

Facile Preparation of Benzo[4,5]thieno[2,3-*b*]pyridines and Naphtho[*b*-4,5]thieno[2,3-*b*]pyridines via the Reaction of Barton Esters and Benzynes

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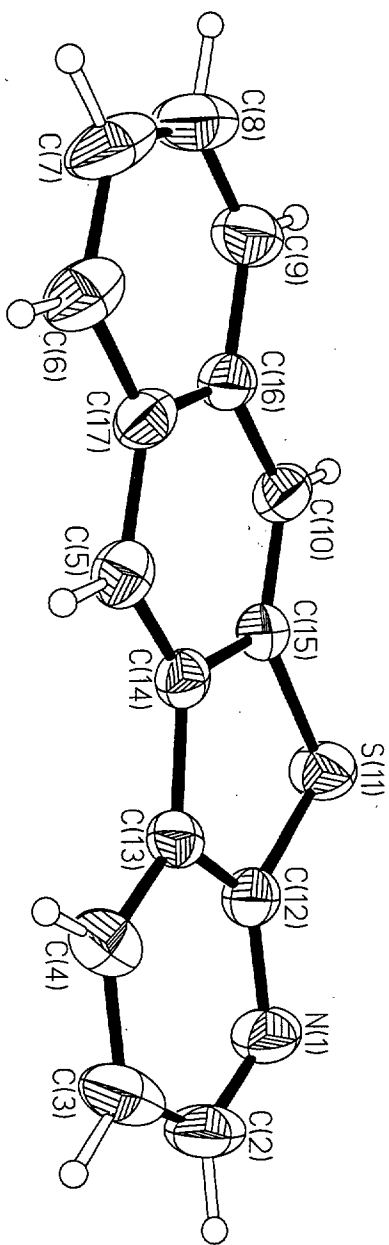


Figure S1: ORTEP of compound 4i

Table S1 Crystal data and structure refinement for 4j.

Identification code	un-128
Empirical formula	C ₁₅ H ₉ N S
Formula weight	235.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 11.770(1) Å alpha = 90 deg. b = 8.865(1) Å beta = 102.957(6) deg. c = 10.948(1) Å gamma = 90 deg.
Volume, Z	1113.2(2) Å ³ , 4
Density (calculated)	1.404 Mg/m ³
Absorption coefficient	0.262 mm ⁻¹
F(000)	488
Crystal size	0.35 x 0.35 x 0.05 mm
Theta range for data collection	1.78 to 25.00 deg.
Limiting indices	-13<=h<=13, -10<=k<=1, -1<=l<=13
Reflections collected	2595
Independent reflections	1957 [R(int) = 0.028]
Absorption correction	N/a
Max. and min. transmission	n/a and n/a
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1800 / 0 / 154
Goodness-of-fit on F ²	1.05
Final R indices [F>4sigma(F)]	R1 = 0.052, wR2 = 0.139
R indices (all data)	R1 = 0.078, wR2 = 0.166
Largest diff. peak and hole	0.52 and -0.23 e.Å ⁻³

Table S2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4i**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	2099(2)	2817(3)	4602(3)	61(1)
C(2)	1468(3)	3735(5)	5132(4)	70(1)
C(3)	1926(3)	4772(5)	6049(3)	69(1)
C(4)	3108(3)	4879(4)	6482(3)	57(1)
C(5)	5919(3)	4467(4)	7078(3)	50(1)
C(6)	8003(3)	4823(5)	8094(3)	66(1)
C(7)	9137(3)	4426(5)	8213(4)	79(1)
C(8)	9451(3)	3321(5)	7441(4)	77(1)
C(9)	8632(3)	2629(4)	6574(4)	65(1)
C(10)	6563(3)	2236(4)	5523(3)	53(1)
S(11)	4208(1)	1796(1)	4432(1)	59(1)
C(12)	3254(3)	2941(3)	5031(3)	47(1)
C(13)	3818(2)	3938(3)	5970(2)	42(1)
C(14)	5075(2)	3747(3)	6231(3)	43(1)
C(15)	5415(2)	2608(3)	5455(3)	42(1)
C(16)	7436(3)	2984(4)	6426(3)	48(1)
C(17)	7108(2)	4106(4)	7200(3)	49(1)

Table S3 Selected bond lengths [Å] and angles [deg] for 4j

N(1)-C(2)	1.320(5)
N(1)-C(12)	1.340(4)
C(2)-C(3)	1.379(6)
C(3)-C(4)	1.370(4)
C(4)-C(13)	1.384(4)
C(5)-C(14)	1.357(4)
C(5)-C(17)	1.412(4)
C(6)-C(7)	1.358(5)
C(6)-C(17)	1.417(4)
C(7)-C(8)	1.397(6)
C(8)-C(9)	1.340(5)
C(9)-C(16)	1.415(4)
C(10)-C(15)	1.377(4)
C(10)-C(16)	1.421(4)
S(11)-C(12)	1.747(3)
S(11)-C(15)	1.755(3)
C(12)-C(13)	1.405(4)
C(13)-C(14)	1.453(4)
C(14)-C(15)	1.433(4)
C(16)-C(17)	1.416(4)
C(2)-N(1)-C(12)	115.0(3)
N(1)-C(2)-C(3)	124.4(3)
C(4)-C(3)-C(2)	119.9(3)
C(3)-C(4)-C(13)	118.5(3)
C(14)-C(5)-C(17)	121.1(3)
C(7)-C(6)-C(17)	120.8(4)
C(6)-C(7)-C(8)	120.8(3)
C(9)-C(8)-C(7)	120.2(3)
C(8)-C(9)-C(16)	121.3(4)
C(15)-C(10)-C(16)	118.2(3)
C(12)-S(11)-C(15)	91.05(14)
N(1)-C(12)-C(13)	125.7(3)
N(1)-C(12)-S(11)	120.5(3)
C(13)-C(12)-S(11)	113.8(2)
C(4)-C(13)-C(12)	116.6(3)
C(4)-C(13)-C(14)	132.1(3)
C(12)-C(13)-C(14)	111.3(3)
C(5)-C(14)-C(15)	118.5(3)
C(5)-C(14)-C(13)	129.6(3)
C(15)-C(14)-C(13)	111.9(2)
C(10)-C(15)-C(14)	122.6(3)
C(10)-C(15)-S(11)	125.5(2)
C(14)-C(15)-S(11)	111.9(2)
C(9)-C(16)-C(17)	119.1(3)
C(9)-C(16)-C(10)	121.4(3)
C(17)-C(16)-C(10)	119.5(3)
C(5)-C(17)-C(16)	120.0(3)
C(5)-C(17)-C(6)	122.1(3)
C(16)-C(17)-C(6)	117.9(3)

Symmetry transformations used to generate equivalent atoms:

Table S4 Bond lengths [Å] and angles [deg] for 4j

N(1)-C(2)	1.320(5)
N(1)-C(12)	1.340(4)
C(2)-C(3)	1.379(6)
C(3)-C(4)	1.370(4)
C(4)-C(13)	1.384(4)
C(5)-C(14)	1.357(4)
C(5)-C(17)	1.412(4)
C(6)-C(7)	1.358(5)
C(6)-C(17)	1.417(4)
C(7)-C(8)	1.397(6)
C(8)-C(9)	1.340(5)
C(9)-C(16)	1.415(4)
C(10)-C(15)	1.377(4)
C(10)-C(16)	1.421(4)
S(11)-C(12)	1.747(3)
S(11)-C(15)	1.755(3)
C(12)-C(13)	1.405(4)
C(13)-C(14)	1.453(4)
C(14)-C(15)	1.433(4)
C(16)-C(17)	1.416(4)
C(2)-N(1)-C(12)	115.0(3)
N(1)-C(2)-C(3)	124.4(3)
C(4)-C(3)-C(2)	119.9(3)
C(3)-C(4)-C(13)	118.5(3)
C(14)-C(5)-C(17)	121.1(3)
C(7)-C(6)-C(17)	120.8(4)
C(6)-C(7)-C(8)	120.8(3)
C(9)-C(8)-C(7)	120.2(3)
C(8)-C(9)-C(16)	121.3(4)
C(15)-C(10)-C(16)	118.2(3)
C(12)-S(11)-C(15)	91.05(14)
N(1)-C(12)-C(13)	125.7(3)
N(1)-C(12)-S(11)	120.5(3)
C(13)-C(12)-S(11)	113.8(2)
C(4)-C(13)-C(12)	116.6(3)
C(4)-C(13)-C(14)	132.1(3)
C(12)-C(13)-C(14)	111.3(3)
C(5)-C(14)-C(15)	118.5(3)
C(5)-C(14)-C(13)	129.6(3)
C(15)-C(14)-C(13)	111.9(2)
C(10)-C(15)-C(14)	122.6(3)
C(10)-C(15)-S(11)	125.5(2)
C(14)-C(15)-S(11)	111.9(2)
C(9)-C(16)-C(17)	119.1(3)
C(9)-C(16)-C(10)	121.4(3)
C(17)-C(16)-C(10)	119.5(3)
C(5)-C(17)-C(16)	120.0(3)
C(5)-C(17)-C(6)	122.1(3)
C(16)-C(17)-C(6)	117.9(3)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4j**
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	41(1)	72(2)	66(2)	9(2)	0(1)	-4(1)
C(2)	35(2)	95(3)	78(2)	25(2)	8(2)	9(2)
C(3)	51(2)	89(3)	70(2)	14(2)	21(2)	26(2)
C(4)	58(2)	62(2)	50(2)	6(2)	15(2)	13(2)
C(5)	55(2)	49(2)	45(2)	0(1)	12(1)	-6(1)
C(6)	62(2)	80(2)	55(2)	-3(2)	6(2)	-23(2)
C(7)	55(2)	112(3)	59(2)	15(2)	-8(2)	-38(2)
C(8)	39(2)	113(3)	75(2)	30(2)	5(2)	-4(2)
C(9)	49(2)	74(2)	73(2)	13(2)	15(2)	7(2)
C(10)	49(2)	52(2)	56(2)	5(2)	4(1)	-9(1)
S(11)	48(1)	58(1)	66(1)	-15(1)	3(1)	-2(1)
C(12)	46(2)	50(2)	46(2)	10(1)	12(1)	0(1)
C(13)	41(1)	45(2)	41(1)	12(1)	10(1)	4(1)
C(14)	45(2)	41(2)	42(1)	7(1)	10(1)	-3(1)
C(15)	45(2)	37(1)	42(1)	0(1)	10(1)	0(1)
C(16)	42(2)	51(2)	50(2)	11(1)	9(1)	-2(1)
C(17)	43(2)	54(2)	47(2)	8(1)	5(1)	-11(1)

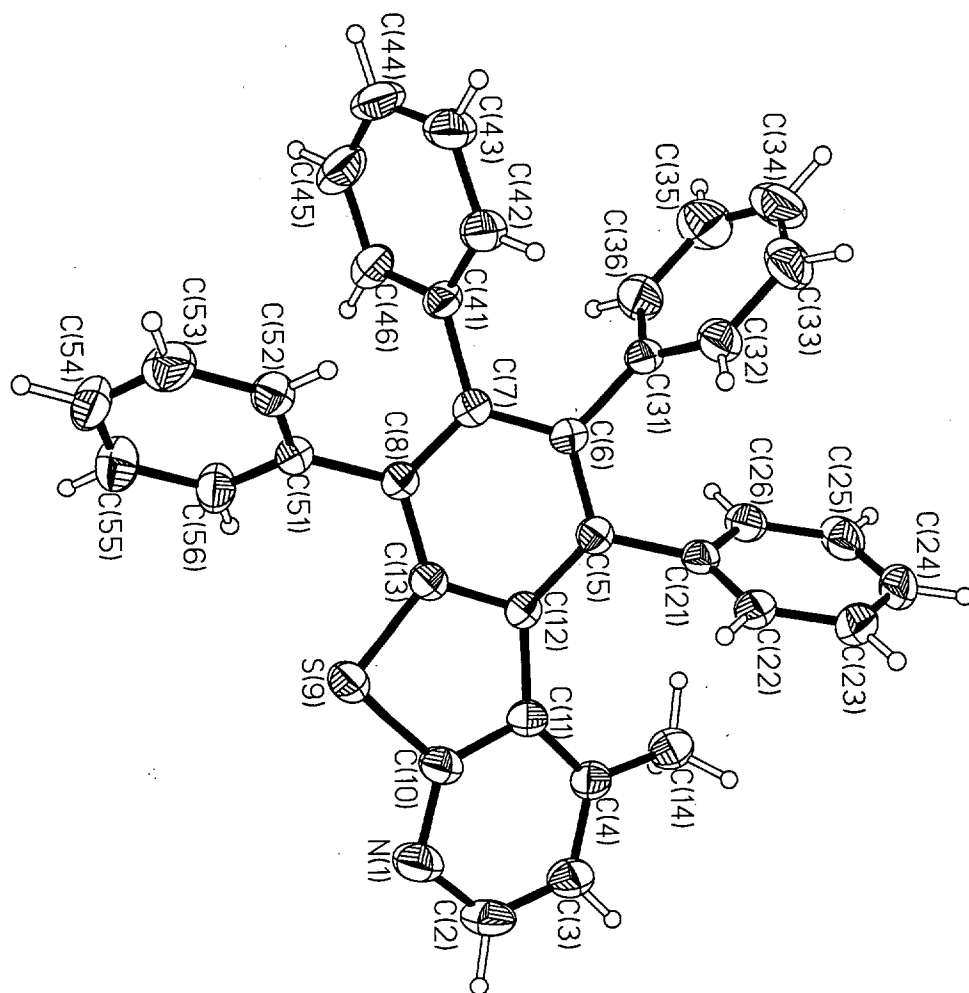


Figure S2 ORTEP for Compound 4f

Table S6 Crystal data and structure refinement for 4f.

Identification code	un-173_3
Empirical formula	C36 H25 N S
Formula weight	503.63
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.5548(6) Å alpha = 93.767(5) deg. b = 11.3399(8) Å beta = 108.738(4) deg. c = 11.6741(6) Å gamma = 90.062(5) deg.
Volume, Z	1319.99(14) Å ³ , 2
Density (calculated)	1.267 Mg/m ³
Absorption coefficient	0.149 mm ⁻¹
F(000)	528
Crystal size	0.30 x 0.25 x 0.10 mm
Theta range for data collection	1.80 to 24.99 deg.
Limiting indices	0 ≤ h ≤ 12, -11 ≤ k ≤ 11, -12 ≤ l ≤ 11
Reflections collected	3618
Independent reflections	3400 [R(int) = 0.0233]
Absorption correction	N/a
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3129 / 0 / 344
Goodness-of-fit on F ²	1.04
Final R indices [F > 4σ(F)]	R1 = 0.041, wR2 = 0.096
R indices (all data)	R1 = 0.064, wR2 = 0.108
Extinction coefficient	0.019(2)
Largest diff. peak and hole	0.23 and -0.15 e.Å ⁻³

Table 2. Atomic coordinates (× 10⁴) and equivalent isotropic

Table S7 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4f. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
N(1)	104(2)	9468(2)	6677(2)	63(1)
C(2)	-951(3)	9095(3)	5738(3)	67(1)
C(3)	-1816(3)	8218(3)	5797(2)	58(1)
C(4)	-1695(2)	7681(2)	6855(2)	47(1)
C(5)	-862(2)	7234(2)	9893(2)	41(1)
C(6)	-158(2)	7072(2)	11114(2)	42(1)
C(7)	1147(2)	7526(2)	11672(2)	42(1)
C(8)	1748(2)	8223(2)	11039(2)	42(1)
S(9)	1606(1)	9316(1)	8957(1)	61(1)
C(10)	193(3)	8972(2)	7708(2)	51(1)
C(11)	-679(2)	8132(2)	7909(2)	43(1)
C(12)	-228(2)	7850(2)	9199(2)	40(1)
C(13)	1036(2)	8376(2)	9821(2)	45(1)
C(14)	-2584(3)	6617(3)	6750(2)	60(1)
C(21)	-2307(2)	6870(2)	9427(2)	42(1)
C(22)	-3270(2)	7718(2)	9115(2)	50(1)
C(23)	-4619(3)	7412(3)	8770(2)	61(1)
C(24)	-5013(3)	6254(3)	8736(2)	68(1)
C(25)	-4075(3)	5396(3)	9031(2)	62(1)
C(26)	-2722(3)	5696(2)	9379(2)	51(1)
C(31)	-819(2)	6442(2)	11868(2)	45(1)
C(32)	-1817(3)	6980(3)	12222(2)	58(1)
C(33)	-2406(3)	6416(4)	12944(3)	77(1)
C(34)	-1983(4)	5335(4)	13343(3)	90(1)
C(35)	-998(4)	4795(3)	12998(3)	88(1)
C(36)	-429(3)	5342(3)	12254(3)	65(1)
C(41)	1914(2)	7308(2)	12963(2)	44(1)
C(42)	1496(3)	7738(2)	13913(2)	56(1)
C(43)	2261(4)	7570(3)	15103(3)	73(1)
C(44)	3435(4)	6980(3)	15341(3)	82(1)
C(45)	3852(3)	6535(3)	14413(3)	76(1)
C(46)	3101(3)	6698(2)	13225(3)	56(1)
C(51)	3093(2)	8806(2)	11614(2)	44(1)
C(52)	3346(3)	9564(2)	12648(2)	52(1)
C(53)	4610(3)	10069(3)	13196(3)	70(1)
C(54)	5609(3)	9838(3)	12708(3)	78(1)
C(55)	5364(3)	9111(3)	11683(3)	75(1)
C(56)	4121(2)	8588(3)	11143(3)	59(1)

Table S8 Selected bond lengths [Å] and angles [deg] for 4f.

N(1)-C(2)	1.332(4)
N(1)-C(10)	1.339(3)
C(2)-C(3)	1.370(4)
C(3)-C(4)	1.382(4)
C(4)-C(11)	1.413(3)
C(4)-C(14)	1.501(4)
C(5)-C(6)	1.404(3)
C(5)-C(12)	1.419(3)
C(5)-C(21)	1.493(3)
C(6)-C(7)	1.402(3)
C(6)-C(31)	1.500(3)
C(7)-C(8)	1.397(3)
C(7)-C(41)	1.501(3)
C(8)-C(13)	1.401(3)
C(8)-C(51)	1.493(3)
S(9)-C(10)	1.740(3)
S(9)-C(13)	1.745(2)
C(10)-C(11)	1.406(3)
C(11)-C(12)	1.483(3)
C(12)-C(13)	1.407(3)
C(2)-N(1)-C(10)	114.2(2)
N(1)-C(2)-C(3)	123.0(3)
C(2)-C(3)-C(4)	122.5(3)
C(3)-C(4)-C(11)	116.8(2)
C(3)-C(4)-C(14)	116.7(2)
C(11)-C(4)-C(14)	126.3(2)
C(6)-C(5)-C(12)	119.2(2)
C(6)-C(5)-C(21)	117.6(2)
C(12)-C(5)-C(21)	122.8(2)
C(7)-C(6)-C(5)	121.6(2)
C(7)-C(6)-C(31)	118.3(2)
C(5)-C(6)-C(31)	120.0(2)
C(8)-C(7)-C(6)	120.1(2)
C(8)-C(7)-C(41)	118.5(2)
C(6)-C(7)-C(41)	121.3(2)
C(7)-C(8)-C(13)	117.5(2)
C(7)-C(8)-C(51)	122.6(2)
C(13)-C(8)-C(51)	119.9(2)
C(10)-S(9)-C(13)	90.65(12)
N(1)-C(10)-C(11)	128.2(2)
N(1)-C(10)-S(9)	117.6(2)
C(11)-C(10)-S(9)	114.0(2)
C(10)-C(11)-C(4)	114.7(2)
C(10)-C(11)-C(12)	110.4(2)
C(4)-C(11)-C(12)	134.6(2)
C(13)-C(12)-C(5)	117.1(2)
C(13)-C(12)-C(11)	110.7(2)
C(5)-C(12)-C(11)	132.1(2)
C(8)-C(13)-C(12)	123.9(2)
C(8)-C(13)-S(9)	122.4(2)
C(12)-C(13)-S(9)	113.6(2)

Table S9 Bond lengths [Å] and angles [deg] for 4f.

N(1)-C(2)	1.332(4)
N(1)-C(10)	1.339(3)
C(2)-C(3)	1.370(4)
C(3)-C(4)	1.382(4)
C(4)-C(11)	1.413(3)
C(4)-C(14)	1.501(4)
C(5)-C(6)	1.404(3)
C(5)-C(12)	1.419(3)
C(5)-C(21)	1.493(3)
C(6)-C(7)	1.402(3)
C(6)-C(31)	1.500(3)
C(7)-C(8)	1.397(3)
C(7)-C(41)	1.501(3)
C(8)-C(13)	1.401(3)
C(8)-C(51)	1.493(3)
S(9)-C(10)	1.740(3)
S(9)-C(13)	1.745(2)
C(10)-C(11)	1.406(3)
C(11)-C(12)	1.483(3)
C(12)-C(13)	1.407(3)
C(21)-C(22)	1.379(3)
C(21)-C(26)	1.393(3)
C(22)-C(23)	1.386(3)
C(23)-C(24)	1.372(4)
C(24)-C(25)	1.368(4)
C(25)-C(26)	1.388(4)
C(31)-C(36)	1.372(4)
C(31)-C(32)	1.379(4)
C(32)-C(33)	1.383(4)
C(33)-C(34)	1.365(5)
C(34)-C(35)	1.363(5)
C(35)-C(36)	1.380(4)
C(41)-C(42)	1.382(4)
C(41)-C(46)	1.387(3)
C(42)-C(43)	1.390(4)
C(43)-C(44)	1.365(5)
C(44)-C(45)	1.363(5)
C(45)-C(46)	1.383(4)
C(51)-C(56)	1.380(3)
C(51)-C(52)	1.387(4)
C(52)-C(53)	1.385(4)
C(53)-C(54)	1.368(4)
C(54)-C(55)	1.360(5)
C(55)-C(56)	1.375(4)
C(2)-N(1)-C(10)	114.2(2)
N(1)-C(2)-C(3)	123.0(3)
C(2)-C(3)-C(4)	122.5(3)
C(3)-C(4)-C(11)	116.8(2)
C(3)-C(4)-C(14)	116.7(2)
C(11)-C(4)-C(14)	126.3(2)
C(6)-C(5)-C(12)	119.2(2)
C(6)-C(5)-C(21)	117.6(2)
C(12)-C(5)-C(21)	122.8(2)

Table S9; con't

C(7)-C(6)-C(5)	121.6(2)
C(7)-C(6)-C(31)	118.3(2)
C(5)-C(6)-C(31)	120.0(2)
C(8)-C(7)-C(6)	120.1(2)
C(8)-C(7)-C(41)	118.5(2)
C(6)-C(7)-C(41)	121.3(2)
C(7)-C(8)-C(13)	117.5(2)
C(7)-C(8)-C(51)	122.6(2)
C(13)-C(8)-C(51)	119.9(2)
C(10)-S(9)-C(13)	90.65(12)
N(1)-C(10)-C(11)	128.2(2)
N(1)-C(10)-S(9)	117.6(2)
C(11)-C(10)-S(9)	114.0(2)
C(10)-C(11)-C(4)	114.7(2)
C(10)-C(11)-C(12)	110.4(2)
C(4)-C(11)-C(12)	134.6(2)
C(13)-C(12)-C(5)	117.1(2)
C(13)-C(12)-C(11)	110.7(2)
C(5)-C(12)-C(11)	132.1(2)
C(8)-C(13)-C(12)	123.9(2)
C(8)-C(13)-S(9)	122.4(2)
C(12)-C(13)-S(9)	113.6(2)
C(22)-C(21)-C(26)	118.4(2)
C(22)-C(21)-C(5)	119.7(2)
C(26)-C(21)-C(5)	121.7(2)
C(21)-C(22)-C(23)	120.8(3)
C(24)-C(23)-C(22)	120.1(3)
C(25)-C(24)-C(23)	120.0(3)
C(24)-C(25)-C(26)	120.2(3)
C(25)-C(26)-C(21)	120.4(3)
C(36)-C(31)-C(32)	118.3(3)
C(36)-C(31)-C(6)	121.6(2)
C(32)-C(31)-C(6)	120.1(2)
C(31)-C(32)-C(33)	120.4(3)
C(34)-C(33)-C(32)	120.5(3)
C(35)-C(34)-C(33)	119.5(3)
C(34)-C(35)-C(36)	120.2(3)
C(31)-C(36)-C(35)	121.1(3)
C(42)-C(41)-C(46)	118.5(2)
C(42)-C(41)-C(7)	121.6(2)
C(46)-C(41)-C(7)	119.8(2)
C(41)-C(42)-C(43)	120.3(3)
C(44)-C(43)-C(42)	120.2(3)
C(45)-C(44)-C(43)	120.2(3)
C(44)-C(45)-C(46)	120.2(3)
C(45)-C(46)-C(41)	120.6(3)
C(56)-C(51)-C(52)	118.4(2)
C(56)-C(51)-C(8)	120.9(2)
C(52)-C(51)-C(8)	120.7(2)
C(53)-C(52)-C(51)	120.2(3)
C(54)-C(53)-C(52)	120.2(3)
C(55)-C(54)-C(53)	120.1(3)
C(54)-C(55)-C(56)	120.3(3)
C(55)-C(56)-C(51)	120.9(3)

Table S10 Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4f.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
N(1)	75(2)	74(2)	42(1)	14(1)	18(1)	-9(1)
C(2)	86(2)	76(2)	38(2)	15(2)	18(2)	2(2)
C(3)	64(2)	71(2)	36(2)	3(1)	10(1)	-3(2)
C(4)	47(2)	57(2)	36(1)	0(1)	12(1)	0(1)
C(5)	41(1)	43(2)	39(1)	3(1)	11(1)	-2(1)
C(6)	41(1)	46(2)	37(1)	7(1)	10(1)	0(1)
C(7)	40(1)	46(2)	39(1)	4(1)	11(1)	2(1)
C(8)	39(1)	48(2)	37(1)	2(1)	11(1)	-4(1)
S(9)	59(1)	77(1)	45(1)	10(1)	13(1)	-24(1)
C(10)	56(2)	60(2)	38(2)	8(1)	16(1)	-6(1)
C(11)	46(1)	49(2)	34(1)	2(1)	12(1)	0(1)
C(12)	38(1)	45(2)	36(1)	2(1)	9(1)	-4(1)
C(13)	44(1)	52(2)	39(2)	3(1)	14(1)	-7(1)
C(14)	59(2)	75(2)	37(2)	-5(1)	8(1)	-11(2)
C(21)	44(1)	51(2)	30(1)	3(1)	10(1)	-8(1)
C(22)	48(2)	60(2)	38(1)	4(1)	9(1)	-6(1)
C(23)	46(2)	91(2)	43(2)	7(2)	10(1)	2(2)
C(24)	45(2)	108(3)	49(2)	1(2)	11(1)	-23(2)
C(25)	68(2)	70(2)	49(2)	-4(2)	20(2)	-30(2)
C(26)	56(2)	53(2)	42(2)	4(1)	14(1)	-9(1)
C(31)	42(1)	52(2)	36(1)	8(1)	7(1)	-7(1)
C(32)	60(2)	68(2)	48(2)	2(1)	21(2)	-7(2)
C(33)	77(2)	106(3)	57(2)	-16(2)	37(2)	-25(2)
C(34)	110(3)	100(3)	64(2)	14(2)	35(2)	-44(3)
C(35)	102(3)	73(2)	89(3)	33(2)	24(2)	-17(2)
C(36)	64(2)	61(2)	73(2)	24(2)	21(2)	-2(2)
C(41)	43(2)	47(2)	36(1)	5(1)	4(1)	-9(1)
C(42)	59(2)	62(2)	43(2)	7(1)	11(1)	-8(1)
C(43)	86(2)	87(2)	40(2)	5(2)	12(2)	-29(2)
C(44)	85(3)	91(3)	47(2)	27(2)	-13(2)	-27(2)
C(45)	60(2)	70(2)	75(2)	25(2)	-14(2)	-6(2)
C(46)	48(2)	53(2)	58(2)	6(1)	1(1)	-1(1)
C(51)	41(1)	50(2)	39(1)	8(1)	8(1)	-4(1)
C(52)	53(2)	53(2)	47(2)	4(1)	13(1)	-6(1)
C(53)	78(2)	62(2)	57(2)	1(2)	3(2)	-20(2)
C(54)	46(2)	91(3)	80(2)	18(2)	-4(2)	-21(2)
C(55)	45(2)	93(3)	86(2)	11(2)	19(2)	0(2)
C(56)	43(2)	70(2)	63(2)	-2(2)	18(2)	-6(1)

Table S11 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4f.

	x	y	z	U(eq)
H(2)	-1106(3)	9447(3)	5008(3)	80
H(3)	-2511(3)	7974(3)	5099(2)	70
H(14A)	-2414(3)	6320(3)	7535(2)	89
H(14B)	-2402(3)	6016(3)	6210(2)	89
H(14C)	-3504(3)	6836(3)	6439(2)	89
H(14D)	-3132(3)	6461(3)	5920(2)	89
H(14E)	-3145(3)	6765(3)	7246(2)	89
H(14F)	-2043(3)	5945(3)	7017(2)	89
H(22)	-3011(2)	8506(2)	9135(2)	60
H(23)	-5258(3)	7993(3)	8561(2)	73
H(24)	-5918(3)	6051(3)	8512(2)	82
H(25)	-4344(3)	4610(3)	8998(2)	75
H(26)	-2089(3)	5109(2)	9582(2)	61
H(32)	-2095(3)	7726(3)	11973(2)	69
H(33)	-3095(3)	6777(4)	13160(3)	93
H(34)	-2364(4)	4969(4)	13848(3)	107
H(35)	-708(4)	4057(3)	13263(3)	106
H(36)	230(3)	4959(3)	12010(3)	79
H(42)	698(3)	8143(2)	13756(2)	67
H(43)	1973(4)	7861(3)	15739(3)	88
H(44)	3951(4)	6882(3)	16139(3)	98
H(45)	4643(3)	6120(3)	14579(3)	91
H(46)	3395(3)	6397(2)	12597(3)	68
H(52)	2665(3)	9734(2)	12974(2)	62
H(53)	4780(3)	10567(3)	13896(3)	84
H(54)	6457(3)	10179(3)	13078(3)	93
H(55)	6041(3)	8967(3)	11346(3)	90
H(56)	3969(2)	8081(3)	10451(3)	71