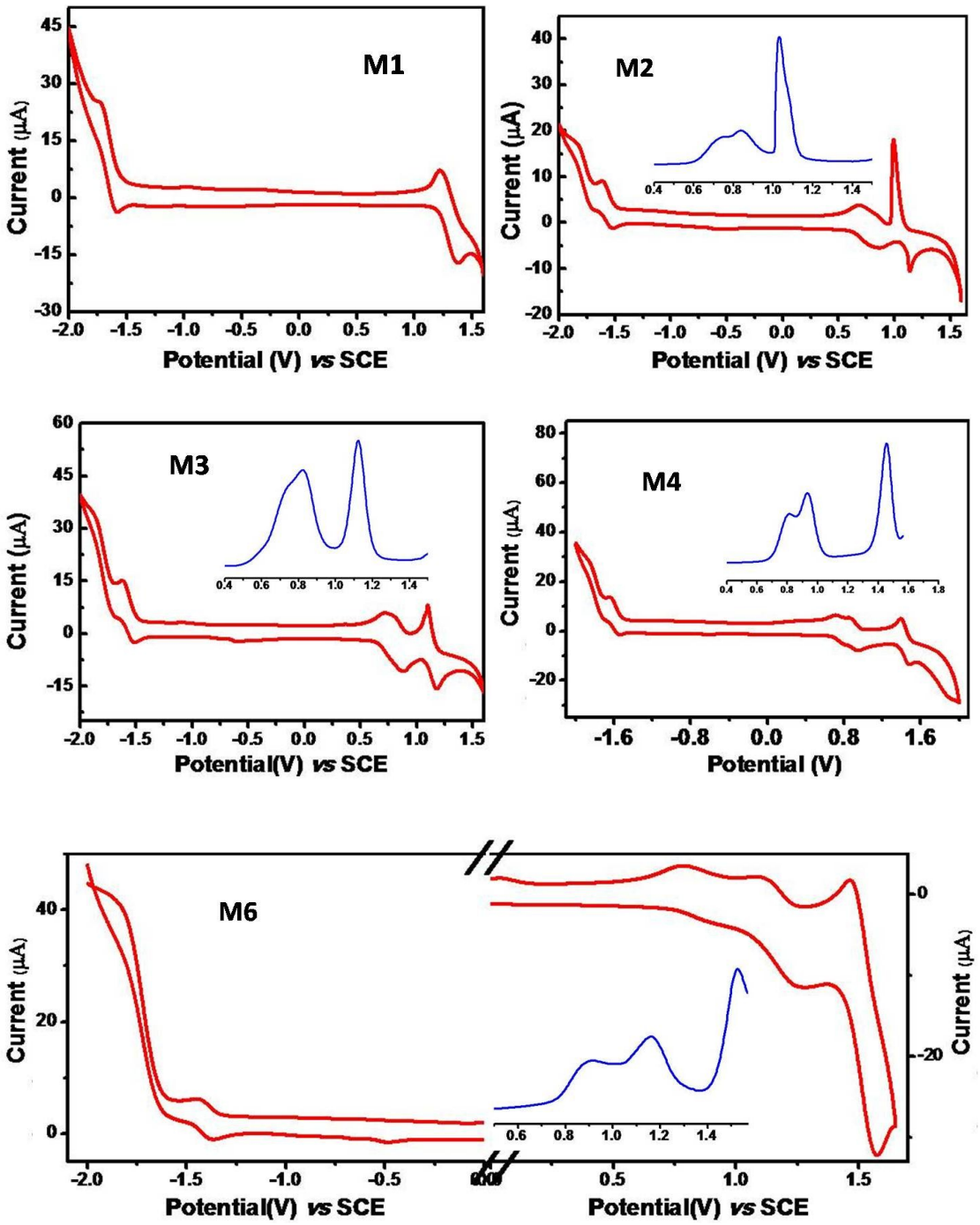

Figure S2. Cyclic voltammograms of compounds **M2-M4** and **M6** (red curves)**.** Inset: corresponding differential pulse voltammograms in the anodic region (blue curves).

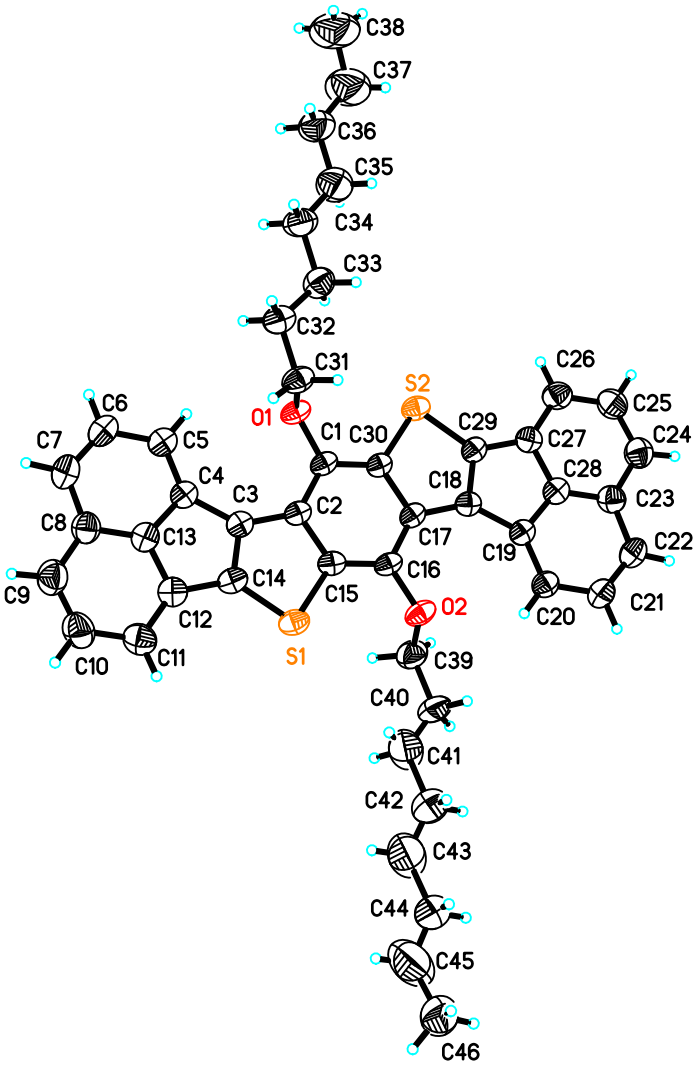

Figure S3. Molecular structure of compound **M2** showing thermal ellipsoids at the 50% probability level.

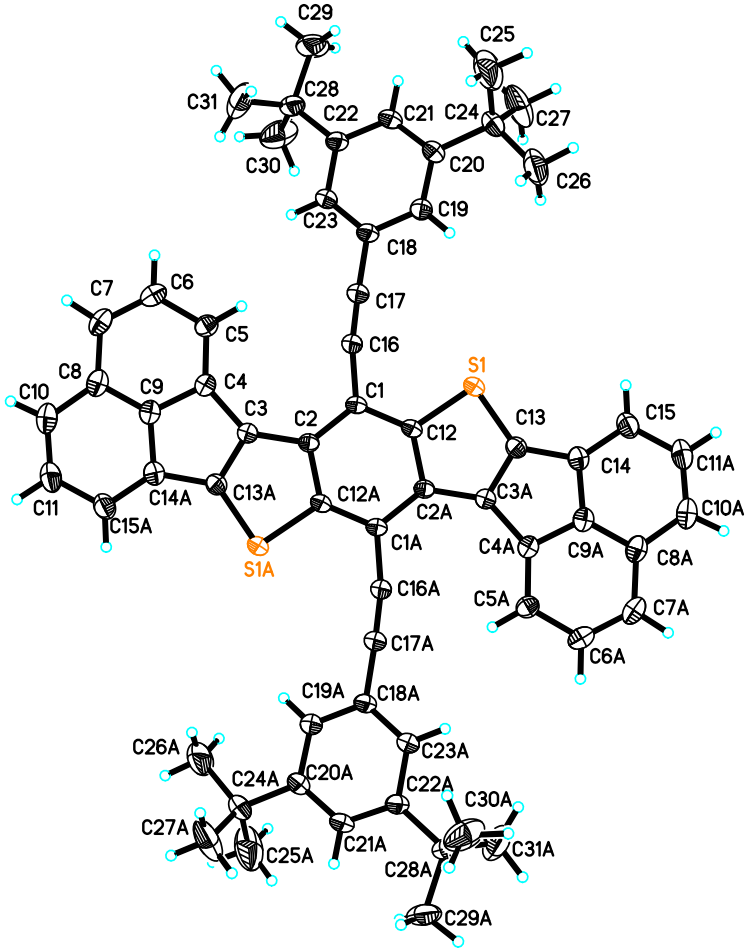

Figure S4. Molecular structure of compound **M6** showing thermal ellipsoids at the 50% probability level.

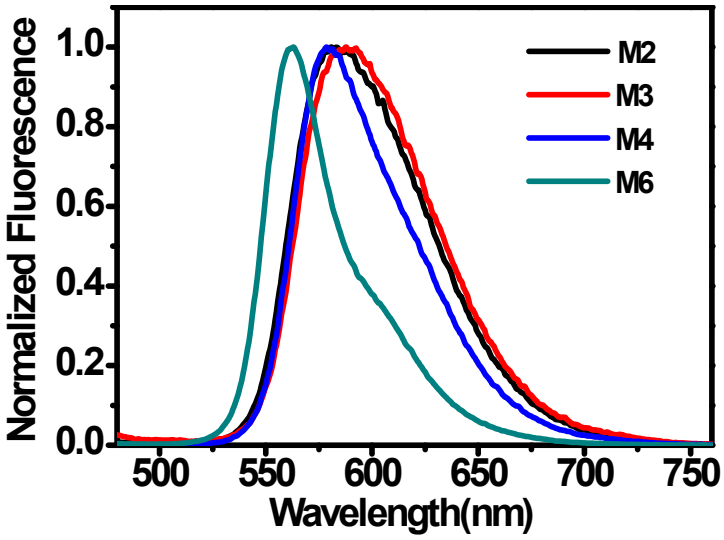

Figure S5. The fluorescence spectra of compounds **M2-M4** and **M6** in CH_2Cl_2 solution (λ_{exc} = 405 nm)

Table S1. Electrochemical Data and HOMO/LUMO Energy Levels for Compounds **M1**-**M4** and **M6**.

Compd	$E_{1/2}^{ox1}$ [a] (V)	$E_{1/2}^{ox2}$ (V)	$E_{1/2}^{ox3}$ (V)	$E_{1/2}^{red1}$ (V)	$E_{1/2}^{red2}$ (V)	HOMO(eV)	LUMO(eV)
M1	1.29			-1.65		-5.65	-2.71
M2	0.67	0.78	1.07	-1.58	-1.77	-5.14	-2.78
M3	0.68	0.80	1.09	-1.57	-1.78	-5.16	-2.79
M4	0.70	0.80	1.30	-1.59	-1.81	-5.16	-2.77
M6	0.80	1.12	1.50	-1.41	-1.74	-5.38	-2.95

[a] The electrode potentials are given in Volt vs SCE. The concentration of the parent compounds in dichloromethane/n-Bu_4NPF_6 was 10^{-3} M.

Table S2. Crystal data and structure refinement for **M2**.

Identification code	**M2**
Empirical formula	C46 H46 O2 S2
Formula weight	694.95
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.0940(7) Å alpha = 76.383(2)°
	b = 14.5388(8) Å beta = 82.5890(10)°
	c = 20.6868(12) Å gamma = 80.352(2)°
Volume	3756.8(4) $Å^3$
Z, Calculated density	4, 1.229 Mg/m^3
Absorption coefficient	0.180 mm^{-1}
F(000)	1480
Crystal size	0.22×0.20×0.15 mm
Theta range for data collection	1.46 to 25.01°
Limiting indices	-15≤h≤15, -17≤k≤17, -24≤l≤21
Reflections collected / unique	26100 / 13010 [*R*(int) = 0.0520]
Completeness to theta = 25.01	98.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9736 and 0.9616
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13010 / 68 / 901
Goodness-of-fit on F^2	0.998
Final R indices [I>2sigma(I)]	R_1 = 0.0713, wR_2 = 0.1635
R indices (all data)	R_1 = 0.1660, wR_2 = 0.2127
Largest diff. peak and hole	0.416 and -0.412 $eÅ^{-3}$

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **M2**. U(eq) is defined as one third of the trace of the orthogonalizedUij tensor.

	x	y	z	U(eq)
S(1)	5067(1)	2245(1)	970(1)	69(1)
S(2)	6131(1)	-1933(1)	580(1)	65(1)
S(3)	-60(1)	2559(1)	5717(1)	59(1)
S(4)	1147(1)	-82(1)	3694(1)	56(1)
O(1)	7333(2)	-288(2)	-91(1)	61(1)
O(2)	3932(2)	544(2)	1711(2)	71(1)
O(3)	2328(2)	-102(2)	4863(1)	52(1)
O(4)	-1185(2)	2666(2)	4486(1)	55(1)
C(1)	6456(3)	-36(3)	320(2)	55(1)
C(2)	6164(3)	895(3)	410(2)	52(1)
C(3)	6608(3)	1757(3)	118(2)	56(1)
C(4)	7441(3)	2103(3)	-382(2)	60(1)
C(5)	8179(4)	1744(3)	-816(2)	70(1)
C(6)	8853(4)	2347(4)	-1232(3)	86(2)
C(7)	8774(4)	3297(4)	-1221(3)	91(2)
C(8)	8003(4)	3694(4)	-793(3)	81(2)
C(9)	7788(5)	4668(4)	-734(3)	102(2)
C(10)	7000(5)	4957(4)	-301(3)	103(2)
C(11)	6346(4)	4328(4)	117(3)	89(2)
C(12)	6536(4)	3386(4)	72(2)	70(1)
C(13)	7369(4)	3086(4)	-381(3)	68(1)
C(14)	6090(3)	2516(3)	376(2)	65(1)
C(15)	5293(3)	1063(3)	878(2)	56(1)
C(16)	4722(3)	352(3)	1224(2)	55(1)
C(17)	4990(3)	-564(3)	1116(2)	56(1)
C(18)	4558(3)	-1432(3)	1403(2)	56(1)
C(19)	3710(3)	-1790(3)	1900(2)	59(1)
C(20)	2958(3)	-1434(3)	2339(2)	68(1)
C(21)	2310(4)	-2053(4)	2760(3)	78(2)
C(22)	2398(4)	-2997(4)	2749(3)	81(2)
C(23)	3167(4)	-3401(4)	2311(3)	77(1)
C(24)	3396(4)	-4367(4)	2253(3)	92(2)
C(25)	4201(5)	-4643(4)	1816(3)	93(2)
C(26)	4838(4)	-4002(4)	1403(3)	81(2)
C(27)	4627(4)	-3056(3)	1443(2)	65(1)
C(28)	3796(3)	-2772(3)	1896(2)	65(1)
C(29)	5076(3)	-2189(3)	1153(2)	59(1)

C(30)	5871(3)	-743(3)	652(2)	52(1)
C(31)	8264(3)	-531(4)	252(2)	78(1)
C(32)	9131(4)	-1001(4)	-145(3)	85(2)
C(33)	9063(4)	-1998(4)	-182(3)	94(2)
C(34)	9959(4)	-2474(4)	-567(3)	105(2)
C(35)	9979(5)	-3437(5)	-635(4)	132(2)
C(36)	10869(5)	-3903(5)	-999(4)	134(3)
C(37)	10972(7)	-4856(6)	-1075(5)	189(4)
C(38)	11843(7)	-5343(6)	-1369(5)	215(5)
C(39)	2986(4)	1021(4)	1469(3)	95(2)
C(40)	2296(6)	1386(5)	1983(4)	172(4)
C(41)	2324(8)	2298(5)	2083(4)	184(4)
C(42)	1663(8)	2653(6)	2630(4)	195(4)
C(43)	1229(8)	3569(6)	2635(4)	181(4)
C(44)	658(6)	3884(5)	3228(4)	159(3)
C(45)	235(10)	4773(6)	3290(6)	235(5)
C(46)	-252(7)	5013(5)	3880(4)	173(4)
C(47)	1433(3)	553(3)	4808(2)	47(1)
C(48)	1102(3)	1137(3)	5262(2)	44(1)
C(49)	1507(3)	1191(3)	5860(2)	48(1)
C(50)	2336(3)	681(3)	6283(2)	51(1)
C(51)	3075(3)	-99(3)	6305(2)	59(1)
C(52)	3747(3)	-353(3)	6830(3)	73(1)
C(53)	3669(4)	151(4)	7320(3)	74(1)
C(54)	2894(4)	949(3)	7324(2)	64(1)
C(55)	2671(4)	1523(4)	7803(2)	79(2)
C(56)	1847(4)	2252(4)	7753(2)	78(2)
C(57)	1198(4)	2470(3)	7231(2)	70(1)
C(58)	1407(3)	1939(3)	6750(2)	56(1)
C(59)	2247(3)	1182(3)	6808(2)	55(1)
C(60)	963(3)	1906(3)	6145(2)	52(1)
C(61)	217(3)	1840(3)	5130(2)	50(1)
C(62)	-356(3)	1945(3)	4591(2)	49(1)
C(63)	-44(3)	1334(3)	4151(2)	47(1)
C(64)	-450(3)	1258(3)	3555(2)	51(1)
C(65)	-1284(3)	1751(3)	3130(2)	55(1)
C(66)	-2044(3)	2524(3)	3097(2)	68(1)
C(67)	-2716(4)	2754(3)	2578(3)	81(2)
C(68)	-2608(4)	2242(4)	2098(3)	78(2)
C(69)	-1820(4)	1454(4)	2092(2)	68(1)
C(70)	-1602(4)	843(4)	1637(3)	80(2)
C(71)	-795(4)	111(4)	1700(2)	75(1)
C(72)	-147(3)	-85(3)	2219(2)	65(1)
C(73)	-334(3)	478(3)	2684(2)	55(1)

C(74)	-1168(3)	1238(3)	2610(2)	57(1)
C(75)	102(3)	536(3)	3280(2)	56(1)
C(76)	854(3)	631(3)	4287(2)	47(1)
C(77)	3244(3)	331(3)	4556(2)	65(1)
C(78)	4140(3)	-440(3)	4513(2)	69(1)
C(79)	4107(3)	-1011(3)	3990(2)	70(1)
C(80)	5002(3)	-1822(3)	4002(2)	70(1)
C(81)	5027(3)	-2405(3)	3485(3)	78(1)
C(82)	5883(4)	-3244(3)	3525(3)	88(2)
C(83)	5917(5)	-3829(4)	3006(3)	112(2)
C(84)	6702(7)	-4674(4)	3071(4)	174(4)
C(85)	-2139(3)	2408(3)	4855(3)	77(1)
C(86)	-2891(4)	3291(4)	4850(3)	94(2)
C(87)	-2594(5)	3962(4)	5226(3)	112(2)
C(88)	-3374(6)	4808(5)	5280(4)	167(3)
C(89)	-3045(8)	5472(6)	5631(5)	221(5)
C(90)	-4123(9)	6251(9)	5895(8)	257(7)
C(91)	-3599(14)	6842(10)	5896(13)	393(15)
C(92)	-4639(9)	7453(7)	6272(6)	234(5)

Table S4. Bond lengths [Å] and angles [deg] for **M2**.

S(1)-C(14)	1.727(5)	C(17)-C(30)	1.432(5)
S(1)-C(15)	1.745(4)	C(17)-C(18)	1.437(5)
S(2)-C(29)	1.730(4)	C(18)-C(29)	1.366(5)
S(2)-C(30)	1.744(4)	C(18)-C(19)	1.486(6)
S(3)-C(60)	1.721(4)	C(19)-C(20)	1.372(5)
S(3)-C(61)	1.748(4)	C(19)-C(28)	1.415(6)
S(4)-C(75)	1.715(4)	C(20)-C(21)	1.410(6)
S(4)-C(76)	1.753(4)	C(20)-H(20A)	0.9300
O(1)-C(1)	1.389(4)	C(21)-C(22)	1.362(6)
O(1)-C(31)	1.441(5)	C(21)-H(21A)	0.9300
O(2)-C(16)	1.389(4)	C(22)-C(23)	1.413(6)
O(2)-C(39)	1.405(5)	C(22)-H(22A)	0.9300
O(3)-C(47)	1.379(4)	C(23)-C(28)	1.398(6)
O(3)-C(77)	1.450(4)	C(23)-C(24)	1.416(6)
O(4)-C(62)	1.376(4)	C(24)-C(25)	1.368(7)
O(4)-C(85)	1.436(5)	C(24)-H(24A)	0.9300
C(1)-C(30)	1.382(5)	C(25)-C(26)	1.414(7)
C(1)-C(2)	1.393(5)	C(25)-H(25A)	0.9300
C(2)-C(15)	1.427(5)	C(26)-C(27)	1.377(6)
C(2)-C(3)	1.439(6)	C(26)-H(26A)	0.9300
C(3)-C(14)	1.377(5)	C(27)-C(28)	1.414(6)
C(3)-C(4)	1.470(6)	C(27)-C(29)	1.448(6)
C(4)-C(5)	1.357(5)	C(31)-C(32)	1.482(6)
C(4)-C(13)	1.417(6)	C(31)-H(31A)	0.9700
C(5)-C(6)	1.413(6)	C(31)-H(31B)	0.9700
C(5)-H(5A)	0.9300	C(32)-C(33)	1.487(6)
C(6)-C(7)	1.373(6)	C(32)-H(32A)	0.9700
C(6)-H(6A)	0.9300	C(32)-H(32B)	0.9700
C(7)-C(8)	1.397(7)	C(33)-C(34)	1.494(6)
C(7)-H(7A)	0.9300	C(33)-H(33A)	0.9700
C(8)-C(13)	1.380(6)	C(33)-H(33B)	0.9700
C(8)-C(9)	1.427(7)	C(34)-C(35)	1.436(7)
C(9)-C(10)	1.355(7)	C(34)-H(34A)	0.9700
C(9)-H(9A)	0.9300	C(34)-H(34B)	0.9700
C(10)-C(11)	1.420(7)	C(35)-C(36)	1.460(7)
C(10)-H(10A)	0.9300	C(35)-H(35A)	0.9700
C(11)-C(12)	1.373(6)	C(35)-H(35B)	0.9700
C(11)-H(11A)	0.9300	C(36)-C(37)	1.413(8)
C(12)-C(13)	1.424(6)	C(36)-H(36A)	0.9700
C(12)-C(14)	1.454(6)	C(36)-H(36B)	0.9700
C(15)-C(16)	1.383(5)	C(37)-C(38)	1.387(9)
C(16)-C(17)	1.381(5)	C(37)-H(37A)	0.9700

C(37)-H(37B)	0.9700	C(55)-C(56)	1.375(6)
C(38)-H(38A)	0.9600	C(55)-H(55A)	0.9300
C(38)-H(38B)	0.9600	C(56)-C(57)	1.406(6)
C(38)-H(38C)	0.9600	C(56)-H(56A)	0.9300
C(39)-C(40)	1.445(7)	C(57)-C(58)	1.373(5)
C(39)-H(39A)	0.9700	C(57)-H(57A)	0.9300
C(39)-H(39B)	0.9700	C(58)-C(59)	1.414(5)
C(40)-C(41)	1.395(6)	C(58)-C(60)	1.460(5)
C(40)-H(40A)	0.9700	C(61)-C(62)	1.388(5)
C(40)-H(40B)	0.9700	C(62)-C(63)	1.395(5)
C(41)-C(42)	1.472(8)	C(63)-C(76)	1.433(5)
C(41)-H(41A)	0.9700	C(63)-C(64)	1.438(5)
C(41)-H(41B)	0.9700	C(64)-C(75)	1.367(5)
C(42)-C(43)	1.359(7)	C(64)-C(65)	1.472(5)
C(42)-H(42A)	0.9700	C(65)-C(66)	1.366(5)
C(42)-H(42B)	0.9700	C(65)-C(74)	1.425(5)
C(43)-C(44)	1.479(9)	C(66)-C(67)	1.420(6)
C(43)-H(43A)	0.9700	C(66)-H(66A)	0.9300
C(43)-H(43B)	0.9700	C(67)-C(68)	1.355(6)
C(44)-C(45)	1.347(7)	C(67)-H(67A)	0.9300
C(44)-H(44A)	0.9700	C(68)-C(69)	1.408(6)
C(44)-H(44B)	0.9700	C(68)-H(68A)	0.9300
C(45)-C(46)	1.395(10)	C(69)-C(74)	1.401(6)
C(45)-H(45A)	0.9700	C(69)-C(70)	1.413(6)
C(45)-H(45B)	0.9700	C(70)-C(71)	1.363(6)
C(46)-H(46A)	0.9600	C(70)-H(70A)	0.9300
C(46)-H(46B)	0.9600	C(71)-C(72)	1.401(6)
C(46)-H(46C)	0.9600	C(71)-H(71A)	0.9300
C(47)-C(76)	1.370(5)	C(72)-C(73)	1.378(5)
C(47)-C(48)	1.391(5)	C(72)-H(72A)	0.9300
C(48)-C(61)	1.419(5)	C(73)-C(74)	1.413(5)
C(48)-C(49)	1.432(5)	C(73)-C(75)	1.450(5)
C(49)-C(60)	1.366(5)	C(77)-C(78)	1.490(5)
C(49)-C(50)	1.470(5)	C(77)-H(77A)	0.9700
C(50)-C(51)	1.358(5)	C(77)-H(77B)	0.9700
C(50)-C(59)	1.427(5)	C(78)-C(79)	1.520(5)
C(51)-C(52)	1.426(6)	C(78)-H(78A)	0.9700
C(51)-H(51A)	0.9300	C(78)-H(78B)	0.9700
C(52)-C(53)	1.368(6)	C(79)-C(80)	1.515(5)
C(52)-H(52A)	0.9300	C(79)-H(79A)	0.9700
C(53)-C(54)	1.409(6)	C(79)-H(79B)	0.9700
C(53)-H(53A)	0.9300	C(80)-C(81)	1.508(6)
C(54)-C(59)	1.392(6)	C(80)-H(80A)	0.9700
C(54)-C(55)	1.415(6)	C(80)-H(80B)	0.9700

C(81)-C(82)	1.506(6)	C(30)-C(1)-O(1)	118.2(4)
C(81)-H(81A)	0.9700	C(30)-C(1)-C(2)	119.8(4)
C(81)-H(81B)	0.9700	O(1)-C(1)-C(2)	122.0(4)
C(82)-C(83)	1.512(6)	C(1)-C(2)-C(15)	117.5(4)
C(82)-H(82A)	0.9700	C(1)-C(2)-C(3)	131.3(4)
C(82)-H(82B)	0.9700	C(15)-C(2)-C(3)	111.2(4)
C(83)-C(84)	1.456(7)	C(14)-C(3)-C(2)	111.5(4)
C(83)-H(83A)	0.9700	C(14)-C(3)-C(4)	108.2(4)
C(83)-H(83B)	0.9700	C(2)-C(3)-C(4)	140.3(4)
C(84)-H(84A)	0.9600	C(5)-C(4)-C(13)	117.6(4)
C(84)-H(84B)	0.9600	C(5)-C(4)-C(3)	137.5(4)
C(84)-H(84C)	0.9600	C(13)-C(4)-C(3)	104.8(4)
C(85)-C(86)	1.480(6)	C(4)-C(5)-C(6)	119.4(5)
C(85)-H(85A)	0.9700	C(4)-C(5)-H(5A)	120.3
C(85)-H(85B)	0.9700	C(6)-C(5)-H(5A)	120.3
C(86)-C(87)	1.507(7)	C(7)-C(6)-C(5)	122.0(5)
C(86)-H(86A)	0.9700	C(7)-C(6)-H(6A)	119.0
C(86)-H(86B)	0.9700	C(5)-C(6)-H(6A)	119.0
C(87)-C(88)	1.478(7)	C(6)-C(7)-C(8)	119.8(5)
C(87)-H(87A)	0.9700	C(6)-C(7)-H(7A)	120.1
C(87)-H(87B)	0.9700	C(8)-C(7)-H(7A)	120.1
C(88)-C(89)	1.483(10)	C(13)-C(8)-C(7)	117.0(5)
C(88)-H(88A)	0.9700	C(13)-C(8)-C(9)	115.7(5)
C(88)-H(88B)	0.9700	C(7)-C(8)-C(9)	127.2(6)
C(89)-C(90)	1.770(14)	C(10)-C(9)-C(8)	120.8(6)
C(89)-H(89A)	0.9700	C(10)-C(9)-H(9A)	119.6
C(89)-H(89B)	0.9700	C(8)-C(9)-H(9A)	119.6
C(90)-C(91)	1.187(12)	C(9)-C(10)-C(11)	123.1(6)
C(90)-H(90A)	0.9700	C(9)-C(10)-H(10A)	118.4
C(90)-H(90B)	0.9700	C(11)-C(10)-H(10A)	118.4
C(91)-C(92)	1.70(2)	C(12)-C(11)-C(10)	117.4(5)
C(91)-H(91A)	0.9700	C(12)-C(11)-H(11A)	121.3
C(91)-H(91B)	0.9700	C(10)-C(11)-H(11A)	121.3
C(92)-H(92A)	0.9600	C(11)-C(12)-C(13)	119.2(5)
C(92)-H(92B)	0.9600	C(11)-C(12)-C(14)	137.1(5)
C(92)-H(92C)	0.9600	C(13)-C(12)-C(14)	103.7(4)
C(14)-S(1)-C(15)	90.3(2)	C(8)-C(13)-C(4)	124.0(5)
C(29)-S(2)-C(30)	89.7(2)	C(8)-C(13)-C(12)	123.8(5)
C(60)-S(3)-C(61)	90.09(19)	C(4)-C(13)-C(12)	112.2(4)
C(75)-S(4)-C(76)	90.2(2)	C(3)-C(14)-C(12)	111.1(4)
C(1)-O(1)-C(31)	112.4(3)	C(3)-C(14)-S(1)	114.8(4)
C(16)-O(2)-C(39)	115.2(4)	C(12)-C(14)-S(1)	134.2(4)
C(47)-O(3)-C(77)	111.9(3)	C(16)-C(15)-C(2)	122.7(4)
C(62)-O(4)-C(85)	113.3(3)	C(16)-C(15)-S(1)	125.1(3)

C(2)-C(15)-S(1)	112.2(3)	C(1)-C(30)-S(2)	124.9(3)
C(17)-C(16)-C(15)	119.7(4)	C(17)-C(30)-S(2)	112.9(3)
C(17)-C(16)-O(2)	120.2(4)	O(1)-C(31)-C(32)	111.0(4)
C(15)-C(16)-O(2)	119.9(4)	O(1)-C(31)-H(31A)	109.4
C(16)-C(17)-C(30)	118.0(4)	C(32)-C(31)-H(31A)	109.4
C(16)-C(17)-C(18)	131.9(4)	O(1)-C(31)-H(31B)	109.4
C(30)-C(17)-C(18)	110.1(4)	C(32)-C(31)-H(31B)	109.4
C(29)-C(18)-C(17)	112.4(4)	H(31A)-C(31)-H(31B)	108.0
C(29)-C(18)-C(19)	107.4(4)	C(31)-C(32)-C(33)	116.4(4)
C(17)-C(18)-C(19)	140.2(4)	C(31)-C(32)-H(32A)	108.2
C(20)-C(19)-C(28)	117.8(4)	C(33)-C(32)-H(32A)	108.2
C(20)-C(19)-C(18)	137.4(4)	C(31)-C(32)-H(32B)	108.2
C(28)-C(19)-C(18)	104.7(4)	C(33)-C(32)-H(32B)	108.2
C(19)-C(20)-C(21)	119.0(4)	H(32A)-C(32)-H(32B)	107.3
C(19)-C(20)-H(20A)	120.5	C(32)-C(33)-C(34)	115.8(5)
C(21)-C(20)-H(20A)	120.5	C(32)-C(33)-H(33A)	108.3
C(22)-C(21)-C(20)	122.6(5)	C(34)-C(33)-H(33A)	108.3
C(22)-C(21)-H(21A)	118.7	C(32)-C(33)-H(33B)	108.3
C(20)-C(21)-H(21A)	118.7	C(34)-C(33)-H(33B)	108.3
C(21)-C(22)-C(23)	120.6(5)	H(33A)-C(33)-H(33B)	107.4
C(21)-C(22)-H(22A)	119.7	C(35)-C(34)-C(33)	120.7(5)
C(23)-C(22)-H(22A)	119.7	C(35)-C(34)-H(34A)	107.2
C(28)-C(23)-C(22)	115.8(5)	C(33)-C(34)-H(34A)	107.2
C(28)-C(23)-C(24)	116.1(5)	C(35)-C(34)-H(34B)	107.2
C(22)-C(23)-C(24)	128.1(5)	C(33)-C(34)-H(34B)	107.2
C(25)-C(24)-C(23)	120.4(5)	H(34A)-C(34)-H(34B)	106.8
C(25)-C(24)-H(24A)	119.8	C(34)-C(35)-C(36)	120.2(6)
C(23)-C(24)-H(24A)	119.8	C(34)-C(35)-H(35A)	107.3
C(24)-C(25)-C(26)	123.0(5)	C(36)-C(35)-H(35A)	107.3
C(24)-C(25)-H(25A)	118.5	C(34)-C(35)-H(35B)	107.3
C(26)-C(25)-H(25A)	118.5	C(36)-C(35)-H(35B)	107.3
C(27)-C(26)-C(25)	117.9(5)	H(35A)-C(35)-H(35B)	106.9
C(27)-C(26)-H(26A)	121.0	C(37)-C(36)-C(35)	124.3(7)
C(25)-C(26)-H(26A)	121.0	C(37)-C(36)-H(36A)	106.3
C(26)-C(27)-C(28)	119.0(5)	C(35)-C(36)-H(36A)	106.3
C(26)-C(27)-C(29)	136.9(5)	C(37)-C(36)-H(36B)	106.3
C(28)-C(27)-C(29)	104.0(4)	C(35)-C(36)-H(36B)	106.3
C(23)-C(28)-C(27)	123.6(5)	H(36A)-C(36)-H(36B)	106.4
C(23)-C(28)-C(19)	124.2(5)	C(38)-C(37)-C(36)	125.6(8)
C(27)-C(28)-C(19)	112.1(4)	C(38)-C(37)-H(37A)	105.9
C(18)-C(29)-C(27)	111.7(4)	C(36)-C(37)-H(37A)	105.9
C(18)-C(29)-S(2)	114.9(3)	C(38)-C(37)-H(37B)	105.9
C(27)-C(29)-S(2)	133.4(4)	C(36)-C(37)-H(37B)	105.9
C(1)-C(30)-C(17)	122.2(4)	H(37A)-C(37)-H(37B)	106.2

C(37)-C(38)-H(38A)	109.5	C(46)-C(45)-H(45A)	106.1
C(37)-C(38)-H(38B)	109.5	C(44)-C(45)-H(45B)	106.1
H(38A)-C(38)-H(38B)	109.5	C(46)-C(45)-H(45B)	106.1
C(37)-C(38)-H(38C)	109.5	H(45A)-C(45)-H(45B)	106.3
H(38A)-C(38)-H(38C)	109.5	C(45)-C(46)-H(46A)	109.5
H(38B)-C(38)-H(38C)	109.5	C(45)-C(46)-H(46B)	109.5
O(2)-C(39)-C(40)	111.4(5)	H(46A)-C(46)-H(46B)	109.5
O(2)-C(39)-H(39A)	109.3	C(45)-C(46)-H(46C)	109.5
C(40)-C(39)-H(39A)	109.3	H(46A)-C(46)-H(46C)	109.5
O(2)-C(39)-H(39B)	109.3	H(46B)-C(46)-H(46C)	109.5
C(40)-C(39)-H(39B)	109.3	C(76)-C(47)-O(3)	118.6(3)
H(39A)-C(39)-H(39B)	108.0	C(76)-C(47)-C(48)	119.0(4)
C(41)-C(40)-C(39)	120.7(7)	O(3)-C(47)-C(48)	122.4(4)
C(41)-C(40)-H(40A)	107.1	C(47)-C(48)-C(61)	117.8(4)
C(39)-C(40)-H(40A)	107.1	C(47)-C(48)-C(49)	131.8(4)
C(41)-C(40)-H(40B)	107.1	C(61)-C(48)-C(49)	110.4(3)
C(39)-C(40)-H(40B)	107.1	C(60)-C(49)-C(48)	112.7(4)
H(40A)-C(40)-H(40B)	106.8	C(60)-C(49)-C(50)	108.6(3)
C(40)-C(41)-C(42)	121.0(7)	C(48)-C(49)-C(50)	138.7(4)
C(40)-C(41)-H(41A)	107.1	C(51)-C(50)-C(59)	117.5(4)
C(42)-C(41)-H(41A)	107.1	C(51)-C(50)-C(49)	137.9(4)
C(40)-C(41)-H(41B)	107.1	C(59)-C(50)-C(49)	104.6(4)
C(42)-C(41)-H(41B)	107.1	C(50)-C(51)-C(52)	119.1(4)
H(41A)-C(41)-H(41B)	106.8	C(50)-C(51)-H(51A)	120.5
C(43)-C(42)-C(41)	127.6(8)	C(52)-C(51)-H(51A)	120.5
C(43)-C(42)-H(42A)	105.4	C(53)-C(52)-C(51)	122.7(5)
C(41)-C(42)-H(42A)	105.4	C(53)-C(52)-H(52A)	118.6
C(43)-C(42)-H(42B)	105.4	C(51)-C(52)-H(52A)	118.6
C(41)-C(42)-H(42B)	105.4	C(52)-C(53)-C(54)	119.9(5)
H(42A)-C(42)-H(42B)	106.0	C(52)-C(53)-H(53A)	120.0
C(42)-C(43)-C(44)	124.3(8)	C(54)-C(53)-H(53A)	120.0
C(42)-C(43)-H(43A)	106.3	C(59)-C(54)-C(53)	116.3(4)
C(44)-C(43)-H(43A)	106.3	C(59)-C(54)-C(55)	116.0(5)
C(42)-C(43)-H(43B)	106.3	C(53)-C(54)-C(55)	127.6(5)
C(44)-C(43)-H(43B)	106.3	C(56)-C(55)-C(54)	120.5(5)
H(43A)-C(43)-H(43B)	106.4	C(56)-C(55)-H(55A)	119.8
C(45)-C(44)-C(43)	128.8(9)	C(54)-C(55)-H(55A)	119.8
C(45)-C(44)-H(44A)	105.1	C(55)-C(56)-C(57)	122.6(4)
C(43)-C(44)-H(44A)	105.1	C(55)-C(56)-H(56A)	118.7
C(45)-C(44)-H(44B)	105.1	C(57)-C(56)-H(56A)	118.7
C(43)-C(44)-H(44B)	105.1	C(58)-C(57)-C(56)	118.4(5)
H(44A)-C(44)-H(44B)	105.9	C(58)-C(57)-H(57A)	120.8
C(44)-C(45)-C(46)	124.9(9)	C(56)-C(57)-H(57A)	120.8
C(44)-C(45)-H(45A)	106.1	C(57)-C(58)-C(59)	118.8(4)

C(57)-C(58)-C(60)	137.0(4)	C(72)-C(73)-C(74)	118.2(4)
C(59)-C(58)-C(60)	104.2(4)	C(72)-C(73)-C(75)	137.8(4)
C(54)-C(59)-C(58)	123.8(4)	C(74)-C(73)-C(75)	104.0(4)
C(54)-C(59)-C(50)	124.4(4)	C(69)-C(74)-C(73)	123.9(4)
C(58)-C(59)-C(50)	111.8(4)	C(69)-C(74)-C(65)	123.8(4)
C(49)-C(60)-C(58)	110.8(4)	C(73)-C(74)-C(65)	112.3(4)
C(49)-C(60)-S(3)	114.3(3)	C(64)-C(75)-C(73)	111.0(4)
C(58)-C(60)-S(3)	134.9(3)	C(64)-C(75)-S(4)	114.9(3)
C(62)-C(61)-C(48)	123.5(4)	C(73)-C(75)-S(4)	134.1(3)
C(62)-C(61)-S(3)	124.0(3)	C(47)-C(76)-C(63)	123.5(4)
C(48)-C(61)-S(3)	112.4(3)	C(47)-C(76)-S(4)	124.2(3)
O(4)-C(62)-C(61)	119.8(4)	C(63)-C(76)-S(4)	112.2(3)
O(4)-C(62)-C(63)	121.7(4)	O(3)-C(77)-C(78)	108.9(3)
C(61)-C(62)-C(63)	118.5(4)	O(3)-C(77)-H(77A)	109.9
C(62)-C(63)-C(76)	117.5(4)	C(78)-C(77)-H(77A)	109.9
C(62)-C(63)-C(64)	132.4(4)	O(3)-C(77)-H(77B)	109.9
C(76)-C(63)-C(64)	110.1(3)	C(78)-C(77)-H(77B)	109.9
C(75)-C(64)-C(63)	112.6(4)	H(77A)-C(77)-H(77B)	108.3
C(75)-C(64)-C(65)	108.6(4)	C(77)-C(78)-C(79)	115.1(4)
C(63)-C(64)-C(65)	138.8(4)	C(77)-C(78)-H(78A)	108.5
C(66)-C(65)-C(74)	117.5(4)	C(79)-C(78)-H(78A)	108.5
C(66)-C(65)-C(64)	138.4(4)	C(77)-C(78)-H(78B)	108.5
C(74)-C(65)-C(64)	104.1(4)	C(79)-C(78)-H(78B)	108.5
C(65)-C(66)-C(67)	119.6(4)	H(78A)-C(78)-H(78B)	107.5
C(65)-C(66)-H(66A)	120.2	C(78)-C(79)-C(80)	112.4(4)
C(67)-C(66)-H(66A)	120.2	C(78)-C(79)-H(79A)	109.1
C(68)-C(67)-C(66)	121.8(5)	C(80)-C(79)-H(79A)	109.1
C(68)-C(67)-H(67A)	119.1	C(78)-C(79)-H(79B)	109.1
C(66)-C(67)-H(67A)	119.1	C(80)-C(79)-H(79B)	109.1
C(67)-C(68)-C(69)	121.3(5)	H(79A)-C(79)-H(79B)	107.9
C(67)-C(68)-H(68A)	119.3	C(81)-C(80)-C(79)	115.1(4)
C(69)-C(68)-H(68A)	119.3	C(81)-C(80)-H(80A)	108.5
C(74)-C(69)-C(68)	115.9(4)	C(79)-C(80)-H(80A)	108.5
C(74)-C(69)-C(70)	115.3(5)	C(81)-C(80)-H(80B)	108.5
C(68)-C(69)-C(70)	128.8(5)	C(79)-C(80)-H(80B)	108.5
C(71)-C(70)-C(69)	121.3(5)	H(80A)-C(80)-H(80B)	107.5
C(71)-C(70)-H(70A)	119.3	C(82)-C(81)-C(80)	114.8(4)
C(69)-C(70)-H(70A)	119.3	C(82)-C(81)-H(81A)	108.6
C(70)-C(71)-C(72)	122.3(5)	C(80)-C(81)-H(81A)	108.6
C(70)-C(71)-H(71A)	118.9	C(82)-C(81)-H(81B)	108.6
C(72)-C(71)-H(71A)	118.9	C(80)-C(81)-H(81B)	108.6
C(73)-C(72)-C(71)	118.9(5)	H(81A)-C(81)-H(81B)	107.6
C(73)-C(72)-H(72A)	120.5	C(81)-C(82)-C(83)	115.1(5)
C(71)-C(72)-H(72A)	120.5	C(81)-C(82)-H(82A)	108.5

C(83)-C(82)-H(82A)	108.5	H(87A)-C(87)-H(87B)	107.5
C(81)-C(82)-H(82B)	108.5	C(89)-C(88)-C(87)	114.1(7)
C(83)-C(82)-H(82B)	108.5	C(89)-C(88)-H(88A)	108.7
H(82A)-C(82)-H(82B)	107.5	C(87)-C(88)-H(88A)	108.7
C(84)-C(83)-C(82)	115.1(6)	C(89)-C(88)-H(88B)	108.7
C(84)-C(83)-H(83A)	108.5	C(87)-C(88)-H(88B)	108.7
C(82)-C(83)-H(83A)	108.5	H(88A)-C(88)-H(88B)	107.6
C(84)-C(83)-H(83B)	108.5	C(88)-C(89)-C(90)	111.2(9)
C(82)-C(83)-H(83B)	108.5	C(88)-C(89)-H(89A)	109.4
H(83A)-C(83)-H(83B)	107.5	C(90)-C(89)-H(89A)	109.4
C(83)-C(84)-H(84A)	109.5	C(88)-C(89)-H(89B)	109.4
C(83)-C(84)-H(84B)	109.5	C(90)-C(89)-H(89B)	109.4
H(84A)-C(84)-H(84B)	109.5	H(89A)-C(89)-H(89B)	108.0
C(83)-C(84)-H(84C)	109.5	C(91)-C(90)-C(89)	92.5(15)
H(84A)-C(84)-H(84C)	109.5	C(91)-C(90)-H(90A)	113.2
H(84B)-C(84)-H(84C)	109.5	C(89)-C(90)-H(90A)	113.2
O(4)-C(85)-C(86)	108.4(4)	C(91)-C(90)-H(90B)	113.2
O(4)-C(85)-H(85A)	110.0	C(89)-C(90)-H(90B)	113.2
C(86)-C(85)-H(85A)	110.0	H(90A)-C(90)-H(90B)	110.6
O(4)-C(85)-H(85B)	110.0	C(90)-C(91)-C(92)	88.9(16)
C(86)-C(85)-H(85B)	110.0	C(90)-C(91)-H(91A)	113.9
H(85A)-C(85)-H(85B)	108.4	C(92)-C(91)-H(91A)	113.8
C(85)-C(86)-C(87)	114.2(5)	C(90)-C(91)-H(91B)	113.8
C(85)-C(86)-H(86A)	108.7	C(92)-C(91)-H(91B)	113.8
C(87)-C(86)-H(86A)	108.7	H(91A)-C(91)-H(91B)	111.0
C(85)-C(86)-H(86B)	108.7	C(91)-C(92)-H(92A)	109.5
C(87)-C(86)-H(86B)	108.7	C(91)-C(92)-H(92B)	109.5
H(86A)-C(86)-H(86B)	107.6	H(92A)-C(92)-H(92B)	109.5
C(88)-C(87)-C(86)	115.4(6)	C(91)-C(92)-H(92C)	109.5
C(88)-C(87)-H(87A)	108.4	H(92A)-C(92)-H(92C)	109.5
C(86)-C(87)-H(87A)	108.4	H(92B)-C(92)-H(92C)	109.5
C(88)-C(87)-H(87B)	108.4		
C(86)-C(87)-H(87B)	108.4		

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for **M6**.

Identification code	**M6**
Empirical formula	C62 H54 S2
Formula weight	863.17
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 41.379(8) Å alpha = 90 °
	b = 6.0824(12) Å beta = 106.27(3) °
	c = 20.059(4) Å gamma = 90 °
Volume	4846.4(17) $Å^3$
Z, Calculated density	4, 1.183 Mg/m^3
Absorption coefficient	0.149 mm^{-1}
F(000)	1832
Crystal size	0.38×0.18×0.16 mm
Theta range for data collection	3.08 to 27.49 °
Limiting indices	-53≤h≤53, -7≤k≤7, -25≤l≤26
Reflections collected / unique	16037 / 5539 [*R*(int) = 0.0271]
Completeness to theta = 27.49	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6720
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5539 / 105 / 317
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R_1 = 0.0492, wR_2 = 0.1345
R indices (all data)	R_1 = 0.0673, wR_2 = 0.1505
Largest diff. peak and hole	0.468 and -0.279 e $Å^{-3}$

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **M6**.

	x	y	z	U(eq)
S(1)	1799(1)	3794(1)	153(1)	41(1)
C(1)	2221(1)	1126(3)	-339(1)	34(1)
C(2)	2546(1)	599(3)	-387(1)	34(1)
C(3)	2666(1)	-1132(3)	-736(1)	36(1)
C(4)	2545(1)	-3111(3)	-1162(1)	38(1)
C(5)	2247(1)	-4228(3)	-1410(1)	44(1)
C(6)	2242(1)	-6169(3)	-1807(1)	51(1)
C(7)	2522(1)	-6979(4)	-1955(1)	53(1)
C(8)	2833(1)	-5868(3)	-1714(1)	49(1)
C(9)	2833(1)	-3982(3)	-1323(1)	42(1)
C(10)	3146(1)	-6440(4)	-1828(1)	62(1)
C(11)	3424(1)	-5185(4)	-1563(1)	67(1)
C(12)	2186(1)	2976(3)	44(1)	35(1)
C(13)	1992(1)	5955(3)	659(1)	40(1)
C(14)	1877(1)	7709(3)	1032(1)	44(1)
C(15)	1579(1)	8291(4)	1157(1)	57(1)
C(16)	1923(1)	-96(3)	-657(1)	39(1)
C(17)	1650(1)	-869(3)	-874(1)	45(1)
C(18)	1315(1)	-1759(3)	-1106(1)	44(1)
C(19)	1084(1)	-1190(3)	-745(1)	48(1)
C(20)	757(1)	-1952(4)	-953(1)	49(1)
C(21)	668(1)	-3325(4)	-1533(1)	50(1)
C(22)	891(1)	-3941(3)	-1905(1)	46(1)
C(23)	1218(1)	-3130(3)	-1680(1)	46(1)
C(24)	495(1)	-1322(4)	-576(1)	62(1)
C(25)	353(1)	-3318(6)	-332(2)	134(2)
C(26)	642(1)	170(8)	48(2)	132(2)
C(27)	210(1)	-54(7)	-1071(2)	121(1)
C(28)	784(1)	-5408(4)	-2552(1)	58(1)
C(29)	413(1)	-6040(14)	-2738(3)	94(3)
C(30)	841(2)	-4193(14)	-3166(3)	106(3)
C(31)	989(2)	-7482(11)	-2407(4)	104(3)
C(29A)	599(3)	-7454(16)	-2405(6)	107(4)
C(30A)	550(4)	-4050(19)	-3111(5)	153(7)
C(31A)	1073(2)	-6280(30)	-2790(7)	135(6)
H(5A)	2051	-3721	-1320	53
H(6A)	2039	-6921	-1972	61
H(7A)	2508	-8261	-2214	63

H(10A)	3161	-7685	-2087	75
H(11A)	3625	-5591	-1652	80
H(15A)	1385	7463	979	68
H(19A)	1152	-283	-357	58
H(21A)	448	-3853	-1678	60
H(23A)	1373	-3511	-1918	56
H(25A)	190	-2886	-98	201
H(25B)	531	-4124	-16	201
H(25C)	247	-4229	-722	201
H(26A)	471	515	270	198
H(26B)	723	1503	-106	198
H(26C)	825	-570	371	198
H(27A)	45	332	-838	181
H(27B)	108	-952	-1467	181
H(27C)	298	1260	-1220	181
H(29A)	279	-4861	-2991	141
H(29B)	349	-6314	-2320	141
H(29C)	376	-7343	-3019	141
H(30A)	972	-2893	-3007	159
H(30B)	628	-3788	-3479	159
H(30C)	960	-5127	-3403	159
H(31A)	1213	-7185	-2430	156
H(31B)	887	-8575	-2746	156
H(31C)	997	-8012	-1952	156
H(29D)	408	-7014	-2256	160
H(29E)	749	-8313	-2048	160
H(29F)	525	-8318	-2821	160
H(30D)	665	-2753	-3195	229
H(30E)	356	-3634	-2964	229
H(30F)	478	-4898	-3531	229
H(31D)	1200	-5067	-2893	202
H(31E)	988	-7154	-3199	202
H(31F)	1215	-7160	-2429	202

Table S7. Bond lengths [Å] and angles [deg] for **M6**.

S(1)-C(13)	1.7147(19)	C(21)-H(21A)	0.9300
S(1)-C(12)	1.7455(17)	C(22)-C(23)	1.392(2)
C(1)-C(12)	1.393(2)	C(22)-C(28)	1.534(3)
C(1)-C(2)	1.409(2)	C(23)-H(23A)	0.9300
C(1)-C(16)	1.429(2)	C(24)-C(25)	1.490(4)
C(2)-C(12)#1	1.426(2)	C(24)-C(27)	1.521(4)
C(2)-C(3)	1.429(2)	C(24)-C(26)	1.528(4)
C(3)-C(13)#1	1.383(2)	C(25)-H(25A)	0.9600
C(3)-C(4)	1.481(2)	C(25)-H(25B)	0.9600
C(4)-C(5)	1.372(3)	C(25)-H(25C)	0.9600
C(4)-C(9)	1.421(2)	C(26)-H(26A)	0.9600
C(5)-C(6)	1.421(3)	C(26)-H(26B)	0.9600
C(5)-H(5A)	0.9300	C(26)-H(26C)	0.9600
C(6)-C(7)	1.367(3)	C(27)-H(27A)	0.9600
C(6)-H(6A)	0.9300	C(27)-H(27B)	0.9600
C(7)-C(8)	1.412(3)	C(27)-H(27C)	0.9600
C(7)-H(7A)	0.9300	C(28)-C(31A)	1.501(8)
C(8)-C(9)	1.390(3)	C(28)-C(31)	1.502(6)
C(8)-C(10)	1.422(3)	C(28)-C(30A)	1.508(8)
C(9)-C(14)#1	1.411(3)	C(28)-C(30)	1.512(6)
C(10)-C(11)	1.360(4)	C(28)-C(29)	1.526(5)
C(10)-H(10A)	0.9300	C(28)-C(29A)	1.532(8)
C(11)-C(15)#1	1.413(3)	C(29)-H(29A)	0.9600
C(11)-H(11A)	0.9300	C(29)-H(29B)	0.9600
C(12)-C(2)#1	1.426(2)	C(29)-H(29C)	0.9600
C(13)-C(3)#1	1.383(2)	C(30)-H(30A)	0.9600
C(13)-C(14)	1.457(3)	C(30)-H(30B)	0.9600
C(14)-C(15)	1.372(3)	C(30)-H(30C)	0.9600
C(14)-C(9)#1	1.411(3)	C(31)-H(31A)	0.9600
C(15)-C(11)#1	1.413(3)	C(31)-H(31B)	0.9600
C(15)-H(15A)	0.9300	C(31)-H(31C)	0.9600
C(16)-C(17)	1.189(2)	C(29A)-H(29D)	0.9600
C(17)-C(18)	1.437(2)	C(29A)-H(29E)	0.9600
C(18)-C(23)	1.388(3)	C(29A)-H(29F)	0.9600
C(18)-C(19)	1.393(3)	C(30A)-H(30D)	0.9600
C(19)-C(20)	1.381(3)	C(30A)-H(30E)	0.9600
C(19)-H(19A)	0.9300	C(30A)-H(30F)	0.9600
C(20)-C(21)	1.395(3)	C(31A)-H(31D)	0.9600
C(20)-C(24)	1.535(3)	C(31A)-H(31E)	0.9600
C(21)-C(22)	1.391(3)	C(31A)-H(31F)	0.9600
C(13)-S(1)-C(12)	90.12(8)	C(12)-C(1)-C(2)	118.08(14)

C(12)-C(1)-C(16)	117.10(15)	C(17)-C(16)-C(1)	169.50(19)
C(2)-C(1)-C(16)	124.82(16)	C(16)-C(17)-C(18)	177.0(2)
C(1)-C(2)-C(12)#1	117.24(15)	C(23)-C(18)-C(19)	119.99(16)
C(1)-C(2)-C(3)	132.15(15)	C(23)-C(18)-C(17)	121.55(17)
C(12)#1-C(2)-C(3)	110.60(14)	C(19)-C(18)-C(17)	118.46(17)
C(13)#1-C(3)-C(2)	111.99(16)	C(20)-C(19)-C(18)	121.04(19)
C(13)#1-C(3)-C(4)	107.41(15)	C(20)-C(19)-H(19A)	119.5
C(2)-C(3)-C(4)	140.60(15)	C(18)-C(19)-H(19A)	119.5
C(5)-C(4)-C(9)	117.26(17)	C(19)-C(20)-C(21)	117.51(18)
C(5)-C(4)-C(3)	137.49(17)	C(19)-C(20)-C(24)	122.41(19)
C(9)-C(4)-C(3)	105.24(15)	C(21)-C(20)-C(24)	120.08(17)
C(4)-C(5)-C(6)	119.03(19)	C(22)-C(21)-C(20)	123.18(17)
C(4)-C(5)-H(5A)	120.5	C(22)-C(21)-H(21A)	118.4
C(6)-C(5)-H(5A)	120.5	C(20)-C(21)-H(21A)	118.4
C(7)-C(6)-C(5)	122.75(19)	C(21)-C(22)-C(23)	117.57(18)
C(7)-C(6)-H(6A)	118.6	C(21)-C(22)-C(28)	122.23(17)
C(5)-C(6)-H(6A)	118.6	C(23)-C(22)-C(28)	120.19(18)
C(6)-C(7)-C(8)	119.94(19)	C(18)-C(23)-C(22)	120.71(18)
C(6)-C(7)-H(7A)	120.0	C(18)-C(23)-H(23A)	119.6
C(8)-C(7)-H(7A)	120.0	C(22)-C(23)-H(23A)	119.6
C(9)-C(8)-C(7)	116.35(19)	C(25)-C(24)-C(27)	108.9(3)
C(9)-C(8)-C(10)	116.0(2)	C(25)-C(24)-C(26)	108.5(3)
C(7)-C(8)-C(10)	127.7(2)	C(27)-C(24)-C(26)	107.0(3)
C(8)-C(9)-C(14)#1	123.44(18)	C(25)-C(24)-C(20)	110.9(2)
C(8)-C(9)-C(4)	124.66(18)	C(27)-C(24)-C(20)	109.3(2)
C(14)#1-C(9)-C(4)	111.90(16)	C(26)-C(24)-C(20)	112.15(19)
C(11)-C(10)-C(8)	120.7(2)	C(24)-C(25)-H(25A)	109.5
C(11)-C(10)-H(10A)	119.7	C(24)-C(25)-H(25B)	109.5
C(8)-C(10)-H(10A)	119.7	H(25A)-C(25)-H(25B)	109.5
C(10)-C(11)-C(15)#1	122.7(2)	C(24)-C(25)-H(25C)	109.5
C(10)-C(11)-H(11A)	118.7	H(25A)-C(25)-H(25C)	109.5
C(15)#1-C(11)-H(11A)	118.7	H(25B)-C(25)-H(25C)	109.5
C(1)-C(12)-C(2)#1	124.68(15)	C(24)-C(26)-H(26A)	109.5
C(1)-C(12)-S(1)	122.72(12)	C(24)-C(26)-H(26B)	109.5
C(2)#1-C(12)-S(1)	112.61(13)	H(26A)-C(26)-H(26B)	109.5
C(3)#1-C(13)-C(14)	110.88(16)	C(24)-C(26)-H(26C)	109.5
C(3)#1-C(13)-S(1)	114.65(14)	H(26A)-C(26)-H(26C)	109.5
C(14)-C(13)-S(1)	134.46(14)	H(26B)-C(26)-H(26C)	109.5
C(15)-C(14)-C(9)#1	119.23(18)	C(24)-C(27)-H(27A)	109.5
C(15)-C(14)-C(13)	136.21(19)	C(24)-C(27)-H(27B)	109.5
C(9)#1-C(14)-C(13)	104.55(15)	H(27A)-C(27)-H(27B)	109.5
C(14)-C(15)-C(11)#1	118.0(2)	C(24)-C(27)-H(27C)	109.5
C(14)-C(15)-H(15A)	121.0	H(27A)-C(27)-H(27C)	109.5
C(11)#1-C(15)-H(15A)	121.0	H(27B)-C(27)-H(27C)	109.5

C(31A)-C(28)-C(31)	46.4(6)	H(29E)-C(29A)-H(29F)	109.5
C(31A)-C(28)-C(30A)	111.1(7)	C(28)-C(30A)-H(30D)	109.5
C(31)-C(28)-C(30A)	144.6(5)	C(28)-C(30A)-H(30E)	109.5
C(31A)-C(28)-C(30)	65.9(6)	H(30D)-C(30A)-H(30E)	109.5
C(31)-C(28)-C(30)	111.1(5)	C(28)-C(30A)-H(30F)	109.5
C(30A)-C(28)-C(30)	48.7(6)	H(30D)-C(30A)-H(30F)	109.5
C(31A)-C(28)-C(29)	132.1(4)	H(30E)-C(30A)-H(30F)	109.5
C(31)-C(28)-C(29)	108.1(4)	C(28)-C(31A)-H(31D)	109.5
C(30A)-C(28)-C(29)	64.0(7)	C(28)-C(31A)-H(31E)	109.5
C(30)-C(28)-C(29)	107.5(4)	H(31D)-C(31A)-H(31E)	109.5
C(31A)-C(28)-C(29A)	105.1(7)	C(28)-C(31A)-H(31F)	109.5
C(31)-C(28)-C(29A)	64.2(5)	H(31D)-C(31A)-H(31F)	109.5
C(30A)-C(28)-C(29A)	109.6(8)	H(31E)-C(31A)-H(31F)	109.5
C(30)-C(28)-C(29A)	138.9(5)		
C(29)-C(28)-C(29A)	47.1(4)		
C(31A)-C(28)-C(22)	114.1(4)		
C(31)-C(28)-C(22)	108.2(3)		
C(30A)-C(28)-C(22)	106.5(4)		
C(30)-C(28)-C(22)	109.4(3)		
C(29)-C(28)-C(22)	112.6(3)		
C(29A)-C(28)-C(22)	110.6(4)		
C(28)-C(29)-H(29A)	109.5		
C(28)-C(29)-H(29B)	109.5		
H(29A)-C(29)-H(29B)	109.5		
C(28)-C(29)-H(29C)	109.5		
H(29A)-C(29)-H(29C)	109.5		
H(29B)-C(29)-H(29C)	109.5		
C(28)-C(30)-H(30A)	109.5		
C(28)-C(30)-H(30B)	109.5		
H(30A)-C(30)-H(30B)	109.5		
C(28)-C(30)-H(30C)	109.5		
H(30A)-C(30)-H(30C)	109.5		
H(30B)-C(30)-H(30C)	109.5		
C(28)-C(31)-H(31A)	109.5		
C(28)-C(31)-H(31B)	109.5		
H(31A)-C(31)-H(31B)	109.5		
C(28)-C(31)-H(31C)	109.5		
H(31A)-C(31)-H(31C)	109.5		
H(31B)-C(31)-H(31C)	109.5		
C(28)-C(29A)-H(29D)	109.5		
C(28)-C(29A)-H(29E)	109.5		
H(29D)-C(29A)-H(29E)	109.5		
C(28)-C(29A)-H(29F)	109.5		
H(29D)-C(29A)-H(29F)	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+1/2,-z