Monomeric Thorium Chalcogenolates with Bipyridine and Terpyridine Ligands

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Supporting Information (SI)

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1. X-ray powder diffraction profiles and the profiles of calculated diffraction patterns for $(bipy)_2Th(SPh)_4$ (1), $(bipy)_2Th(SePh)_4$·py (2), $(bipy)_2Th(SC_6F_5)_4$· 2THF (3), and **$(bipy)_2Th(SeC_6F_5)_4$ · 2THF (4), (py)(terpy)$Th(SPh)_4$· 2py (5).**

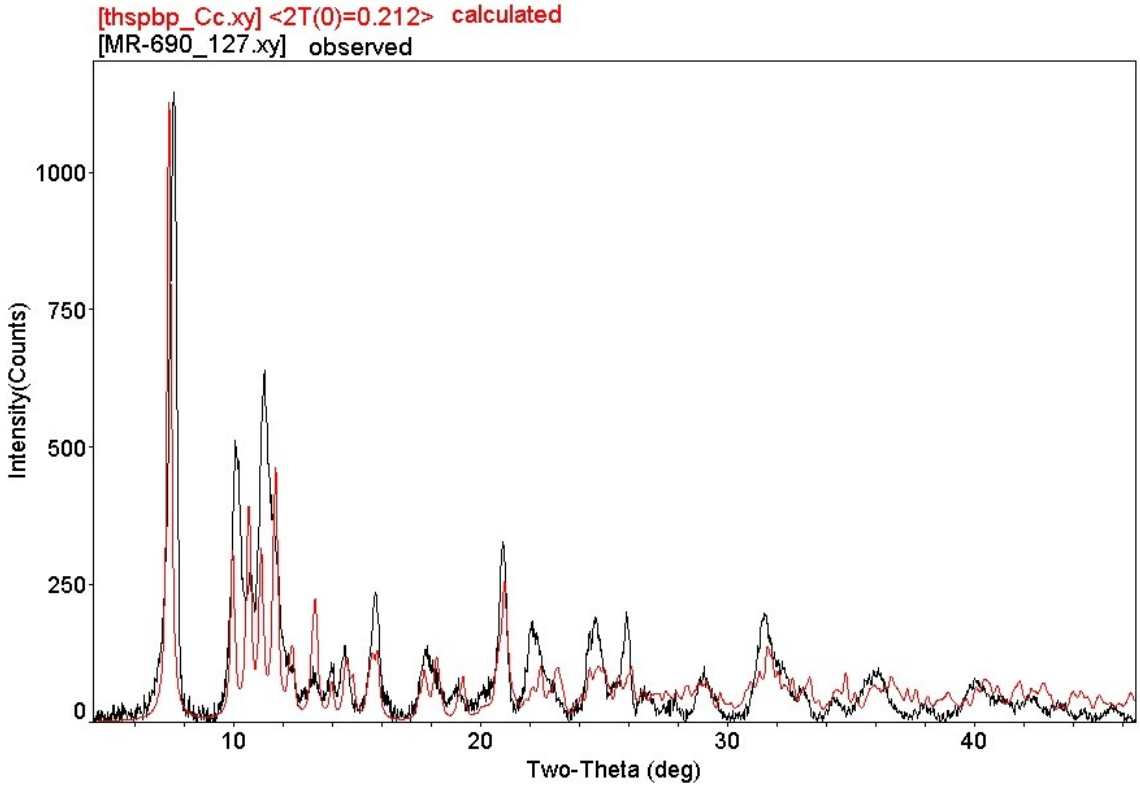

Figure *S*1. PXRD and calculated pattern from single crystal (in red) for **$(bipy)_2Th(SPh)_4$ (1).**

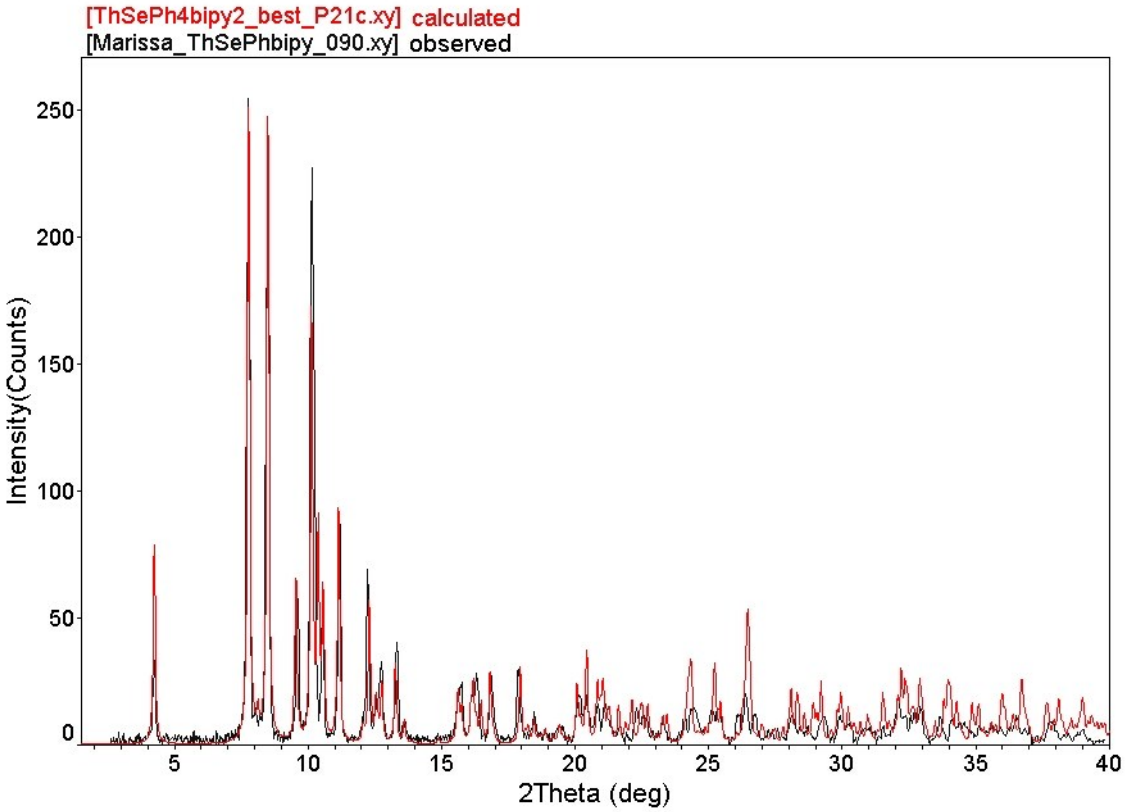

Figure *S*2. PXRD and calculated pattern from single crystal (in red) for **$(bipy)_2Th(SePh)_4py$ (2).**

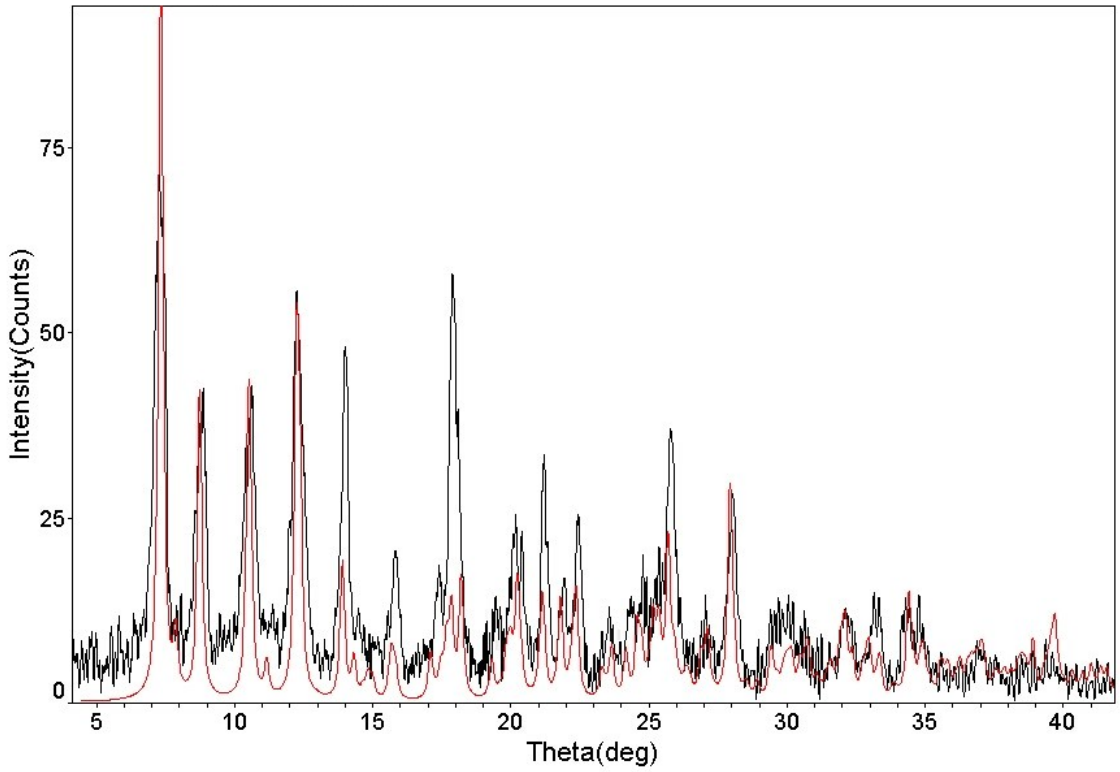

Figure S3. PXRD and calculated pattern from single crystal (in red) for **$(bipy)_2Th(SC_6F_5)_4 \cdot 2THF$ (3).**

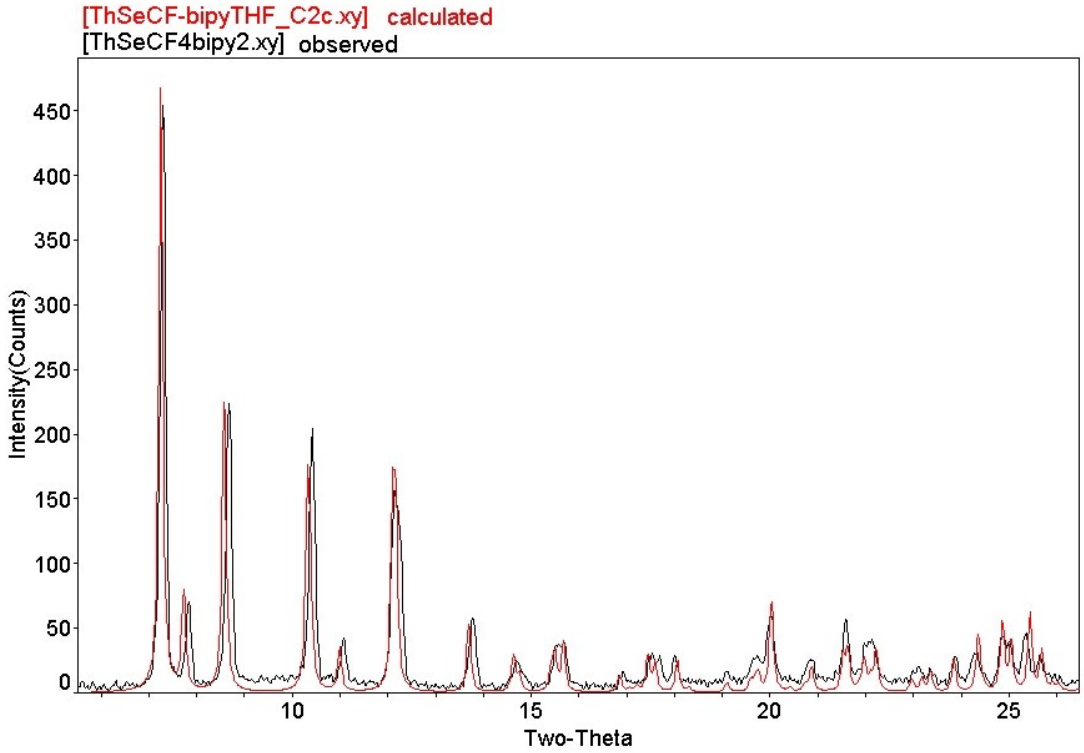

Figure S4. PXRD and calculated pattern from single crystal (in red) for **$(bipy)_2Th(SeC_6F_5)_4 \cdot 2THF$ (4).**

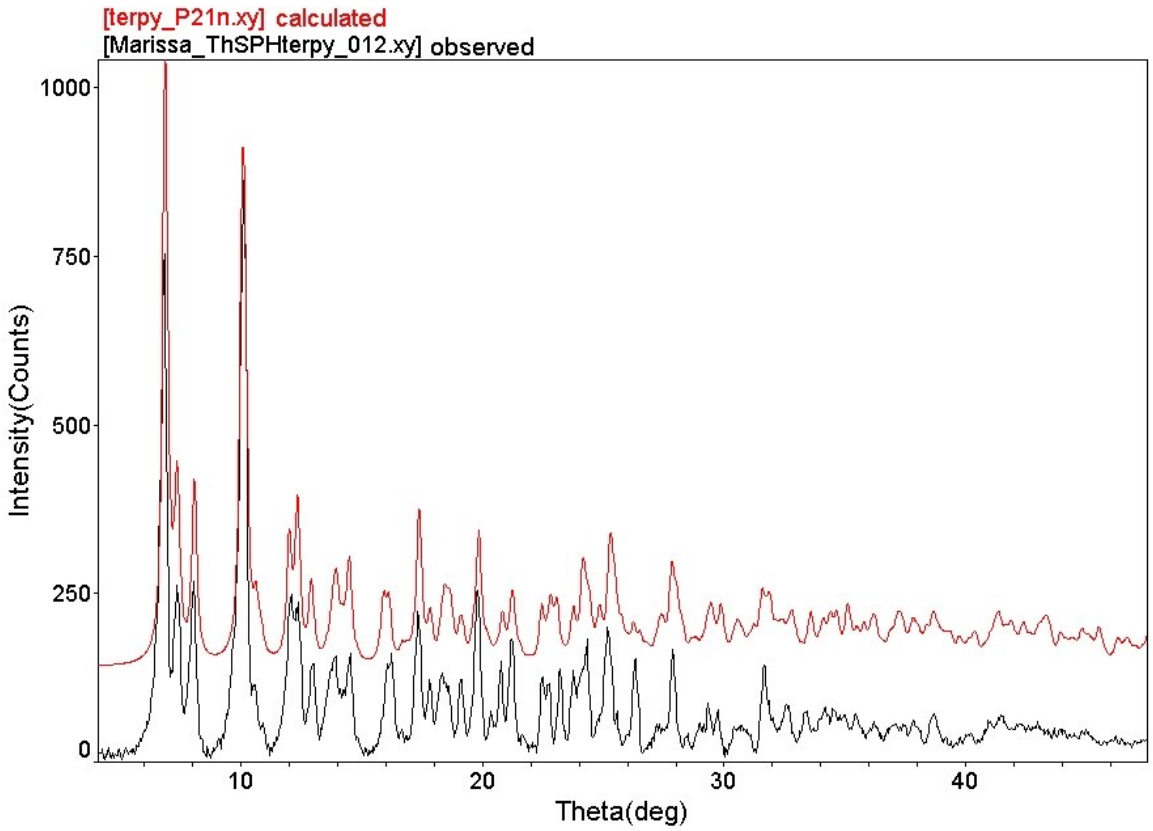

Figure S5. PXRD and calculated pattern from single crystal (in red) for **(py)(terpy)Th(SPh)$_4$·2py (5).**

2. ^{1}H NMR data for all four compounds

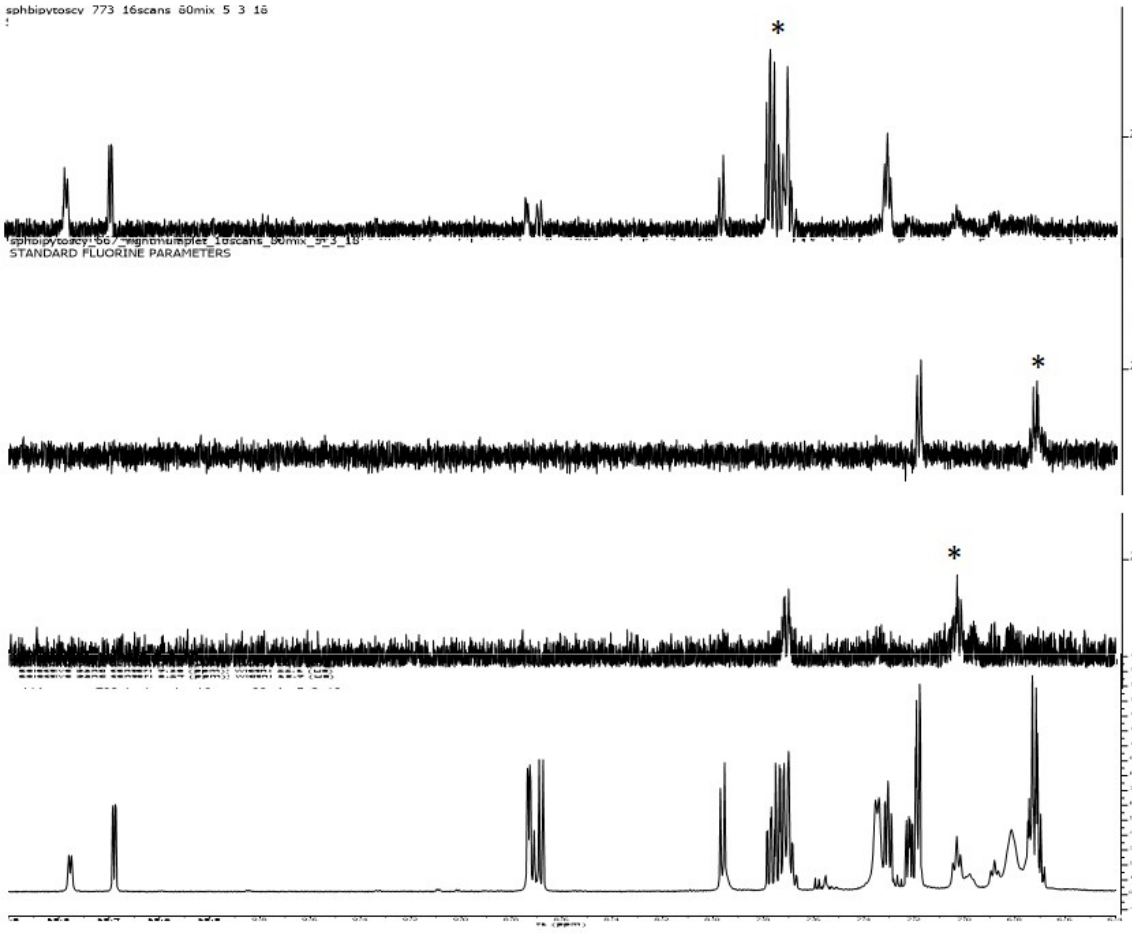

Figure *S*6. ^{1}H NMR (pyridine- d_5) spectrum of **Th(SPh)$_4$(bipy) (1)** (bottom) and 1D TOCSY experiments applied to the SPh (second and third spectra) and bipy (top) resonances respectively. (* indicates excited peak)

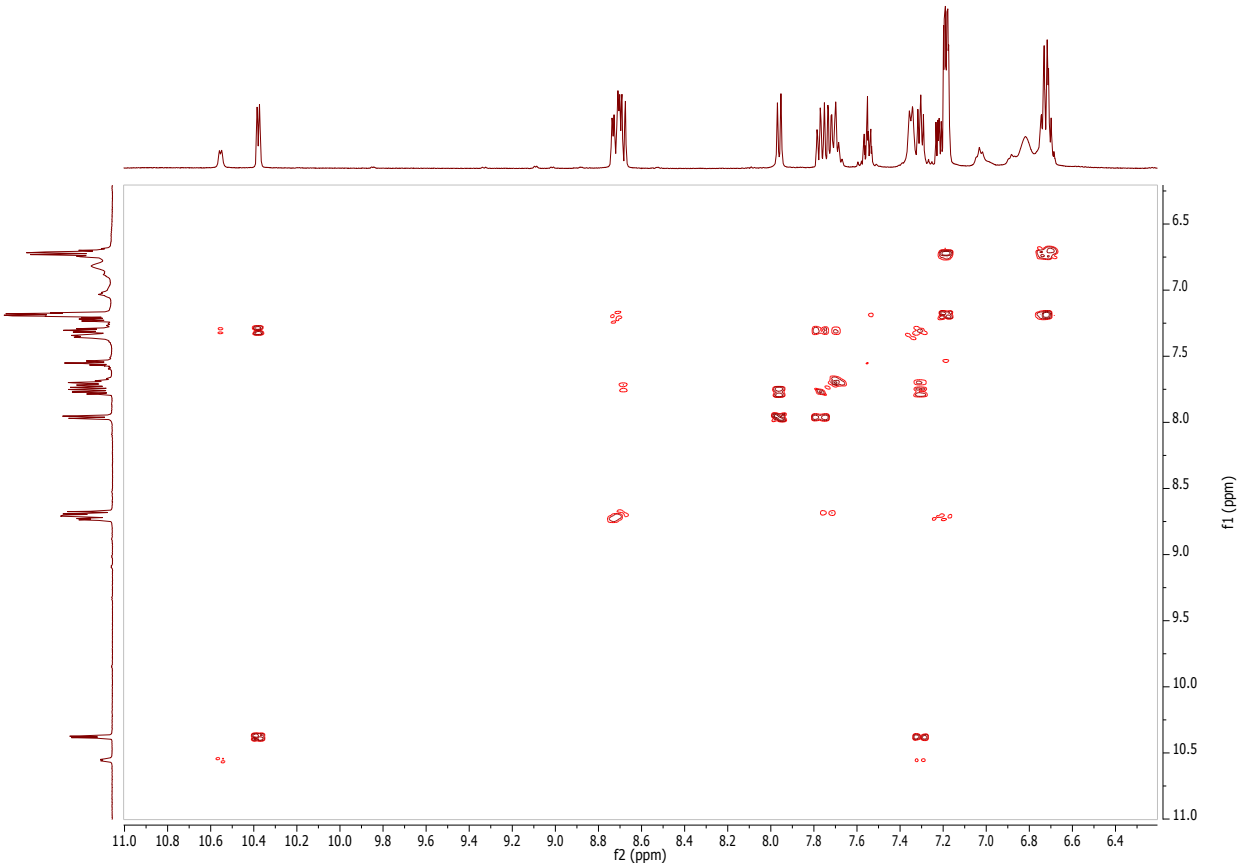

Figure *S*7. Two-dimensional ^{1}H-^{1}H correlation spectroscopy (COSY) NMR (pyridine- d_5) of **Th(SPh)$_4$(bipy) (1).**

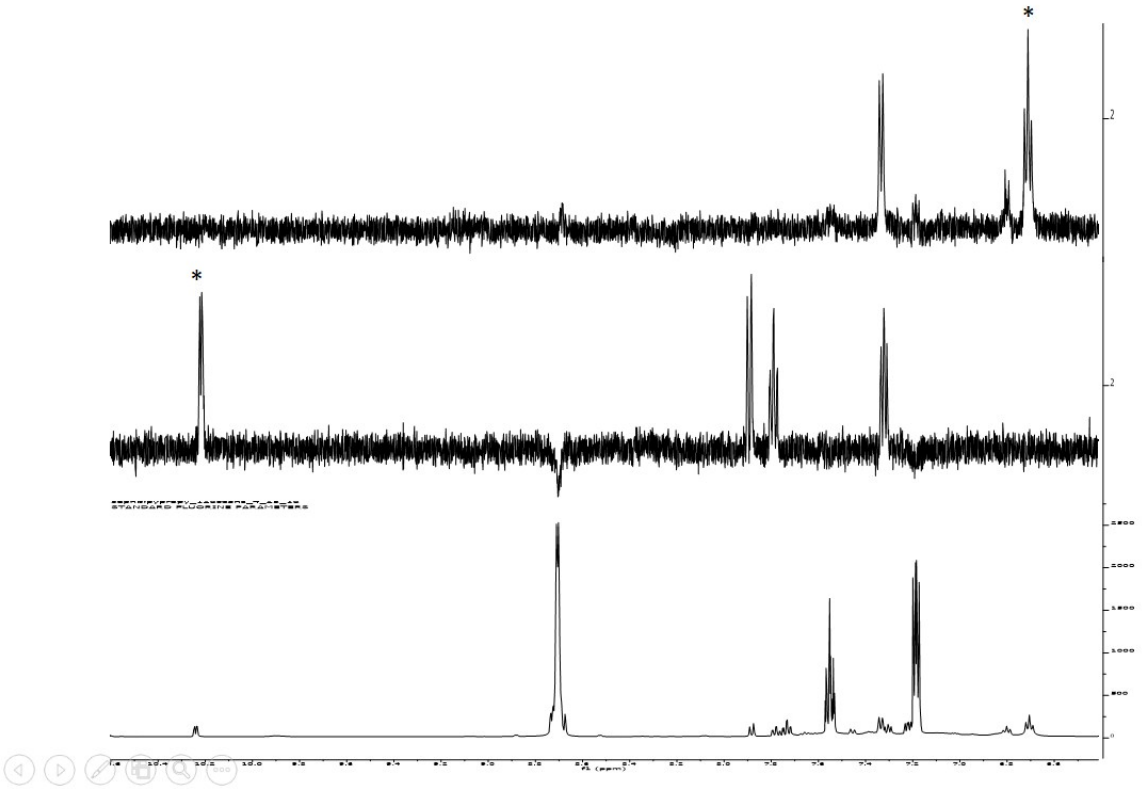

Figure *S*8. ^{1}H NMR (pyridine- d_5) spectrum of **Th(SePh)$_4$(bipy)·Py (2)** (bottom) and 1D TOCSY experiments (top and middle) applied to the SePh and bipy resonances respectively.

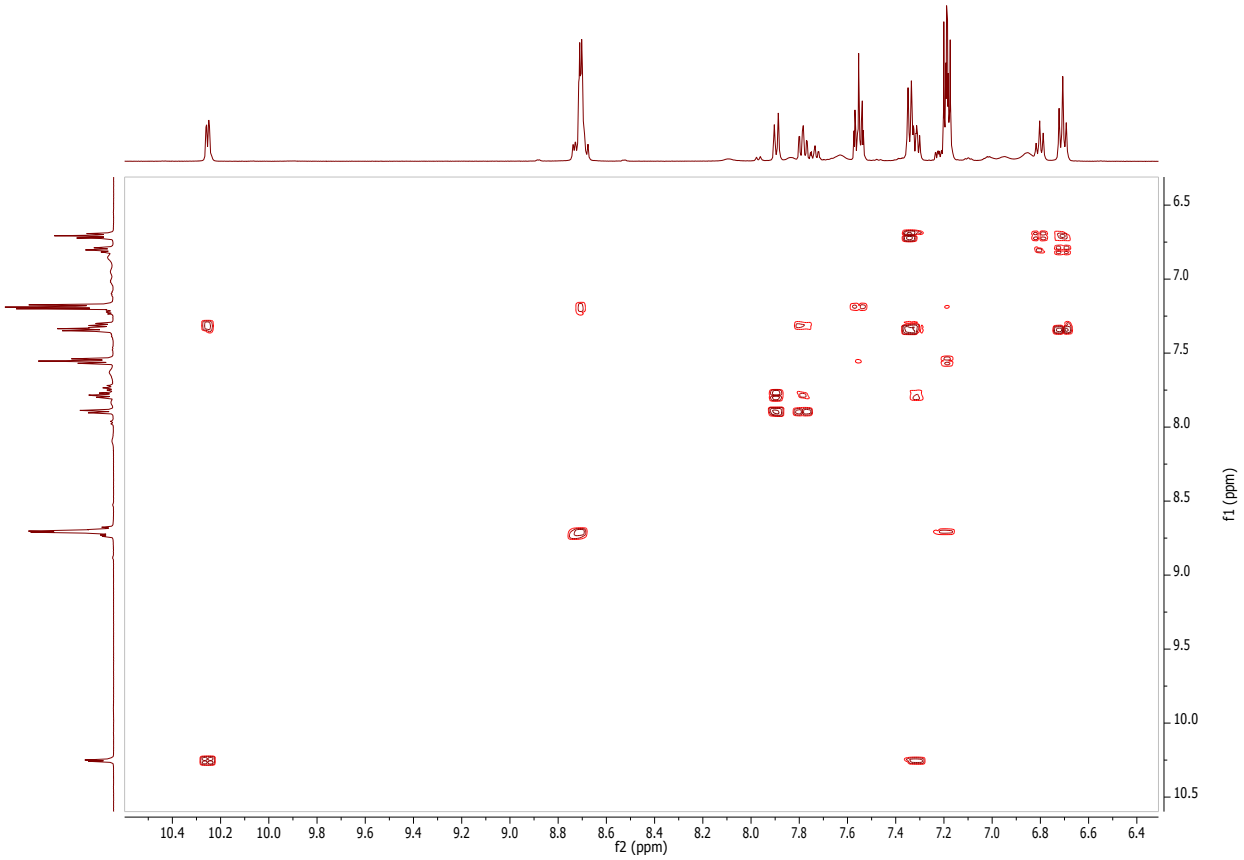

Figure *S*9. Two-dimensional ^{1}H-^{1}H correlation spectroscopy (COSY) NMR (pyridine- d_5) of **Th(SePh)$_4$(bipy) (2).**

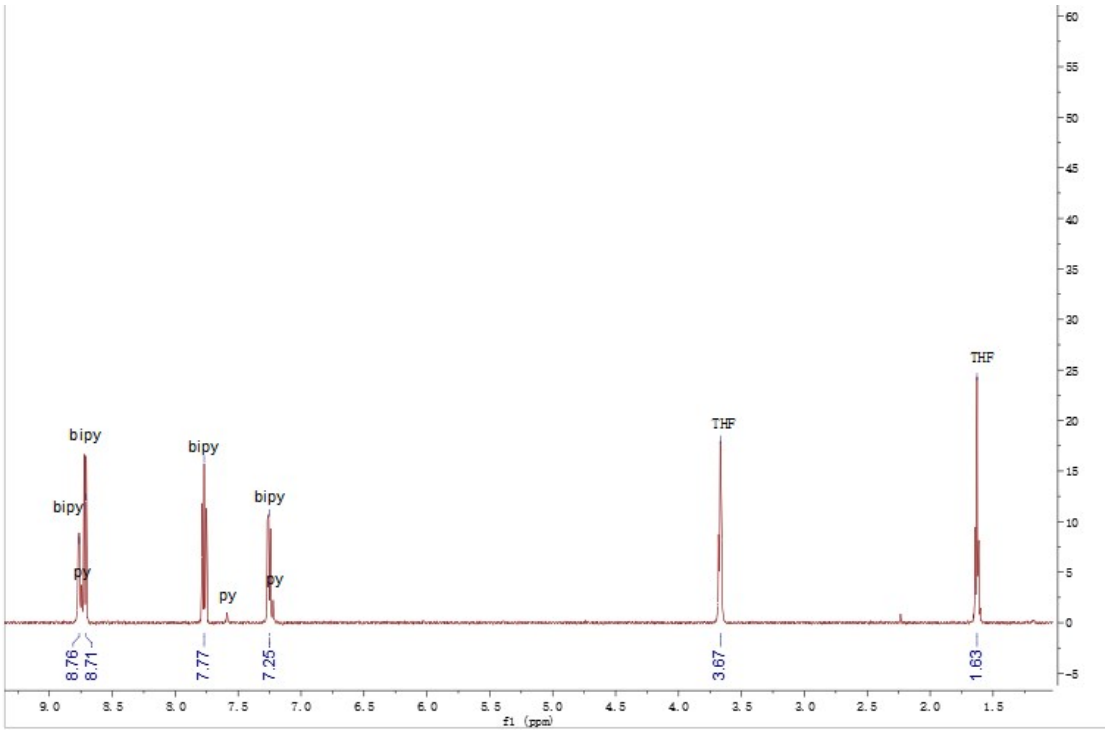

Figure *S*10. ^{1}H NMR (pyridine – d_5) spectrum of **Th(SC$_6$F$_5$)$_4$(bipy)$_2$ (3).**

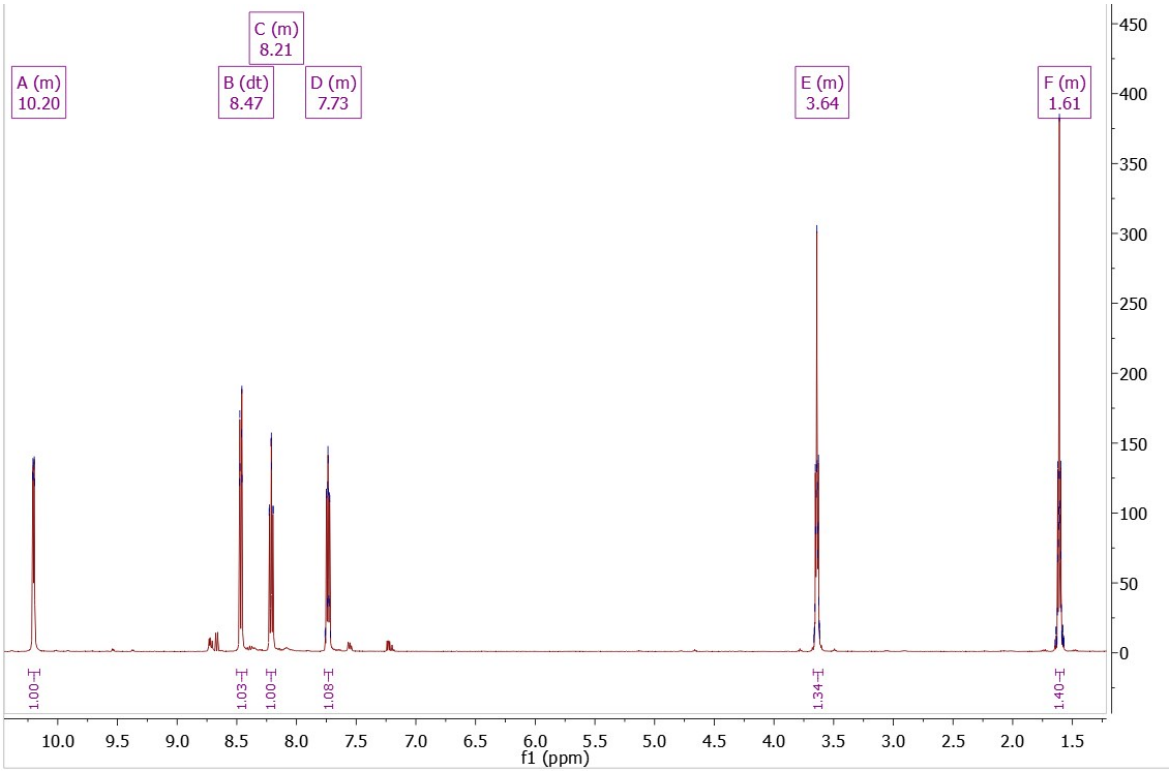

Figure *S*11. ^{1}H NMR (pyridine – d_5) spectrum of **Th(SeC$_6$F$_5$)$_4$(bipy)$_2$ (4).**

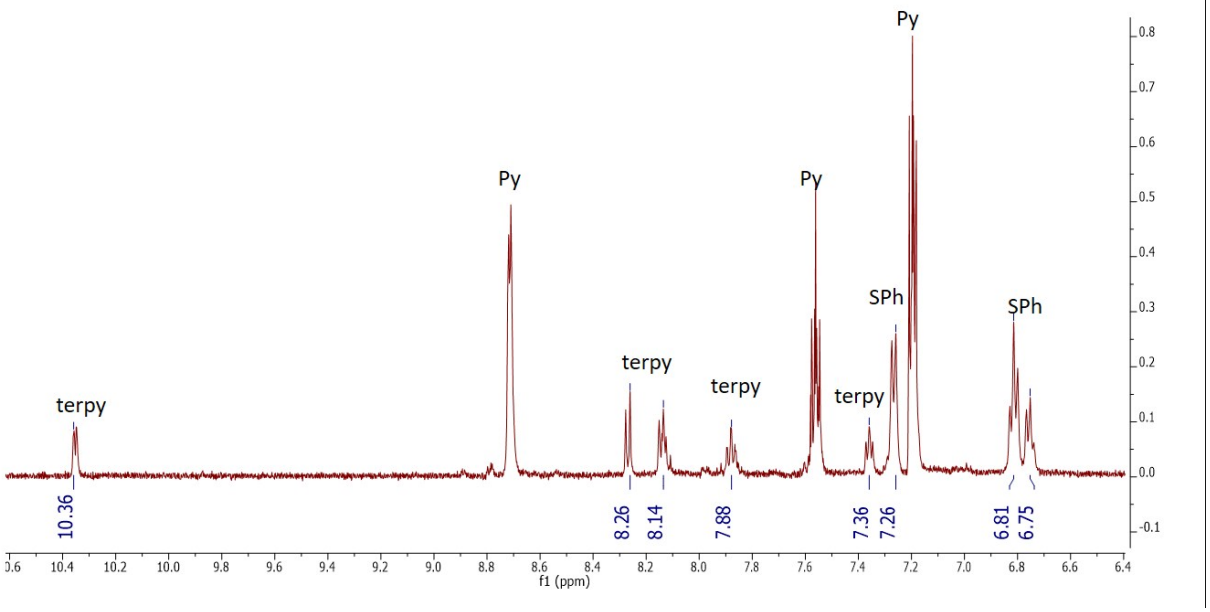

Figure *S*12. ^{1}H NMR (pyridine – d_5) spectrum of **pyTh(SPh)$_4$(terpy) (5).**

3. ^{19}F NMR data for compounds 3 and 4.

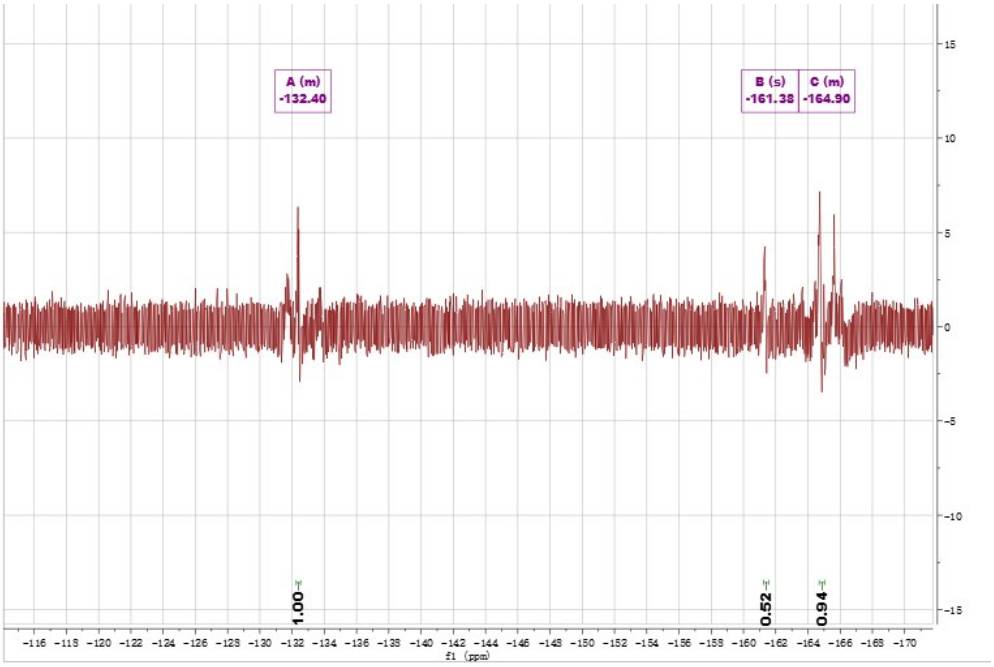

Figure *S*13. ^{19}F NMR (pyridine – d_5) spectrum of **(bipy)$_2$Th(SC$_6$F$_5$)$_4$ (3).**

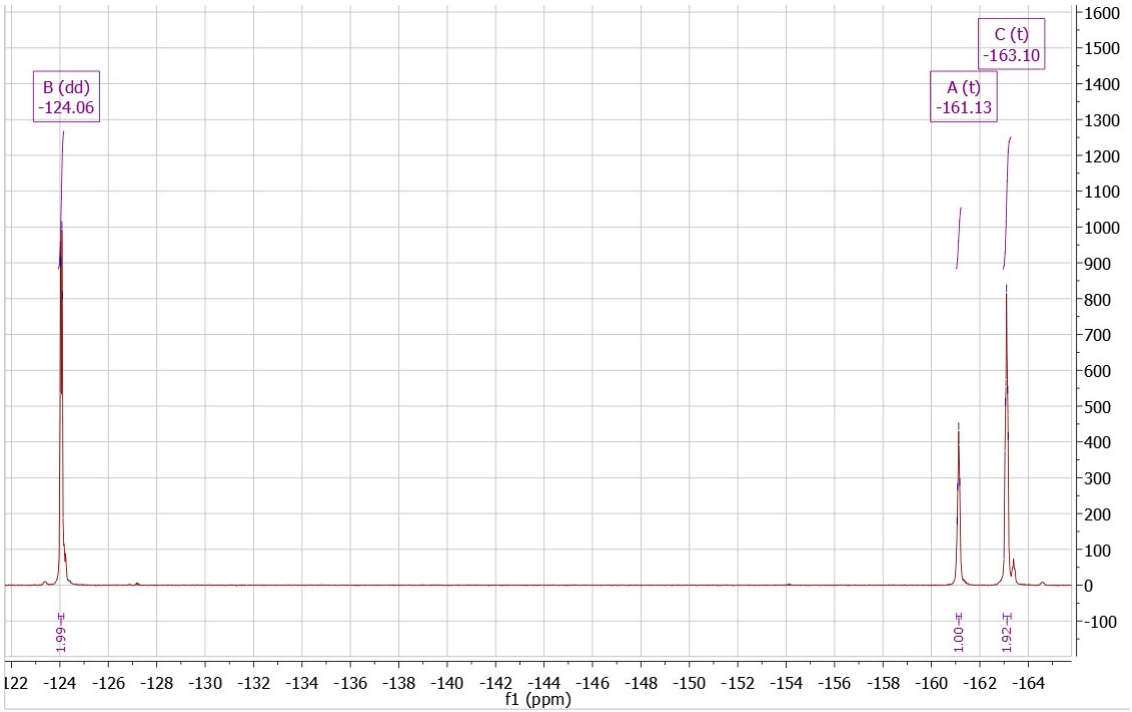

Figure *S*14. ^{19}F NMR (pyridine – d_5) spectrum of **(bipy)$_2$Th(SeC$_6$F$_5$)$_4$ (4).**

4. ^{77}Se NMR for compounds 2 and 4.

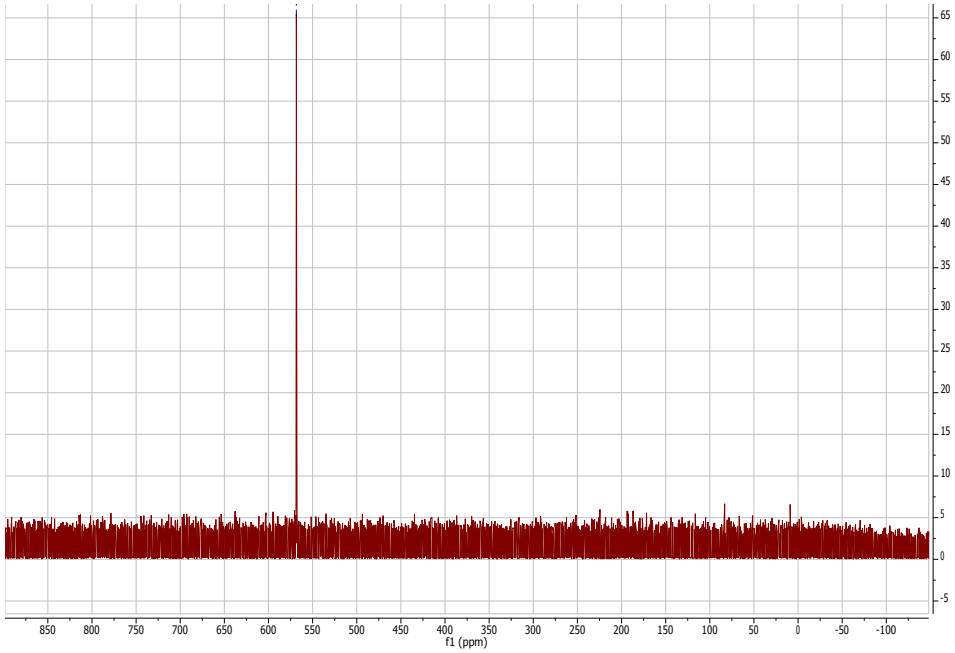

Figure *S*15. ^{77}Se NMR (toluene - d_8) spectrum of **Th(SePh)$_4$(bipy)·Py (2).**

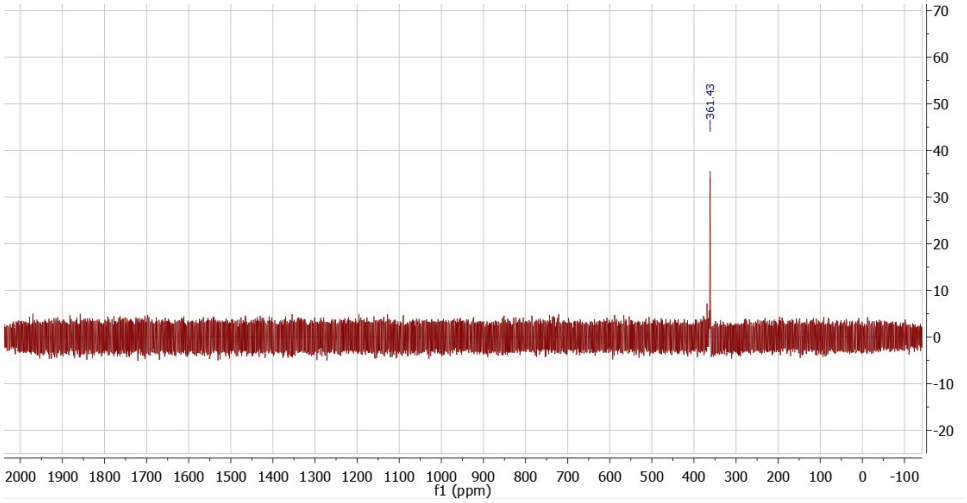

Figure *S*16. ^{77}Se NMR (pyridine – d_5) spectrum of **(bipy)$_2$Th(SeC$_6$F$_5$)$_4$ (4).**

5. IR Spectra for compounds 1, 2, 3, 4, and 5.

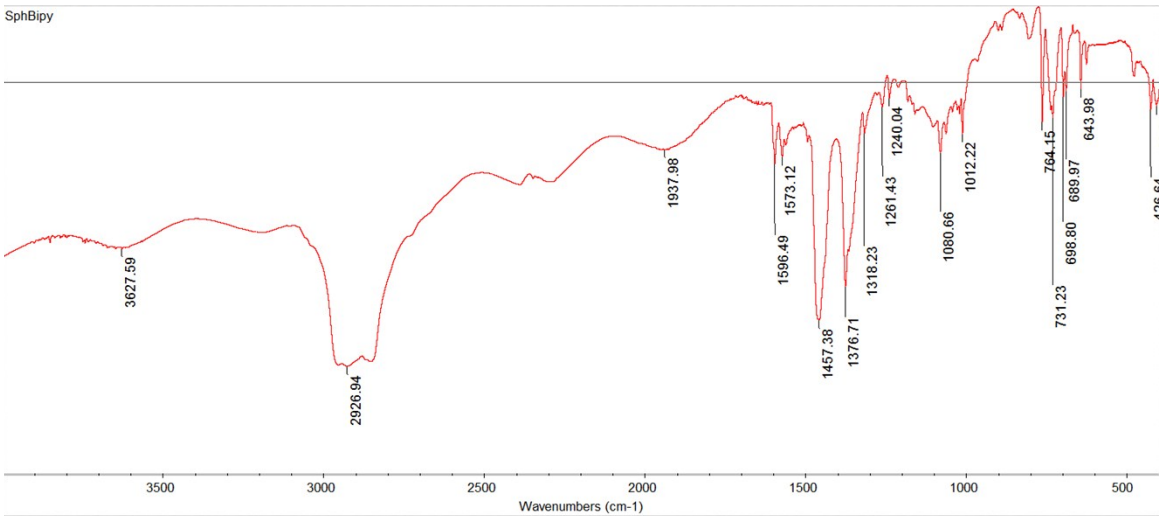

Figure *S*17. IR spectrum for **$(bipy)_2Th(SPh)_4$ (1).**

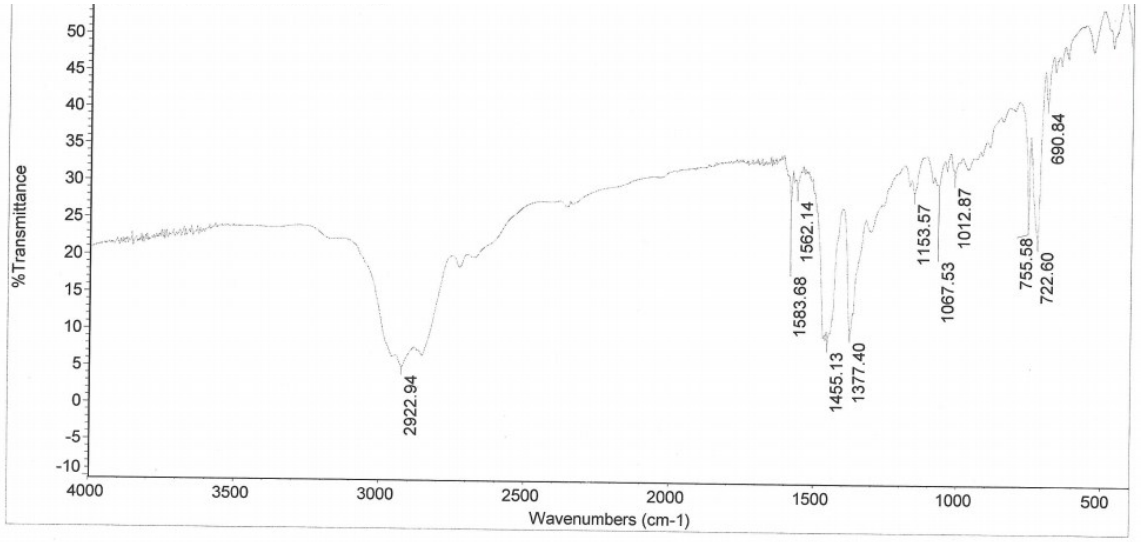

Figure *S*18. IR spectrum for **$Th(SePh)_4(bipy)\cdot Py$ (2).**

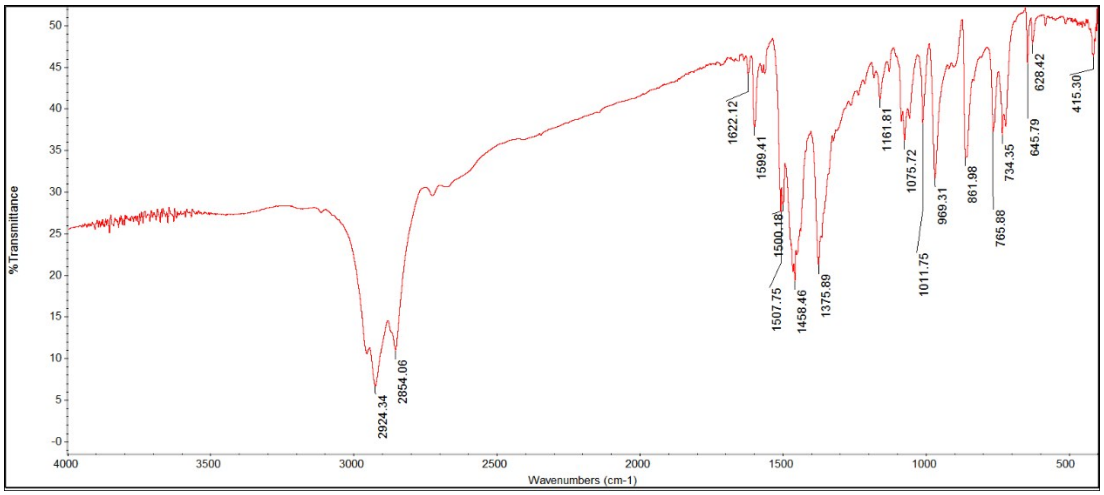

Figure S19. IR spectrum for **$(bipy)_2Th(SC_6F_5)_4$ (3).**

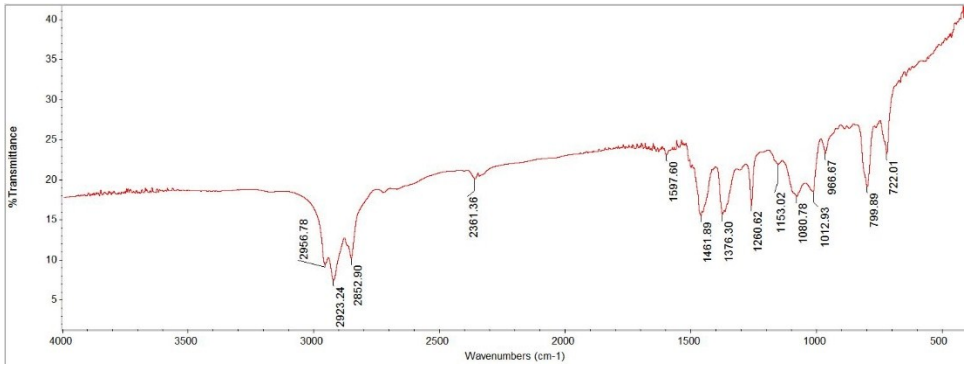

Figure S20. IR spectrum for **$(bipy)_2Th(SeC_6F_5)_4$ (4).**

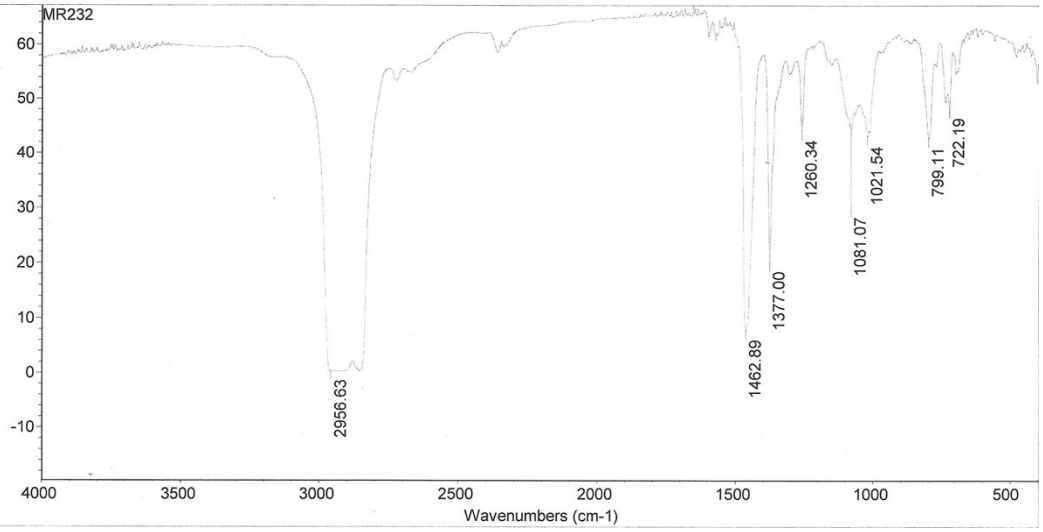

Figure S21. IR spectrum for (**py)(terpy)Th(SPh)$_4$ (5).**

6. Summary of Crystallographic Details for compounds 1- 5, Table S1.

Table *S*1. Summary of Crystallographic Details for compounds **1-5**

	1	**2**	**3**	**4**	**5**
	(bipy)$_2$Th(SPh)$_4$ **E = S**	**(bipy)$_2$Th(SePh)$_4$ · py** **E = Se**	**(bipy)$_2$Th(SC$_6$F$_5$)$_4$ · 2THF** **E = S**	**(bipy)$_2$Th(SeC$_6$F$_5$)$_4$ · 2THF** **E = Se**	**(py)(terpy)Th(SPh)$_4$ · 2py** **E = S**
empirical formula	C_{44} H_{36} N_4 S_4 Th	C_{49} H_{41} N_5 Se_4 Th	C_{52} H_{32} $F_{20}N_4O_2S_4$Th	$C_{52}H_{32}F_{20}N_4O_2Se_4$Th	C_{54} H_{46} N_6 S_4 Th
fw	981.05	1247.75	1485.09	1672.69	1139.25
crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
space group[a]	Cc	$P2_1/c$	C2/c	C2/c	$P2_1/n$
a (Å)	25.426(1)	20.895(2)	26.247(1)	26.340(1)	15.188(1)
b (Å)	25.274(1)	9.473(1)	12.598(1)	12.750(1)	21.632(1)

c (Å)	24.336(1)	22.825(3)	17.213(1)	17.396(1)	15.651(1)
β (deg)	90.948(2)	100.916(1)	114.189(1)	114.296(1)	111.146(1)
V (Å^3)	15636.8(13)	4434.5(9)	5191.9(4)	5324.7(4)	4795.8(5)
Z	16	4	4	4	4
D_{calc} (Mg/cm^3)	1.667	1.869	1.900	2.087	1.578
T (K)	100(2)	100(2)	100(2)	100(2)	100(2)
abs coeff (mm^{-1})	4.066	6.686	3.153	5.652	3.328
R(int)/N_{unique}	0.0879/28537	0.0586/10170	0.0412/7926	0.0357/8110	0.0398/13310
R(F)[b] [I > 2σ(I)]	0.0522	0.0404	0.0290	0.0271	0.0371
$R_w(F^2)$[c] [I>2σ(I)]	0.1175	0.0879	0.0643	0.0605	0.0733
CCDC number	1841858	1841859	1841860	1841861	1841862

[a] Crystal sample for **1** was twinned and absolute structure parameter (Flack) was refined to 0.508(11). Crystal sample for **2** had additional, weaker, and non-overlapping reflections that were consistent with both twinning and an approximate (2**a**,**b**,**c**) supercell, with respect to the unit cell for **2** used here, and were subsequently ignored.

[b] $R(F) = \Sigma||F_O| - |F_C||/\Sigma|F_O|$

[c] $Rw(F^2) = \{\Sigma[w(F_O^2 - F_C^2)^2]/\Sigma[w(F_O^2)^2]\}^{1/2}$

7. Crystallographic tables for compounds 1 (Tables S2-S8), 2 (Tables S9-S15), 2a (Tables S16-S22), 3 (Tables S23-S29), 4 (Tables S30-S36), and 5 (Tables S37-S43).

Table S2. Crystal data and structure refinement for **1**.

Identification code	thsph4bipy2_final_xstl1_Cc	
Empirical formula	C44 H36 N4 S4 Th	
Formula weight	981.05	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 25.4257(12) Å	α= 90°.
	b = 25.2741(12) Å	β= 90.9478(16)°.
	c = 24.3365(12) Å	γ = 90°.
Volume	15636.8(13) $Å^3$	
Z	16	
Density (calculated)	1.667 Mg/m^3	
Absorption coefficient	4.066 mm^{-1}	
F(000)	7712	
Crystal size	.16 x .16 x .016 mm^3	
Theta range for data collection	1.136 to 25.409°.	
Index ranges	-30<=h<=30, -30<=k<=30, -29<=l<=29	
Reflections collected	65333	
Independent reflections	28537 [R(int) = 0.0879]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0921 and 0.0622	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	28537 / 3948 / 1911	
Goodness-of-fit on F^2	0.958	
Final R indices [I>2sigma(I)]	R1 = 0.0522, wR2 = 0.1002	
R indices (all data)	R1 = 0.0957, wR2 = 0.1175	
Absolute structure parameter	0.508(11)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.985 and -1.106 $e.Å^{-3}$	

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	-2949(1)	3924(1)	18(2)	14(1)
S(1)	-4006(2)	3842(1)	-390(2)	18(1)
S(2)	-3025(2)	2870(1)	435(2)	20(1)
S(3)	-2334(2)	4111(2)	980(2)	21(1)
S(4)	-2782(2)	4535(1)	-942(2)	22(1)
N(1)	-3689(2)	4184(1)	719(2)	15(3)
N(2)	-3095(2)	4945(1)	250(2)	17(3)
N(3)	-1933(2)	3774(1)	-235(2)	14(3)
N(4)	-2714(2)	3164(1)	-673(2)	18(3)
C(1)	-4140(3)	3750(3)	-1101(2)	19(4)
C(2)	-4421(8)	3298(5)	-1269(3)	28(4)
C(3)	-4584(8)	3222(6)	-1816(4)	32(4)
C(4)	-4439(8)	3618(6)	-2210(3)	29(4)
C(5)	-4206(8)	4062(5)	-2054(3)	25(4)
C(6)	-4029(7)	4134(5)	-1500(3)	21(4)
C(7)	-3124(3)	2729(2)	1144(2)	19(4)
C(8)	-3585(4)	2452(7)	1280(3)	19(4)
C(9)	-3657(5)	2309(7)	1825(3)	20(4)
C(10)	-3291(6)	2429(8)	2228(3)	25(4)
C(11)	-2835(6)	2704(8)	2096(3)	24(4)
C(12)	-2759(5)	2842(7)	1554(3)	23(4)
C(13)	-2648(3)	4483(2)	1498(2)	23(4)
C(14)	-2566(8)	5019(3)	1567(6)	30(4)
C(15)	-2784(8)	5294(4)	2009(6)	31(4)
C(16)	-3081(8)	5035(5)	2388(6)	31(4)
C(17)	-3165(7)	4497(5)	2334(5)	29(4)
C(18)	-2970(6)	4220(4)	1890(5)	26(4)
C(19)	-2435(3)	4187(2)	-1457(2)	21(4)
C(20)	-1922(3)	4334(6)	-1568(6)	24(4)
C(21)	-1653(4)	4079(7)	-1985(6)	29(4)
C(22)	-1896(5)	3708(7)	-2300(6)	28(4)

C(23)	-2408(5)	3541(6)	-2189(6)	27(4)
C(24)	-2679(4)	3803(6)	-1789(6)	22(4)
C(25)	-3984(5)	3800(2)	943(6)	23(4)
C(26)	-4401(5)	3899(2)	1241(8)	26(4)
C(27)	-4577(5)	4405(3)	1317(8)	23(4)
C(28)	-4282(5)	4830(2)	1102(8)	23(4)
C(29)	-3825(4)	4687(1)	814(6)	17(3)
C(30)	-3490(4)	5120(1)	582(6)	17(3)
C(31)	-3541(5)	5645(2)	720(7)	19(4)
C(32)	-3189(5)	6006(1)	511(7)	25(4)
C(33)	-2774(5)	5839(2)	202(7)	23(4)
C(34)	-2735(5)	5303(1)	84(7)	19(4)
C(35)	-1574(2)	4132(4)	-72(7)	17(4)
C(36)	-1047(2)	4098(5)	-225(7)	20(4)
C(37)	-897(2)	3701(5)	-545(7)	20(4)
C(38)	-1270(2)	3331(5)	-731(7)	19(4)
C(39)	-1799(2)	3380(4)	-581(6)	16(3)
C(40)	-2217(2)	3033(4)	-783(6)	18(3)
C(41)	-2089(3)	2576(4)	-1090(7)	20(4)
C(42)	-2506(3)	2268(5)	-1289(8)	21(4)
C(43)	-3026(3)	2410(5)	-1186(8)	23(4)
C(44)	-3098(2)	2855(4)	-874(6)	20(4)
Th(2)	-467(1)	6424(1)	19(2)	15(1)
S(5)	-1509(2)	6328(1)	-417(2)	19(1)
S(6)	-537(2)	5368(1)	437(2)	18(1)
S(7)	127(2)	6621(1)	989(2)	22(1)
S(8)	-285(2)	7033(1)	-941(2)	22(1)
N(5)	-1215(2)	6684(1)	707(2)	16(3)
N(6)	-608(2)	7440(1)	270(2)	20(3)
N(7)	537(2)	6282(1)	-222(2)	19(3)
N(8)	-218(2)	5654(1)	-669(2)	16(3)
C(45)	-1621(3)	6270(3)	-1132(2)	20(4)
C(46)	-1866(7)	5807(4)	-1342(3)	21(4)
C(47)	-2000(8)	5779(5)	-1901(3)	27(4)
C(48)	-1899(9)	6190(5)	-2253(3)	25(4)
C(49)	-1690(8)	6639(5)	-2052(3)	26(4)

C(50)	-1541(8)	6691(4)	-1505(3)	22(4)
C(51)	-626(3)	5249(2)	1152(2)	20(4)
C(52)	-1083(4)	4971(7)	1310(3)	21(4)
C(53)	-1155(6)	4841(8)	1857(3)	30(4)
C(54)	-786(6)	4966(8)	2241(3)	30(4)
C(55)	-328(6)	5246(9)	2100(3)	31(4)
C(56)	-250(5)	5378(7)	1541(3)	23(4)
C(57)	-198(3)	6995(2)	1505(2)	21(4)
C(58)	-68(6)	7528(3)	1581(6)	20(4)
C(59)	-294(7)	7806(3)	2009(6)	21(4)
C(60)	-627(7)	7564(5)	2361(6)	25(4)
C(61)	-750(7)	7041(5)	2305(5)	28(4)
C(62)	-543(6)	6761(4)	1876(5)	27(4)
C(63)	79(3)	6668(2)	-1430(2)	20(4)
C(64)	612(3)	6786(6)	-1492(6)	18(4)
C(65)	915(4)	6509(7)	-1874(7)	23(4)
C(66)	681(5)	6132(7)	-2203(7)	23(4)
C(67)	154(5)	6021(6)	-2130(6)	24(4)
C(68)	-149(4)	6297(6)	-1769(6)	22(4)
C(69)	-1537(5)	6293(2)	916(6)	21(4)
C(70)	-1966(5)	6391(2)	1223(8)	22(4)
C(71)	-2113(5)	6914(3)	1316(8)	23(4)
C(72)	-1803(5)	7312(2)	1117(8)	23(4)
C(73)	-1348(4)	7199(1)	815(6)	19(3)
C(74)	-994(4)	7598(1)	606(6)	21(3)
C(75)	-1042(5)	8116(2)	763(7)	23(4)
C(76)	-681(5)	8490(2)	592(7)	24(4)
C(77)	-257(5)	8331(2)	253(7)	23(4)
C(78)	-238(5)	7809(2)	116(7)	24(4)
C(79)	899(2)	6645(5)	-48(7)	21(4)
C(80)	1426(2)	6618(5)	-172(8)	23(4)
C(81)	1610(2)	6192(5)	-487(7)	22(4)
C(82)	1235(2)	5825(5)	-661(7)	19(4)
C(83)	710(2)	5873(4)	-549(6)	18(3)
C(84)	295(2)	5513(4)	-759(6)	20(3)
C(85)	423(2)	5061(4)	-1051(7)	22(4)

C(86)	28(3)	4759(5)	-1268(8)	24(4)
C(87)	-507(3)	4910(5)	-1200(7)	20(4)
C(88)	-591(2)	5351(4)	-873(6)	21(4)
Th(3)	412(1)	2307(1)	-37(2)	14(1)
S(9)	1468(2)	2382(1)	387(2)	19(1)
S(10)	491(2)	3364(1)	-440(2)	19(1)
S(11)	-190(2)	2118(2)	-1012(2)	21(1)
S(12)	217(2)	1711(1)	928(2)	19(1)
N(9)	1162(2)	2029(1)	-713(2)	19(3)
N(10)	523(2)	1301(1)	-279(2)	15(3)
N(11)	-587(2)	2438(1)	206(2)	22(4)
N(12)	154(2)	3059(1)	658(2)	18(3)
C(89)	1605(3)	2487(3)	1100(2)	20(4)
C(90)	1876(8)	2953(5)	1267(3)	24(4)
C(91)	2021(9)	3042(6)	1792(4)	32(4)
C(92)	1883(9)	2691(6)	2182(3)	31(4)
C(93)	1606(8)	2224(6)	2036(2)	28(4)
C(94)	1483(8)	2128(5)	1499(3)	26(4)
C(95)	658(3)	3489(2)	-1127(2)	19(4)
C(96)	1106(5)	3751(8)	-1249(3)	27(4)
C(97)	1247(6)	3892(8)	-1777(3)	28(4)
C(98)	930(6)	3741(8)	-2213(3)	27(4)
C(99)	481(6)	3460(8)	-2117(2)	24(4)
C(100)	316(5)	3318(7)	-1577(2)	22(4)
C(101)	122(3)	1710(2)	-1504(2)	19(4)
C(102)	-20(7)	1191(3)	-1555(6)	25(4)
C(103)	197(7)	861(4)	-1947(7)	28(4)
C(104)	586(7)	1043(5)	-2281(7)	29(4)
C(105)	750(6)	1575(5)	-2222(6)	26(4)
C(106)	514(6)	1909(4)	-1845(6)	23(4)
C(107)	-99(3)	2079(2)	1438(2)	24(4)
C(108)	-645(3)	2034(6)	1530(6)	25(4)
C(109)	-875(4)	2332(7)	1942(6)	29(4)
C(110)	-589(5)	2678(7)	2264(6)	30(4)
C(111)	-54(5)	2717(6)	2190(6)	25(4)
C(112)	185(4)	2434(6)	1767(6)	21(4)

C(113)	1466(5)	2410(2)	-919(7)	21(4)
C(114)	1912(5)	2297(2)	-1236(7)	19(4)
C(115)	2051(5)	1787(3)	-1327(8)	24(4)
C(116)	1729(5)	1391(2)	-1104(8)	23(4)
C(117)	1306(4)	1519(1)	-803(6)	18(3)
C(118)	933(4)	1119(1)	-584(6)	16(3)
C(119)	997(5)	582(2)	-697(8)	21(4)
C(120)	630(5)	211(1)	-502(7)	23(4)
C(121)	221(5)	401(1)	-204(8)	22(4)
C(122)	185(5)	935(1)	-112(7)	18(4)
C(123)	-958(2)	2095(5)	36(7)	22(4)
C(124)	-1476(2)	2105(5)	165(7)	23(4)
C(125)	-1639(2)	2522(5)	492(7)	26(4)
C(126)	-1290(2)	2889(5)	680(7)	25(4)
C(127)	-756(2)	2834(4)	528(6)	20(3)
C(128)	-355(2)	3202(4)	759(6)	19(3)
C(129)	-459(2)	3638(4)	1073(7)	19(4)
C(130)	-77(3)	3946(5)	1310(8)	25(4)
C(131)	441(3)	3797(5)	1202(8)	22(4)
C(132)	535(2)	3363(5)	880(6)	18(4)
Th(4)	2926(1)	4800(1)	32(2)	14(1)
S(13)	3980(2)	4883(1)	447(2)	18(1)
S(14)	2983(2)	5841(1)	-425(2)	18(1)
S(15)	2333(2)	4573(1)	-934(2)	18(1)
S(16)	2744(2)	4226(1)	1021(2)	20(1)
N(13)	3676(2)	4538(1)	-632(2)	18(3)
N(14)	3067(2)	3782(1)	-188(2)	21(3)
N(15)	1931(2)	4941(1)	263(2)	17(3)
N(16)	2681(2)	5569(1)	701(2)	16(3)
C(133)	4131(3)	5011(3)	1151(2)	20(3)
C(134)	4437(7)	5465(4)	1266(3)	17(3)
C(135)	4605(7)	5570(5)	1802(3)	21(3)
C(136)	4481(7)	5214(6)	2228(3)	20(3)
C(137)	4171(8)	4788(6)	2102(3)	23(3)
C(138)	4006(7)	4684(5)	1576(2)	21(3)
C(139)	3013(3)	5923(2)	-1144(2)	22(3)

C(140)	3461(4)	6164(7)	-1375(3)	22(3)
C(141)	3498(5)	6277(8)	-1916(3)	25(3)
C(142)	3081(6)	6164(8)	-2283(3)	24(3)
C(143)	2618(5)	5937(8)	-2055(3)	22(3)
C(144)	2609(4)	5828(8)	-1510(3)	22(3)
C(145)	2701(3)	4219(2)	-1422(2)	22(4)
C(146)	2626(7)	3670(3)	-1493(7)	28(4)
C(147)	2898(7)	3379(4)	-1891(7)	30(4)
C(148)	3263(7)	3657(5)	-2209(7)	31(4)
C(149)	3335(6)	4172(5)	-2155(6)	26(4)
C(150)	3065(6)	4483(4)	-1760(6)	23(4)
C(151)	2332(2)	4574(2)	1489(2)	15(4)
C(152)	1792(3)	4451(6)	1496(6)	21(4)
C(153)	1466(3)	4729(6)	1847(7)	24(4)
C(154)	1667(4)	5113(7)	2187(7)	25(4)
C(155)	2191(4)	5233(6)	2182(6)	23(4)
C(156)	2533(3)	4952(6)	1831(6)	19(4)
C(157)	3964(5)	4904(2)	-860(6)	20(3)
C(158)	4416(5)	4791(2)	-1176(8)	22(3)
C(159)	4545(5)	4274(3)	-1249(8)	22(3)
C(160)	4265(5)	3888(2)	-1019(7)	20(4)
C(161)	3823(4)	4018(1)	-716(5)	17(3)
C(162)	3459(4)	3614(1)	-509(6)	20(3)
C(163)	3510(5)	3069(2)	-631(7)	20(4)
C(164)	3141(5)	2708(2)	-451(7)	23(4)
C(165)	2727(5)	2899(2)	-155(8)	22(4)
C(166)	2719(5)	3427(2)	-32(7)	21(4)
C(167)	1564(2)	4592(5)	96(7)	18(4)
C(168)	1030(2)	4628(5)	198(8)	24(4)
C(169)	880(2)	5068(5)	508(7)	24(4)
C(170)	1233(2)	5431(5)	703(7)	20(4)
C(171)	1769(2)	5369(4)	568(6)	17(3)
C(172)	2178(2)	5704(4)	803(6)	18(3)
C(173)	2055(2)	6165(4)	1124(7)	20(4)
C(174)	2466(3)	6463(5)	1348(8)	23(3)
C(175)	2953(3)	6306(5)	1254(7)	23(3)

C(176)	3059(2)	5873(5)	941(6)	21(3)
Th(1B)	2910	-189	-122	20
S(1B)	3959	-110	310	20
S(2B)	2996	868	-531	20
S(3B)	2316	-370	-1100	20
S(4B)	2722	-805	828	20
N(1B)	3665	-445	-808	20
N(2B)	3060	-1209	-357	20
N(3B)	1889	-40	107	20
N(4B)	2661	567	567	20
C(201)	4078	-41	1026	20
C(202)	4425	356	1211	20
C(203)	4602	385	1758	20
C(204)	4388	10	2140	20
C(205)	4079	-379	1971	20
C(206)	3891	-403	1416	20
C(207)	3118	1013	-1235	20
C(208)	3550	1342	-1348	20
C(209)	3632	1492	-1889	20
C(210)	3293	1344	-2308	20
C(211)	2873	1008	-2200	20
C(212)	2795	849	-1664	20
C(213)	2622	-779	-1593	20
C(214)	2546	-1319	-1613	20
C(215)	2798	-1632	-2006	20
C(216)	3109	-1406	-2393	20
C(217)	3193	-866	-2383	20
C(218)	2945	-547	-2004	20
C(219)	2372	-456	1341	20
C(220)	1850	-585	1431	20
C(221)	1573	-316	1833	20
C(222)	1819	45	2159	20
C(223)	2342	188	2075	20
C(224)	2619	-85	1687	20
C(225)	3969	-61	-1018	20
C(226)	4399	-159	-1296	20

C(227)	4541	-666	-1426	20
C(228)	4226	-1090	-1242	20
C(229)	3799	-948	-909	20
C(230)	3449	-1381	-699	20
C(231)	3478	-1898	-871	20
C(232)	3095	-2250	-707	20
C(233)	2713	-2093	-350	20
C(234)	2712	-1571	-175	20
C(235)	1533	-395	-69	20
C(236)	1008	-379	96	20
C(237)	850	18	411	20
C(238)	1217	396	596	20
C(239)	1748	351	453	20
C(240)	2161	698	666	20
C(241)	2027	1154	972	20
C(242)	2438	1479	1151	20
C(243)	2961	1338	1061	20
C(244)	3040	878	776	20
Th(2B)	5481	2400	11	20
S(5B)	6531	2506	426	20
S(6B)	5539	3452	-421	20
S(7B)	4870	2190	-944	20
S(8B)	5320	1803	983	20
N(5B)	6218	2136	-689	20
N(6B)	5622	1383	-230	20
N(7B)	4482	2542	271	20
N(8B)	5242	3178	695	20
C(245)	6660	2521	1139	20
C(246)	7007	2910	1357	20
C(247)	7156	2889	1912	20
C(248)	6961	2510	2258	20
C(249)	6639	2134	2053	20
C(250)	6490	2122	1503	20
C(251)	5619	3564	-1138	20
C(252)	6064	3856	-1304	20
C(253)	6159	3931	-1858	20

C(254)	5826	3730	-2244	20
C(255)	5387	3425	-2095	20
C(256)	5292	3339	-1529	20
C(257)	5175	1781	-1445	20
C(258)	5026	1249	-1491	20
C(259)	5208	952	-1928	20
C(260)	5527	1170	-2310	20
C(261)	5697	1681	-2262	20
C(262)	5518	1984	-1835	20
C(263)	4957	2168	1472	20
C(264)	4440	2015	1577	20
C(265)	4134	2302	1948	20
C(266)	4349	2730	2218	20
C(267)	4872	2848	2136	20
C(268)	5172	2580	1765	20
C(269)	6534	2526	-909	20
C(270)	6943	2427	-1243	20
C(271)	7073	1903	-1359	20
C(272)	6788	1506	-1121	20
C(273)	6351	1620	-794	20
C(274)	6003	1222	-571	20
C(275)	6051	703	-721	20
C(276)	5706	326	-523	20
C(277)	5280	489	-189	20
C(278)	5257	1013	-63	20
C(279)	4119	2174	111	20
C(280)	3593	2203	241	20
C(281)	3418	2619	575	20
C(282)	3791	2997	725	20
C(283)	4314	2955	595	20
C(284)	4731	3319	792	20
C(285)	4606	3771	1085	20
C(286)	5003	4078	1289	20
C(287)	5538	3928	1213	20
C(288)	5618	3485	888	20
Th(3B)	4600	6477	-39	20

S(9B)	3541	6383	-448	20
S(10B)	4535	5431	395	20
S(11B)	5210	6698	923	20
S(12B)	4779	7050	-1024	20
N(9B)	3854	6767	637	20
N(10B)	4481	7489	175	20
N(11B)	5597	6349	-291	20
N(12B)	4857	5710	-716	20
C(289)	3397	6243	-1154	20
C(290)	3109	5779	-1292	20
C(291)	2916	5691	-1800	20
C(292)	2998	6053	-2198	20
C(293)	3311	6505	-2087	20
C(294)	3510	6586	-1571	20
C(295)	4379	5322	1088	20
C(296)	3949	5039	1224	20
C(297)	3840	4874	1754	20
C(298)	4167	5032	2179	20
C(299)	4600	5333	2070	20
C(300)	4728	5504	1528	20
C(301)	4891	7096	1417	20
C(302)	4975	7630	1427	20
C(303)	4755	7956	1821	20
C(304)	4463	7744	2234	20
C(305)	4360	7193	2223	20
C(306)	4564	6874	1813	20
C(307)	5101	6674	-1523	20
C(308)	5655	6672	-1566	20
C(309)	5889	6390	-1987	20
C(310)	5600	6092	-2357	20
C(311)	5061	6074	-2308	20
C(312)	4813	6381	-1909	20
C(313)	3555	6389	856	20
C(314)	3121	6507	1189	20
C(315)	2987	7018	1279	20
C(316)	3286	7410	1016	20

C(317)	3707	7278	714	20
C(318)	4076	7675	484	20
C(319)	4025	8211	607	20
C(320)	4379	8582	386	20
C(321)	4775	8389	70	20
C(322)	4815	7853	-7	20
C(323)	5970	6690	-120	20
C(324)	6489	6671	-239	20
C(325)	6646	6269	-588	20
C(326)	6297	5900	-770	20
C(327)	5766	5948	-605	20
C(328)	5367	5568	-819	20
C(329)	5474	5096	-1067	20
C(330)	5094	4748	-1237	20
C(331)	4575	4914	-1164	20
C(332)	4478	5390	-915	20
Th(4B)	-2975	-1021	-44	20
S(13B)	-4029	-1105	-459	20
S(14B)	-3031	-2062	412	20
S(15B)	-2382	-794	921	20
S(16B)	-2794	-447	-1033	20
N(13B)	-3725	-759	620	20
N(14B)	-3117	-3	176	20
N(15B)	-1980	-1162	-276	20
N(16B)	-2730	-1790	-714	20
C(333)	-4181	-1213	-1167	20
C(334)	-4523	-1637	-1292	20
C(335)	-4671	-1738	-1835	20
C(336)	-4464	-1427	-2262	20
C(337)	-4150	-1007	-2121	20
C(338)	-4012	-902	-1587	20
C(339)	-3092	-2143	1129	20
C(340)	-3491	-2477	1333	20
C(341)	-3508	-2636	1863	20
C(342)	-3128	-2463	2249	20
C(343)	-2739	-2102	2056	20

C(344)	-2741	-1964	1518	20
C(345)	-2735	-401	1390	20
C(346)	-2593	133	1480	20
C(347)	-2816	436	1901	20
C(348)	-3182	183	2238	20
C(349)	-3340	-308	2143	20
C(350)	-3136	-624	1713	20
C(351)	-2407	-807	-1515	20
C(352)	-1871	-678	-1562	20
C(353)	-1555	-988	-1893	20
C(354)	-1759	-1418	-2166	20
C(355)	-2283	-1532	-2137	20
C(356)	-2617	-1216	-1809	20
C(357)	-4012	-1126	850	20
C(358)	-4442	-1012	1196	20
C(359)	-4572	-495	1270	20
C(360)	-4305	-110	1021	20
C(361)	-3870	-240	708	20
C(362)	-3505	164	502	20
C(363)	-3541	705	645	20
C(364)	-3197	1072	429	20
C(365)	-2795	885	112	20
C(366)	-2773	353	12	20
C(367)	-1609	-829	-82	20
C(368)	-1075	-869	-179	20
C(369)	-929	-1288	-520	20
C(370)	-1282	-1653	-714	20
C(371)	-1818	-1591	-580	20
C(372)	-2227	-1925	-815	20
C(373)	-2104	-2395	-1123	20
C(374)	-2514	-2719	-1303	20
C(375)	-3002	-2559	-1217	20
C(376)	-3108	-2102	-943	20

Table S4. Bond lengths [Å] and angles [°] for **1**.

Th(1)-N(4)	2.6269(11)	C(8)-H(8)	0.9500
Th(1)-N(1)	2.6445(11)	C(9)-C(10)	1.3757(14)
Th(1)-N(2)	2.6692(11)	C(9)-H(9)	0.9500
Th(1)-N(3)	2.6910(11)	C(10)-C(11)	1.3927(14)
Th(1)-S(3)	2.8348(12)	C(10)-H(10)	0.9500
Th(1)-S(4)	2.8355(12)	C(11)-C(12)	1.3824(14)
Th(1)-S(1)	2.8575(12)	C(11)-H(11)	0.9500
Th(1)-S(2)	2.8595(12)	C(12)-H(12)	0.9500
S(1)-C(1)	1.7720(14)	C(13)-C(14)	1.3797(14)
S(2)-C(7)	1.7840(14)	C(13)-C(18)	1.4300(14)
S(3)-C(13)	1.7727(14)	C(14)-C(15)	1.4024(14)
S(4)-C(19)	1.7787(14)	C(14)-H(14)	0.9500
N(1)-C(29)	1.3401(13)	C(15)-C(16)	1.3675(14)
N(1)-C(25)	1.3467(13)	C(15)-H(15)	0.9500
N(2)-C(34)	1.3528(14)	C(16)-C(17)	1.3816(14)
N(2)-C(30)	1.3725(13)	C(16)-H(16)	0.9500
N(3)-C(35)	1.3410(14)	C(17)-C(18)	1.3856(14)
N(3)-C(39)	1.3506(13)	C(17)-H(17)	0.9500
N(4)-C(44)	1.3367(13)	C(18)-H(18)	0.9500
N(4)-C(40)	1.3394(13)	C(19)-C(20)	1.3877(14)
C(1)-C(2)	1.4042(14)	C(19)-C(24)	1.4020(14)
C(1)-C(6)	1.4062(14)	C(20)-C(21)	1.3925(14)
C(2)-C(3)	1.4003(14)	C(20)-H(20)	0.9500
C(2)-H(2)	0.9500	C(21)-C(22)	1.3543(14)
C(3)-C(4)	1.4386(14)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(23)	1.3963(14)
C(4)-C(5)	1.3207(14)	C(22)-H(22)	0.9500
C(4)-H(4)	0.9500	C(23)-C(24)	1.3723(14)
C(5)-C(6)	1.4264(14)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(24)-H(24)	0.9500
C(6)-H(6)	0.9500	C(25)-C(26)	1.3183(14)
C(7)-C(12)	1.3828(14)	C(25)-H(25)	0.9500
C(7)-C(8)	1.4091(14)	C(26)-C(27)	1.3694(14)
C(8)-C(9)	1.3885(14)	C(26)-H(26)	0.9500

C(27)-C(28)	1.4148(14)	Th(2)-S(5)	2.8489(12)
C(27)-H(27)	0.9500	Th(2)-S(6)	2.8638(12)
C(28)-C(29)	1.4117(14)	S(5)-C(45)	1.7631(14)
C(28)-H(28)	0.9500	S(6)-C(51)	1.7830(14)
C(29)-C(30)	1.5044(13)	S(7)-C(57)	1.7843(14)
C(30)-C(31)	1.3757(14)	S(8)-C(63)	1.7763(14)
C(31)-C(32)	1.3809(14)	N(5)-C(73)	1.3719(13)
C(31)-H(31)	0.9500	N(5)-C(69)	1.3856(13)
C(32)-C(33)	1.3719(14)	N(6)-C(74)	1.3484(13)
C(32)-H(32)	0.9500	N(6)-C(78)	1.3815(14)
C(33)-C(34)	1.3868(14)	N(7)-C(79)	1.3614(13)
C(33)-H(33)	0.9500	N(7)-C(83)	1.3805(13)
C(34)-H(34)	0.9500	N(8)-C(88)	1.3120(14)
C(35)-C(36)	1.3998(14)	N(8)-C(84)	1.3727(13)
C(35)-H(35)	0.9500	C(45)-C(50)	1.4145(14)
C(36)-C(37)	1.3290(14)	C(45)-C(46)	1.4172(14)
C(36)-H(36)	0.9500	C(46)-C(47)	1.3992(14)
C(37)-C(38)	1.4019(14)	C(46)-H(46)	0.9500
C(37)-H(37)	0.9500	C(47)-C(48)	1.3715(14)
C(38)-C(39)	1.4047(13)	C(47)-H(47)	0.9500
C(38)-H(38)	0.9500	C(48)-C(49)	1.3441(14)
C(39)-C(40)	1.4566(12)	C(48)-H(48)	0.9500
C(40)-C(41)	1.4162(13)	C(49)-C(50)	1.3840(14)
C(41)-C(42)	1.3940(14)	C(49)-H(49)	0.9500
C(41)-H(41)	0.9500	C(50)-H(50)	0.9500
C(42)-C(43)	1.3961(14)	C(51)-C(56)	1.3743(14)
C(42)-H(42)	0.9500	C(51)-C(52)	1.4162(14)
C(43)-C(44)	1.3712(14)	C(52)-C(53)	1.3870(14)
C(43)-H(43)	0.9500	C(52)-H(52)	0.9500
C(44)-H(44)	0.9500	C(53)-C(54)	1.3514(14)
Th(2)-N(5)	2.6377(11)	C(53)-H(53)	0.9500
Th(2)-N(8)	2.6517(11)	C(54)-C(55)	1.4093(14)
Th(2)-N(7)	2.6539(11)	C(54)-H(54)	0.9500
Th(2)-N(6)	2.6637(11)	C(55)-C(56)	1.4191(14)
Th(2)-S(7)	2.8259(12)	C(55)-H(55)	0.9500
Th(2)-S(8)	2.8412(12)	C(56)-H(56)	0.9500

C(57)-C(62)	1.3982(14)	C(77)-C(78)	1.3605(14)
C(57)-C(58)	1.4008(14)	C(77)-H(77)	0.9500
C(58)-C(59)	1.3896(14)	C(78)-H(78)	0.9500
C(58)-H(58)	0.9500	C(79)-C(80)	1.3805(14)
C(59)-C(60)	1.3608(14)	C(79)-H(79)	0.9500
C(59)-H(59)	0.9500	C(80)-C(81)	1.4054(14)
C(60)-C(61)	1.3651(14)	C(80)-H(80)	0.9500
C(60)-H(60)	0.9500	C(81)-C(82)	1.3911(14)
C(61)-C(62)	1.3741(14)	C(81)-H(81)	0.9500
C(61)-H(61)	0.9500	C(82)-C(83)	1.3738(13)
C(62)-H(62)	0.9500	C(82)-H(82)	0.9500
C(63)-C(68)	1.3704(14)	C(83)-C(84)	1.4780(13)
C(63)-C(64)	1.3993(14)	C(84)-C(85)	1.3859(13)
C(64)-C(65)	1.4034(14)	C(85)-C(86)	1.3602(14)
C(64)-H(64)	0.9500	C(85)-H(85)	0.9500
C(65)-C(66)	1.3737(14)	C(86)-C(87)	1.4265(14)
C(65)-H(65)	0.9500	C(86)-H(86)	0.9500
C(66)-C(67)	1.3816(14)	C(87)-C(88)	1.3873(14)
C(66)-H(66)	0.9500	C(87)-H(87)	0.9500
C(67)-C(68)	1.3687(14)	C(88)-H(88)	0.9500
C(67)-H(67)	0.9500	Th(3)-N(10)	2.6278(11)
C(68)-H(68)	0.9500	Th(3)-N(12)	2.6336(11)
C(69)-C(70)	1.3535(14)	Th(3)-N(9)	2.6353(11)
C(69)-H(69)	0.9500	Th(3)-N(11)	2.6381(11)
C(70)-C(71)	1.3940(14)	Th(3)-S(12)	2.8424(12)
C(70)-H(70)	0.9500	Th(3)-S(11)	2.8425(12)
C(71)-C(72)	1.3725(14)	Th(3)-S(10)	2.8540(12)
C(71)-H(71)	0.9500	Th(3)-S(9)	2.8669(12)
C(72)-C(73)	1.4082(13)	S(9)-C(89)	1.7844(14)
C(72)-H(72)	0.9500	S(10)-C(95)	1.7608(14)
C(73)-C(74)	1.4503(13)	S(11)-C(101)	1.7756(14)
C(74)-C(75)	1.3687(13)	S(12)-C(107)	1.7566(13)
C(75)-C(76)	1.3868(14)	N(9)-C(113)	1.3366(14)
C(75)-H(75)	0.9500	N(9)-C(117)	1.3584(13)
C(76)-C(77)	1.4266(14)	N(10)-C(122)	1.3323(13)
C(76)-H(76)	0.9500	N(10)-C(118)	1.3680(13)

N(11)-C(123)	1.3426(13)	C(106)-H(106)	0.9500
N(11)-C(127)	1.3446(13)	C(107)-C(112)	1.3947(14)
N(12)-C(132)	1.3434(13)	C(107)-C(108)	1.4143(14)
N(12)-C(128)	1.3713(13)	C(108)-C(109)	1.3895(14)
C(89)-C(94)	1.3685(14)	C(108)-H(108)	0.9500
C(89)-C(90)	1.4196(14)	C(109)-C(110)	1.3765(14)
C(90)-C(91)	1.3431(14)	C(109)-H(109)	0.9500
C(90)-H(90)	0.9500	C(110)-C(111)	1.3773(14)
C(91)-C(92)	1.3495(14)	C(110)-H(110)	0.9500
C(91)-H(91)	0.9500	C(111)-C(112)	1.4015(14)
C(92)-C(93)	1.4159(14)	C(111)-H(111)	0.9500
C(92)-H(92)	0.9500	C(112)-H(112)	0.9500
C(93)-C(94)	1.3620(14)	C(113)-C(114)	1.4128(14)
C(93)-H(93)	0.9500	C(113)-H(113)	0.9500
C(94)-H(94)	0.9500	C(114)-C(115)	1.3536(14)
C(95)-C(96)	1.3525(14)	C(114)-H(114)	0.9500
C(95)-C(100)	1.4530(14)	C(115)-C(116)	1.4077(14)
C(96)-C(97)	1.3870(14)	C(115)-H(115)	0.9500
C(96)-H(96)	0.9500	C(116)-C(117)	1.3503(13)
C(97)-C(98)	1.3751(14)	C(116)-H(116)	0.9500
C(97)-H(97)	0.9500	C(117)-C(118)	1.4898(13)
C(98)-C(99)	1.3674(14)	C(118)-C(119)	1.3948(13)
C(98)-H(98)	0.9500	C(119)-C(120)	1.4118(14)
C(99)-C(100)	1.4318(14)	C(119)-H(119)	0.9500
C(99)-H(99)	0.9500	C(120)-C(121)	1.3664(14)
C(100)-H(100)	0.9500	C(120)-H(120)	0.9500
C(101)-C(102)	1.3658(14)	C(121)-C(122)	1.3703(14)
C(101)-C(106)	1.4002(14)	C(121)-H(121)	0.9500
C(102)-C(103)	1.3885(14)	C(122)-H(122)	0.9500
C(102)-H(102)	0.9500	C(123)-C(124)	1.3578(14)
C(103)-C(104)	1.3706(14)	C(123)-H(123)	0.9500
C(103)-H(103)	0.9500	C(124)-C(125)	1.3879(14)
C(104)-C(105)	1.4152(14)	C(124)-H(124)	0.9500
C(104)-H(104)	0.9500	C(125)-C(126)	1.3569(14)
C(105)-C(106)	1.3903(14)	C(125)-H(125)	0.9500
C(105)-H(105)	0.9500	C(126)-C(127)	1.4205(13)

C(126)-H(126)	0.9500	C(136)-C(137)	1.3668(14)
C(127)-C(128)	1.4839(13)	C(136)-H(136)	0.9500
C(128)-C(129)	1.3681(13)	C(137)-C(138)	1.3671(14)
C(129)-C(130)	1.3647(14)	C(137)-H(137)	0.9500
C(129)-H(129)	0.9500	C(138)-H(138)	0.9500
C(130)-C(131)	1.3994(14)	C(139)-C(144)	1.3680(14)
C(130)-H(130)	0.9500	C(139)-C(140)	1.4170(14)
C(131)-C(132)	1.3702(14)	C(140)-C(141)	1.3520(14)
C(131)-H(131)	0.9500	C(140)-H(140)	0.9500
C(132)-H(132)	0.9500	C(141)-C(142)	1.4049(14)
Th(4)-N(13)	2.6065(11)	C(141)-H(141)	0.9500
Th(4)-N(16)	2.6183(11)	C(142)-C(143)	1.4311(14)
Th(4)-N(15)	2.6246(11)	C(142)-H(142)	0.9500
Th(4)-N(14)	2.6527(11)	C(143)-C(144)	1.3544(14)
Th(4)-S(15)	2.8301(12)	C(143)-H(143)	0.9500
Th(4)-S(16)	2.8544(12)	C(144)-H(144)	0.9500
Th(4)-S(13)	2.8563(12)	C(145)-C(146)	1.4129(14)
Th(4)-S(14)	2.8615(12)	C(145)-C(150)	1.4144(14)
S(13)-C(133)	1.7792(14)	C(146)-C(147)	1.4070(14)
S(14)-C(139)	1.7646(14)	C(146)-H(146)	0.9500
S(15)-C(145)	1.7686(14)	C(147)-C(148)	1.4052(14)
S(16)-C(151)	1.7909(13)	C(147)-H(147)	0.9500
N(13)-C(157)	1.3097(13)	C(148)-C(149)	1.3217(14)
N(13)-C(161)	1.3800(13)	C(148)-H(148)	0.9500
N(14)-C(166)	1.3208(13)	C(149)-C(150)	1.4243(14)
N(14)-C(162)	1.3449(13)	C(149)-H(149)	0.9500
N(15)-C(167)	1.3434(13)	C(150)-H(150)	0.9500
N(15)-C(171)	1.3793(13)	C(151)-C(156)	1.3613(14)
N(16)-C(172)	1.3493(13)	C(151)-C(152)	1.4090(14)
N(16)-C(176)	1.3563(13)	C(152)-C(153)	1.3896(14)
C(133)-C(138)	1.3635(14)	C(152)-H(152)	0.9500
C(133)-C(134)	1.4116(14)	C(153)-C(154)	1.3693(14)
C(134)-C(135)	1.3922(14)	C(153)-H(153)	0.9500
C(134)-H(134)	0.9500	C(154)-C(155)	1.3657(14)
C(135)-C(136)	1.4113(14)	C(154)-H(154)	0.9500
C(135)-H(135)	0.9500	C(155)-C(156)	1.4192(14)

C(155)-H(155)	0.9500	Th(1B)-N(4B)	2.6270
C(156)-H(156)	0.9500	Th(1B)-N(1B)	2.6444
C(157)-C(158)	1.4207(14)	Th(1B)-N(2B)	2.6692
C(157)-H(157)	0.9500	Th(1B)-N(3B)	2.6910
C(158)-C(159)	1.3610(14)	Th(1B)-S(3B)	2.8348
C(158)-H(158)	0.9500	Th(1B)-S(4B)	2.8356
C(159)-C(160)	1.3374(14)	Th(1B)-S(1B)	2.8575
C(159)-H(159)	0.9500	Th(1B)-S(2B)	2.8596
C(160)-C(161)	1.3924(13)	S(1B)-C(201)	1.7721
C(160)-H(160)	0.9500	S(2B)-C(207)	1.7839
C(161)-C(162)	1.4739(13)	S(3B)-C(213)	1.7726
C(162)-C(163)	1.4148(13)	S(4B)-C(219)	1.7785
C(163)-C(164)	1.3852(14)	N(1B)-C(229)	1.3401
C(163)-H(163)	0.9500	N(1B)-C(225)	1.3467
C(164)-C(165)	1.3732(14)	N(2B)-C(234)	1.3527
C(164)-H(164)	0.9500	N(2B)-C(230)	1.3724
C(165)-C(166)	1.3684(14)	N(3B)-C(235)	1.3410
C(165)-H(165)	0.9500	N(3B)-C(239)	1.3506
C(166)-H(166)	0.9500	N(4B)-C(244)	1.3368
C(167)-C(168)	1.3859(14)	N(4B)-C(240)	1.3394
C(167)-H(167)	0.9500	C(201)-C(202)	1.4043
C(168)-C(169)	1.4004(14)	C(201)-C(206)	1.4063
C(168)-H(168)	0.9500	C(202)-C(203)	1.4004
C(169)-C(170)	1.3645(14)	C(202)-H(202)	0.9500
C(169)-H(169)	0.9500	C(203)-C(204)	1.4386
C(170)-C(171)	1.4155(14)	C(203)-H(203)	0.9500
C(170)-H(170)	0.9500	C(204)-C(205)	1.3208
C(171)-C(172)	1.4517(13)	C(204)-H(204)	0.9500
C(172)-C(173)	1.4402(13)	C(205)-C(206)	1.4265
C(173)-C(174)	1.3919(14)	C(205)-H(205)	0.9500
C(173)-H(173)	0.9500	C(206)-H(206)	0.9500
C(174)-C(175)	1.3239(14)	C(207)-C(212)	1.3827
C(174)-H(174)	0.9500	C(207)-C(208)	1.4091
C(175)-C(176)	1.3615(14)	C(208)-C(209)	1.3886
C(175)-H(175)	0.9500	C(208)-H(208)	0.9500
C(176)-H(176)	0.9500	C(209)-C(210)	1.3758

C(209)-H(209)	0.9500	C(229)-C(230)	1.5046
C(210)-C(211)	1.3927	C(230)-C(231)	1.3758
C(210)-H(210)	0.9500	C(231)-C(232)	1.3809
C(211)-C(212)	1.3825	C(231)-H(231)	0.9500
C(211)-H(211)	0.9500	C(232)-C(233)	1.3719
C(212)-H(212)	0.9500	C(232)-H(232)	0.9500
C(213)-C(214)	1.3796	C(233)-C(234)	1.3868
C(213)-C(218)	1.4299	C(233)-H(233)	0.9500
C(214)-C(215)	1.4025	C(234)-H(234)	0.9500
C(214)-H(214)	0.9500	C(235)-C(236)	1.3998
C(215)-C(216)	1.3676	C(235)-H(235)	0.9500
C(215)-H(215)	0.9500	C(236)-C(237)	1.3291
C(216)-C(217)	1.3816	C(236)-H(236)	0.9500
C(216)-H(216)	0.9500	C(237)-C(238)	1.4020
C(217)-C(218)	1.3856	C(237)-H(237)	0.9500
C(217)-H(217)	0.9500	C(238)-C(239)	1.4047
C(218)-H(218)	0.9500	C(238)-H(238)	0.9500
C(219)-C(220)	1.3877	C(239)-C(240)	1.4565
C(219)-C(224)	1.4019	C(240)-C(241)	1.4162
C(220)-C(221)	1.3926	C(241)-C(242)	1.3941
C(220)-H(220)	0.9500	C(241)-H(241)	0.9500
C(221)-C(222)	1.3543	C(242)-C(243)	1.3962
C(221)-H(221)	0.9500	C(242)-H(242)	0.9500
C(222)-C(223)	1.3963	C(243)-C(244)	1.3712
C(222)-H(222)	0.9500	C(243)-H(243)	0.9500
C(223)-C(224)	1.3723	C(244)-H(244)	0.9500
C(223)-H(223)	0.9500	Th(2B)-N(5B)	2.6377
C(224)-H(224)	0.9500	Th(2B)-N(8B)	2.6518
C(225)-C(226)	1.3184	Th(2B)-N(7B)	2.6539
C(225)-H(225)	0.9500	Th(2B)-N(6B)	2.6637
C(226)-C(227)	1.3694	Th(2B)-S(7B)	2.8259
C(226)-H(226)	0.9500	Th(2B)-S(8B)	2.8412
C(227)-C(228)	1.4149	Th(2B)-S(5B)	2.8489
C(227)-H(227)	0.9500	Th(2B)-S(6B)	2.8638
C(228)-C(229)	1.4118	S(5B)-C(245)	1.7631
C(228)-H(228)	0.9500	S(6B)-C(251)	1.7830

S(7B)-C(257)	1.7843	C(259)-C(260)	1.3608
S(8B)-C(263)	1.7763	C(259)-H(259)	0.9500
N(5B)-C(273)	1.3719	C(260)-C(261)	1.3651
N(5B)-C(269)	1.3856	C(260)-H(260)	0.9500
N(6B)-C(274)	1.3484	C(261)-C(262)	1.3741
N(6B)-C(278)	1.3815	C(261)-H(261)	0.9500
N(7B)-C(279)	1.3614	C(262)-H(262)	0.9500
N(7B)-C(283)	1.3805	C(263)-C(268)	1.3704
N(8B)-C(288)	1.3120	C(263)-C(264)	1.3993
N(8B)-C(284)	1.3727	C(264)-C(265)	1.4034
C(245)-C(250)	1.4145	C(264)-H(264)	0.9500
C(245)-C(246)	1.4172	C(265)-C(266)	1.3737
C(246)-C(247)	1.3992	C(265)-H(265)	0.9500
C(246)-H(246)	0.9500	C(266)-C(267)	1.3816
C(247)-C(248)	1.3715	C(266)-H(266)	0.9500
C(247)-H(247)	0.9500	C(267)-C(268)	1.3687
C(248)-C(249)	1.3441	C(267)-H(267)	0.9500
C(248)-H(248)	0.9500	C(268)-H(268)	0.9500
C(249)-C(250)	1.3840	C(269)-C(270)	1.3535
C(249)-H(249)	0.9500	C(269)-H(269)	0.9500
C(250)-H(250)	0.9500	C(270)-C(271)	1.3940
C(251)-C(256)	1.3744	C(270)-H(270)	0.9500
C(251)-C(252)	1.4163	C(271)-C(272)	1.3725
C(252)-C(253)	1.3870	C(271)-H(271)	0.9500
C(252)-H(252)	0.9500	C(272)-C(273)	1.4083
C(253)-C(254)	1.3514	C(272)-H(272)	0.9500
C(253)-H(253)	0.9500	C(273)-C(274)	1.4503
C(254)-C(255)	1.4093	C(274)-C(275)	1.3687
C(254)-H(254)	0.9500	C(275)-C(276)	1.3869
C(255)-C(256)	1.4191	C(275)-H(275)	0.9500
C(255)-H(255)	0.9500	C(276)-C(277)	1.4267
C(256)-H(256)	0.9500	C(276)-H(276)	0.9500
C(257)-C(262)	1.3982	C(277)-C(278)	1.3606
C(257)-C(258)	1.4008	C(277)-H(277)	0.9500
C(258)-C(259)	1.3897	C(278)-H(278)	0.9500
C(258)-H(258)	0.9500	C(279)-C(280)	1.3806

C(279)-H(279)	0.9500	C(289)-C(294)	1.3687
C(280)-C(281)	1.4055	C(289)-C(290)	1.4198
C(280)-H(280)	0.9500	C(290)-C(291)	1.3431
C(281)-C(282)	1.3912	C(290)-H(290)	0.9500
C(281)-H(281)	0.9500	C(291)-C(292)	1.3495
C(282)-C(283)	1.3738	C(291)-H(291)	0.9500
C(282)-H(282)	0.9500	C(292)-C(293)	1.4160
C(283)-C(284)	1.4781	C(292)-H(292)	0.9500
C(284)-C(285)	1.3859	C(293)-C(294)	1.3621
C(285)-C(286)	1.3602	C(293)-H(293)	0.9500
C(285)-H(285)	0.9500	C(294)-H(294)	0.9500
C(286)-C(287)	1.4265	C(295)-C(296)	1.3526
C(286)-H(286)	0.9500	C(295)-C(300)	1.4531
C(287)-C(288)	1.3873	C(296)-C(297)	1.3870
C(287)-H(287)	0.9500	C(296)-H(296)	0.9500
C(288)-H(288)	0.9500	C(297)-C(298)	1.3751
Th(3B)-N(10B)	2.6278	C(297)-H(297)	0.9500
Th(3B)-N(12B)	2.6337	C(298)-C(299)	1.3674
Th(3B)-N(9B)	2.6353	C(298)-H(298)	0.9500
Th(3B)-N(11B)	2.6380	C(299)-C(300)	1.4318
Th(3B)-S(12B)	2.8424	C(299)-H(299)	0.9500
Th(3B)-S(11B)	2.8425	C(300)-H(300)	0.9500
Th(3B)-S(10B)	2.8540	C(301)-C(302)	1.3659
Th(3B)-S(9B)	2.8669	C(301)-C(306)	1.4002
S(9B)-C(289)	1.7846	C(302)-C(303)	1.3886
S(10B)-C(295)	1.7609	C(302)-H(302)	0.9500
S(11B)-C(301)	1.7756	C(303)-C(304)	1.3707
S(12B)-C(307)	1.7566	C(303)-H(303)	0.9500
N(9B)-C(313)	1.3367	C(304)-C(305)	1.4153
N(9B)-C(317)	1.3585	C(304)-H(304)	0.9500
N(10B)-C(322)	1.3324	C(305)-C(306)	1.3903
N(10B)-C(318)	1.3680	C(305)-H(305)	0.9500
N(11B)-C(323)	1.3426	C(306)-H(306)	0.9500
N(11B)-C(327)	1.3446	C(307)-C(312)	1.3948
N(12B)-C(332)	1.3438	C(307)-C(308)	1.4143
N(12B)-C(328)	1.3716	C(308)-C(309)	1.3895

C(308)-H(308)	0.9500	C(329)-H(329)	0.9500
C(309)-C(310)	1.3766	C(330)-C(331)	1.3995
C(309)-H(309)	0.9500	C(330)-H(330)	0.9500
C(310)-C(311)	1.3774	C(331)-C(332)	1.3704
C(310)-H(310)	0.9500	C(331)-H(331)	0.9500
C(311)-C(312)	1.4016	C(332)-H(332)	0.9500
C(311)-H(311)	0.9500	Th(4B)-N(13B)	2.6063
C(312)-H(312)	0.9500	Th(4B)-N(16B)	2.6184
C(313)-C(314)	1.4128	Th(4B)-N(15B)	2.6246
C(313)-H(313)	0.9500	Th(4B)-N(14B)	2.6526
C(314)-C(315)	1.3537	Th(4B)-S(15B)	2.8301
C(314)-H(314)	0.9500	Th(4B)-S(16B)	2.8545
C(315)-C(316)	1.4078	Th(4B)-S(13B)	2.8563
C(315)-H(315)	0.9500	Th(4B)-S(14B)	2.8615
C(316)-C(317)	1.3503	S(13B)-C(333)	1.7790
C(316)-H(316)	0.9500	S(14B)-C(339)	1.7647
C(317)-C(318)	1.4899	S(15B)-C(345)	1.7687
C(318)-C(319)	1.3949	S(16B)-C(351)	1.7909
C(319)-C(320)	1.4118	N(13B)-C(357)	1.3097
C(319)-H(319)	0.9500	N(13B)-C(361)	1.3800
C(320)-C(321)	1.3664	N(14B)-C(366)	1.3208
C(320)-H(320)	0.9500	N(14B)-C(362)	1.3449
C(321)-C(322)	1.3703	N(15B)-C(367)	1.3435
C(321)-H(321)	0.9500	N(15B)-C(371)	1.3794
C(322)-H(322)	0.9500	N(16B)-C(372)	1.3494
C(323)-C(324)	1.3578	N(16B)-C(376)	1.3565
C(323)-H(323)	0.9500	C(333)-C(338)	1.3634
C(324)-C(325)	1.3880	C(333)-C(334)	1.4115
C(324)-H(324)	0.9500	C(334)-C(335)	1.3922
C(325)-C(326)	1.3570	C(334)-H(334)	0.9500
C(325)-H(325)	0.9500	C(335)-C(336)	1.4113
C(326)-C(327)	1.4205	C(335)-H(335)	0.9500
C(326)-H(326)	0.9500	C(336)-C(337)	1.3668
C(327)-C(328)	1.4838	C(336)-H(336)	0.9500
C(328)-C(329)	1.3682	C(337)-C(338)	1.3671
C(329)-C(330)	1.3647	C(337)-H(337)	0.9500

C(338)-H(338)	0.9500	C(357)-C(358)	1.4208
C(339)-C(344)	1.3681	C(357)-H(357)	0.9500
C(339)-C(340)	1.4171	C(358)-C(359)	1.3611
C(340)-C(341)	1.3520	C(358)-H(358)	0.9500
C(340)-H(340)	0.9500	C(359)-C(360)	1.3374
C(341)-C(342)	1.4049	C(359)-H(359)	0.9500
C(341)-H(341)	0.9500	C(360)-C(361)	1.3926
C(342)-C(343)	1.4312	C(360)-H(360)	0.9500
C(342)-H(342)	0.9500	C(361)-C(362)	1.4740
C(343)-C(344)	1.3544	C(362)-C(363)	1.4148
C(343)-H(343)	0.9500	C(363)-C(364)	1.3852
C(344)-H(344)	0.9500	C(363)-H(363)	0.9500
C(345)-C(346)	1.4132	C(364)-C(365)	1.3733
C(345)-C(350)	1.4146	C(364)-H(364)	0.9500
C(346)-C(347)	1.4071	C(365)-C(366)	1.3685
C(346)-H(346)	0.9500	C(365)-H(365)	0.9500
C(347)-C(348)	1.4052	C(366)-H(366)	0.9500
C(347)-H(347)	0.9500	C(367)-C(368)	1.3860
C(348)-C(349)	1.3218	C(367)-H(367)	0.9500
C(348)-H(348)	0.9500	C(368)-C(369)	1.4005
C(349)-C(350)	1.4244	C(368)-H(368)	0.9500
C(349)-H(349)	0.9500	C(369)-C(370)	1.3646
C(350)-H(350)	0.9500	C(369)-H(369)	0.9500
C(351)-C(356)	1.3614	C(370)-C(371)	1.4156
C(351)-C(352)	1.4091	C(370)-H(370)	0.9500
C(352)-C(353)	1.3897	C(371)-C(372)	1.4516
C(352)-H(352)	0.9500	C(372)-C(373)	1.4403
C(353)-C(354)	1.3693	C(373)-C(374)	1.3920
C(353)-H(353)	0.9500	C(373)-H(373)	0.9500
C(354)-C(355)	1.3658	C(374)-C(375)	1.3240
C(354)-H(354)	0.9500	C(374)-H(374)	0.9500
C(355)-C(356)	1.4192	C(375)-C(376)	1.3616
C(355)-H(355)	0.9500	C(375)-H(375)	0.9500
C(356)-H(356)	0.9500	C(376)-H(376)	0.9500

N(4)-Th(1)-N(1)	139.97(7)	N(4)-Th(1)-N(2)	151.17(8)

N(1)-Th(1)-N(2)	61.35(5)	C(35)-N(3)-C(39)	120.26(17)
N(4)-Th(1)-N(3)	61.44(5)	C(35)-N(3)-Th(1)	119.25(15)
N(1)-Th(1)-N(3)	151.45(8)	C(39)-N(3)-Th(1)	119.95(11)
N(2)-Th(1)-N(3)	108.79(7)	C(44)-N(4)-C(40)	117.85(15)
N(4)-Th(1)-S(3)	121.53(7)	C(44)-N(4)-Th(1)	119.39(15)
N(1)-Th(1)-S(3)	79.26(6)	C(40)-N(4)-Th(1)	122.27(13)
N(2)-Th(1)-S(3)	74.96(6)	C(2)-C(1)-C(6)	117.84(16)
N(3)-Th(1)-S(3)	72.22(6)	C(2)-C(1)-S(1)	118.74(19)
N(4)-Th(1)-S(4)	80.38(7)	C(6)-C(1)-S(1)	123.1(2)
N(1)-Th(1)-S(4)	120.92(7)	C(3)-C(2)-C(1)	122.08(18)
N(2)-Th(1)-S(4)	70.80(6)	C(3)-C(2)-H(2)	119.0
N(3)-Th(1)-S(4)	74.43(6)	C(1)-C(2)-H(2)	119.0
S(3)-Th(1)-S(4)	120.11(7)	C(2)-C(3)-C(4)	117.5(2)
N(4)-Th(1)-S(1)	86.95(6)	C(2)-C(3)-H(3)	121.3
N(1)-Th(1)-S(1)	64.32(6)	C(4)-C(3)-H(3)	121.3
N(2)-Th(1)-S(1)	90.60(7)	C(5)-C(4)-C(3)	121.3(2)
N(3)-Th(1)-S(1)	144.19(7)	C(5)-C(4)-H(4)	119.4
S(3)-Th(1)-S(1)	143.30(7)	C(3)-C(4)-H(4)	119.4
S(4)-Th(1)-S(1)	84.62(6)	C(4)-C(5)-C(6)	120.9(2)
N(4)-Th(1)-S(2)	64.09(6)	C(4)-C(5)-H(5)	119.6
N(1)-Th(1)-S(2)	87.08(6)	C(6)-C(5)-H(5)	119.6
N(2)-Th(1)-S(2)	144.65(7)	C(1)-C(6)-C(5)	120.02(19)
N(3)-Th(1)-S(2)	91.18(7)	C(1)-C(6)-H(6)	120.0
S(3)-Th(1)-S(2)	84.36(6)	C(5)-C(6)-H(6)	120.0
S(4)-Th(1)-S(2)	144.22(7)	C(12)-C(7)-C(8)	118.99(16)
S(1)-Th(1)-S(2)	89.23(6)	C(12)-C(7)-S(2)	123.5(2)
C(1)-S(1)-Th(1)	120.86(18)	C(8)-C(7)-S(2)	117.30(18)
C(7)-S(2)-Th(1)	122.75(18)	C(9)-C(8)-C(7)	118.48(18)
C(13)-S(3)-Th(1)	115.31(16)	C(9)-C(8)-H(8)	120.8
C(19)-S(4)-Th(1)	113.16(16)	C(7)-C(8)-H(8)	120.8
C(29)-N(1)-C(25)	117.74(15)	C(10)-C(9)-C(8)	121.74(19)
C(29)-N(1)-Th(1)	122.46(14)	C(10)-C(9)-H(9)	119.1
C(25)-N(1)-Th(1)	119.35(16)	C(8)-C(9)-H(9)	119.1
C(34)-N(2)-C(30)	117.72(17)	C(9)-C(10)-C(11)	120.03(19)
C(34)-N(2)-Th(1)	119.10(14)	C(9)-C(10)-H(10)	120.0
C(30)-N(2)-Th(1)	122.79(10)	C(11)-C(10)-H(10)	120.0

C(12)-C(11)-C(10)	118.52(19)	C(24)-C(23)-C(22)	118.2(2)
C(12)-C(11)-H(11)	120.7	C(24)-C(23)-H(23)	120.9
C(10)-C(11)-H(11)	120.7	C(22)-C(23)-H(23)	120.9
C(11)-C(12)-C(7)	122.21(19)	C(23)-C(24)-C(19)	121.3(2)
C(11)-C(12)-H(12)	118.9	C(23)-C(24)-H(24)	119.3
C(7)-C(12)-H(12)	118.9	C(19)-C(24)-H(24)	119.3
C(14)-C(13)-C(18)	117.54(16)	C(26)-C(25)-N(1)	123.05(19)
C(14)-C(13)-S(3)	122.5(2)	C(26)-C(25)-H(25)	118.5
C(18)-C(13)-S(3)	119.79(19)	N(1)-C(25)-H(25)	118.5
C(13)-C(14)-C(15)	121.21(18)	C(25)-C(26)-C(27)	121.2(2)
C(13)-C(14)-H(14)	119.4	C(25)-C(26)-H(26)	119.4
C(15)-C(14)-H(14)	119.4	C(27)-C(26)-H(26)	119.4
C(16)-C(15)-C(14)	120.62(19)	C(26)-C(27)-C(28)	118.89(19)
C(16)-C(15)-H(15)	119.7	C(26)-C(27)-H(27)	120.6
C(14)-C(15)-H(15)	119.7	C(28)-C(27)-H(27)	120.6
C(15)-C(16)-C(17)	119.53(19)	C(29)-C(28)-C(27)	115.74(17)
C(15)-C(16)-H(16)	120.2	C(29)-C(28)-H(28)	122.1
C(17)-C(16)-H(16)	120.2	C(27)-C(28)-H(28)	122.1
C(16)-C(17)-C(18)	120.9(2)	N(1)-C(29)-C(28)	123.11(17)
C(16)-C(17)-H(17)	119.5	N(1)-C(29)-C(30)	118.37(14)
C(18)-C(17)-H(17)	119.5	C(28)-C(29)-C(30)	118.46(18)
C(17)-C(18)-C(13)	120.04(19)	N(2)-C(30)-C(31)	121.86(16)
C(17)-C(18)-H(18)	120.0	N(2)-C(30)-C(29)	114.38(13)
C(13)-C(18)-H(18)	120.0	C(31)-C(30)-C(29)	123.6(2)
C(20)-C(19)-C(24)	118.83(17)	C(30)-C(31)-C(32)	118.84(19)
C(20)-C(19)-S(4)	118.94(19)	C(30)-C(31)-H(31)	120.6
C(24)-C(19)-S(4)	121.9(2)	C(32)-C(31)-H(31)	120.6
C(19)-C(20)-C(21)	119.51(19)	C(33)-C(32)-C(31)	120.4(2)
C(19)-C(20)-H(20)	120.2	C(33)-C(32)-H(32)	119.8
C(21)-C(20)-H(20)	120.2	C(31)-C(32)-H(32)	119.8
C(22)-C(21)-C(20)	120.5(2)	C(32)-C(33)-C(34)	118.27(19)
C(22)-C(21)-H(21)	119.8	C(32)-C(33)-H(33)	120.9
C(20)-C(21)-H(21)	119.8	C(34)-C(33)-H(33)	120.9
C(21)-C(22)-C(23)	121.3(2)	N(2)-C(34)-C(33)	122.61(18)
C(21)-C(22)-H(22)	119.4	N(2)-C(34)-H(34)	118.7
C(23)-C(22)-H(22)	119.4	C(33)-C(34)-H(34)	118.7

N(3)-C(35)-C(36)	122.04(18)	N(5)-Th(2)-S(7)	78.89(6)
N(3)-C(35)-H(35)	119.0	N(8)-Th(2)-S(7)	121.78(7)
C(36)-C(35)-H(35)	119.0	N(7)-Th(2)-S(7)	72.86(6)
C(37)-C(36)-C(35)	119.11(19)	N(6)-Th(2)-S(7)	73.22(6)
C(37)-C(36)-H(36)	120.4	N(5)-Th(2)-S(8)	121.11(7)
C(35)-C(36)-H(36)	120.4	N(8)-Th(2)-S(8)	80.45(6)
C(36)-C(37)-C(38)	119.60(19)	N(7)-Th(2)-S(8)	73.83(6)
C(36)-C(37)-H(37)	120.2	N(6)-Th(2)-S(8)	72.05(6)
C(38)-C(37)-H(37)	120.2	S(7)-Th(2)-S(8)	120.00(7)
C(37)-C(38)-C(39)	120.19(18)	N(5)-Th(2)-S(5)	65.29(6)
C(37)-C(38)-H(38)	119.9	N(8)-Th(2)-S(5)	86.07(6)
C(39)-C(38)-H(38)	119.9	N(7)-Th(2)-S(5)	142.96(7)
N(3)-C(39)-C(38)	118.64(15)	N(6)-Th(2)-S(5)	92.32(7)
N(3)-C(39)-C(40)	117.67(14)	S(7)-Th(2)-S(5)	143.88(7)
C(38)-C(39)-C(40)	123.68(18)	S(8)-Th(2)-S(5)	84.43(6)
N(4)-C(40)-C(41)	122.18(16)	N(5)-Th(2)-S(6)	87.50(6)
N(4)-C(40)-C(39)	117.95(16)	N(8)-Th(2)-S(6)	63.67(6)
C(41)-C(40)-C(39)	119.86(17)	N(7)-Th(2)-S(6)	91.00(7)
C(42)-C(41)-C(40)	117.38(18)	N(6)-Th(2)-S(6)	143.85(7)
C(42)-C(41)-H(41)	121.3	S(7)-Th(2)-S(6)	84.42(6)
C(40)-C(41)-H(41)	121.3	S(8)-Th(2)-S(6)	143.94(7)
C(41)-C(42)-C(43)	120.69(18)	S(5)-Th(2)-S(6)	89.38(6)
C(41)-C(42)-H(42)	119.7	C(45)-S(5)-Th(2)	120.63(18)
C(43)-C(42)-H(42)	119.7	C(51)-S(6)-Th(2)	120.92(17)
C(44)-C(43)-C(42)	116.43(18)	C(57)-S(7)-Th(2)	115.62(17)
C(44)-C(43)-H(43)	121.8	C(63)-S(8)-Th(2)	111.36(15)
C(42)-C(43)-H(43)	121.8	C(73)-N(5)-C(69)	117.20(15)
N(4)-C(44)-C(43)	125.45(19)	C(73)-N(5)-Th(2)	122.73(13)
N(4)-C(44)-H(44)	117.3	C(69)-N(5)-Th(2)	119.51(15)
C(43)-C(44)-H(44)	117.3	C(74)-N(6)-C(78)	118.07(17)
N(5)-Th(2)-N(8)	139.95(7)	C(74)-N(6)-Th(2)	121.76(11)
N(5)-Th(2)-N(7)	151.72(8)	C(78)-N(6)-Th(2)	119.60(15)
N(8)-Th(2)-N(7)	61.32(5)	C(79)-N(7)-C(83)	117.70(16)
N(5)-Th(2)-N(6)	60.91(5)	C(79)-N(7)-Th(2)	119.14(14)
N(8)-Th(2)-N(6)	152.47(8)	C(83)-N(7)-Th(2)	123.00(10)
N(7)-Th(2)-N(6)	108.38(7)	C(88)-N(8)-C(84)	118.06(16)

C(88)-N(8)-Th(2)	119.34(16)	C(51)-C(56)-H(56)	120.1
C(84)-N(8)-Th(2)	121.95(14)	C(55)-C(56)-H(56)	120.1
C(50)-C(45)-C(46)	117.15(16)	C(62)-C(57)-C(58)	118.08(16)
C(50)-C(45)-S(5)	123.2(2)	C(62)-C(57)-S(7)	122.2(2)
C(46)-C(45)-S(5)	119.15(19)	C(58)-C(57)-S(7)	119.38(19)
C(47)-C(46)-C(45)	119.40(18)	C(59)-C(58)-C(57)	119.07(18)
C(47)-C(46)-H(46)	120.3	C(59)-C(58)-H(58)	120.5
C(45)-C(46)-H(46)	120.3	C(57)-C(58)-H(58)	120.5
C(48)-C(47)-C(46)	121.6(2)	C(60)-C(59)-C(58)	121.00(19)
C(48)-C(47)-H(47)	119.2	C(60)-C(59)-H(59)	119.5
C(46)-C(47)-H(47)	119.2	C(58)-C(59)-H(59)	119.5
C(49)-C(48)-C(47)	119.3(2)	C(59)-C(60)-C(61)	121.06(19)
C(49)-C(48)-H(48)	120.4	C(59)-C(60)-H(60)	119.5
C(47)-C(48)-H(48)	120.4	C(61)-C(60)-H(60)	119.5
C(48)-C(49)-C(50)	122.0(2)	C(60)-C(61)-C(62)	119.02(19)
C(48)-C(49)-H(49)	119.0	C(60)-C(61)-H(61)	120.5
C(50)-C(49)-H(49)	119.0	C(62)-C(61)-H(61)	120.5
C(49)-C(50)-C(45)	120.43(18)	C(61)-C(62)-C(57)	121.72(19)
C(49)-C(50)-H(50)	119.8	C(61)-C(62)-H(62)	119.1
C(45)-C(50)-H(50)	119.8	C(57)-C(62)-H(62)	119.1
C(56)-C(51)-C(52)	119.75(17)	C(68)-C(63)-C(64)	118.70(17)
C(56)-C(51)-S(6)	122.3(2)	C(68)-C(63)-S(8)	122.57(19)
C(52)-C(51)-S(6)	117.77(18)	C(64)-C(63)-S(8)	118.62(18)
C(53)-C(52)-C(51)	120.00(18)	C(63)-C(64)-C(65)	120.59(18)
C(53)-C(52)-H(52)	120.0	C(63)-C(64)-H(64)	119.7
C(51)-C(52)-H(52)	120.0	C(65)-C(64)-H(64)	119.7
C(54)-C(53)-C(52)	120.53(19)	C(66)-C(65)-C(64)	119.67(19)
C(54)-C(53)-H(53)	119.7	C(66)-C(65)-H(65)	120.2
C(52)-C(53)-H(53)	119.7	C(64)-C(65)-H(65)	120.2
C(53)-C(54)-C(55)	121.04(19)	C(65)-C(66)-C(67)	118.43(19)
C(53)-C(54)-H(54)	119.5	C(65)-C(66)-H(66)	120.8
C(55)-C(54)-H(54)	119.5	C(67)-C(66)-H(66)	120.8
C(54)-C(55)-C(56)	118.81(19)	C(68)-C(67)-C(66)	122.5(2)
C(54)-C(55)-H(55)	120.6	C(68)-C(67)-H(67)	118.8
C(56)-C(55)-H(55)	120.6	C(66)-C(67)-H(67)	118.8
C(51)-C(56)-C(55)	119.83(18)	C(67)-C(68)-C(63)	119.9(2)

C(67)-C(68)-H(68)	120.1	C(79)-C(80)-H(80)	120.3
C(63)-C(68)-H(68)	120.1	C(81)-C(80)-H(80)	120.3
C(70)-C(69)-N(5)	123.93(19)	C(82)-C(81)-C(80)	116.45(18)
C(70)-C(69)-H(69)	118.0	C(82)-C(81)-H(81)	121.8
N(5)-C(69)-H(69)	118.0	C(80)-C(81)-H(81)	121.8
C(69)-C(70)-C(71)	118.92(19)	C(83)-C(82)-C(81)	122.94(19)
C(69)-C(70)-H(70)	120.5	C(83)-C(82)-H(82)	118.5
C(71)-C(70)-H(70)	120.5	C(81)-C(82)-H(82)	118.5
C(72)-C(71)-C(70)	118.79(19)	C(82)-C(83)-N(7)	119.98(16)
C(72)-C(71)-H(71)	120.6	C(82)-C(83)-C(84)	124.60(17)
C(70)-C(71)-H(71)	120.6	N(7)-C(83)-C(84)	115.42(14)
C(71)-C(72)-C(73)	121.03(18)	N(8)-C(84)-C(85)	121.88(16)
C(71)-C(72)-H(72)	119.5	N(8)-C(84)-C(83)	117.29(17)
C(73)-C(72)-H(72)	119.5	C(85)-C(84)-C(83)	120.78(17)
N(5)-C(73)-C(72)	120.04(16)	C(86)-C(85)-C(84)	118.86(18)
N(5)-C(73)-C(74)	115.82(16)	C(86)-C(85)-H(85)	120.6
C(72)-C(73)-C(74)	124.13(18)	C(84)-C(85)-H(85)	120.6
N(6)-C(74)-C(75)	121.38(16)	C(85)-C(86)-C(87)	120.34(19)
N(6)-C(74)-C(73)	118.03(14)	C(85)-C(86)-H(86)	119.8
C(75)-C(74)-C(73)	120.55(19)	C(87)-C(86)-H(86)	119.8
C(74)-C(75)-C(76)	120.48(19)	C(88)-C(87)-C(86)	115.90(19)
C(74)-C(75)-H(75)	119.8	C(88)-C(87)-H(87)	122.1
C(76)-C(75)-H(75)	119.8	C(86)-C(87)-H(87)	122.1
C(75)-C(76)-C(77)	119.35(18)	N(8)-C(88)-C(87)	124.7(2)
C(75)-C(76)-H(76)	120.3	N(8)-C(88)-H(88)	117.6
C(77)-C(76)-H(76)	120.3	C(87)-C(88)-H(88)	117.6
C(78)-C(77)-C(76)	116.47(18)	N(10)-Th(3)-N(12)	150.59(8)
C(78)-C(77)-H(77)	121.8	N(10)-Th(3)-N(9)	61.29(5)
C(76)-C(77)-H(77)	121.8	N(12)-Th(3)-N(9)	141.59(7)
C(77)-C(78)-N(6)	124.11(18)	N(10)-Th(3)-N(11)	106.25(7)
C(77)-C(78)-H(78)	117.9	N(12)-Th(3)-N(11)	60.98(5)
N(6)-C(78)-H(78)	117.9	N(9)-Th(3)-N(11)	152.07(8)
N(7)-C(79)-C(80)	123.49(18)	N(10)-Th(3)-S(12)	72.10(6)
N(7)-C(79)-H(79)	118.3	N(12)-Th(3)-S(12)	78.63(6)
C(80)-C(79)-H(79)	118.3	N(9)-Th(3)-S(12)	120.80(7)
C(79)-C(80)-C(81)	119.31(19)	N(11)-Th(3)-S(12)	72.49(6)

N(10)-Th(3)-S(11)	73.07(6)	C(90)-C(89)-S(9)	119.19(19)
N(12)-Th(3)-S(11)	121.45(7)	C(91)-C(90)-C(89)	122.30(19)
N(9)-Th(3)-S(11)	79.61(6)	C(91)-C(90)-H(90)	118.8
N(11)-Th(3)-S(11)	72.66(6)	C(89)-C(90)-H(90)	118.8
S(12)-Th(3)-S(11)	120.14(7)	C(90)-C(91)-C(92)	119.3(2)
N(10)-Th(3)-S(10)	145.14(7)	C(90)-C(91)-H(91)	120.3
N(12)-Th(3)-S(10)	64.26(6)	C(92)-C(91)-H(91)	120.3
N(9)-Th(3)-S(10)	88.81(6)	C(91)-C(92)-C(93)	120.33(19)
N(11)-Th(3)-S(10)	91.94(7)	C(91)-C(92)-H(92)	119.8
S(12)-Th(3)-S(10)	142.66(7)	C(93)-C(92)-H(92)	119.8
S(11)-Th(3)-S(10)	84.88(7)	C(94)-C(93)-C(92)	119.67(19)
N(10)-Th(3)-S(9)	92.30(7)	C(94)-C(93)-H(93)	120.2
N(12)-Th(3)-S(9)	87.85(6)	C(92)-C(93)-H(93)	120.2
N(9)-Th(3)-S(9)	63.80(6)	C(93)-C(94)-C(89)	120.73(19)
N(11)-Th(3)-S(9)	144.10(7)	C(93)-C(94)-H(94)	119.6
S(12)-Th(3)-S(9)	84.95(6)	C(89)-C(94)-H(94)	119.6
S(11)-Th(3)-S(9)	143.10(7)	C(96)-C(95)-C(100)	118.41(16)
S(10)-Th(3)-S(9)	89.49(7)	C(96)-C(95)-S(10)	120.85(19)
C(89)-S(9)-Th(3)	121.84(18)	C(100)-C(95)-S(10)	120.74(19)
C(95)-S(10)-Th(3)	120.97(18)	C(95)-C(96)-C(97)	124.1(2)
C(101)-S(11)-Th(3)	114.80(16)	C(95)-C(96)-H(96)	118.0
C(107)-S(12)-Th(3)	113.01(16)	C(97)-C(96)-H(96)	118.0
C(113)-N(9)-C(117)	117.71(16)	C(98)-C(97)-C(96)	118.99(19)
C(113)-N(9)-Th(3)	118.02(15)	C(98)-C(97)-H(97)	120.5
C(117)-N(9)-Th(3)	123.60(14)	C(96)-C(97)-H(97)	120.5
C(122)-N(10)-C(118)	115.78(15)	C(99)-C(98)-C(97)	119.63(19)
C(122)-N(10)-Th(3)	122.06(14)	C(99)-C(98)-H(98)	120.2
C(118)-N(10)-Th(3)	122.15(11)	C(97)-C(98)-H(98)	120.2
C(123)-N(11)-C(127)	115.56(15)	C(98)-C(99)-C(100)	122.92(19)
C(123)-N(11)-Th(3)	121.60(15)	C(98)-C(99)-H(99)	118.5
C(127)-N(11)-Th(3)	122.77(10)	C(100)-C(99)-H(99)	118.5
C(132)-N(12)-C(128)	116.95(15)	C(99)-C(100)-C(95)	115.88(17)
C(132)-N(12)-Th(3)	119.10(15)	C(99)-C(100)-H(100)	122.1
C(128)-N(12)-Th(3)	123.48(13)	C(95)-C(100)-H(100)	122.1
C(94)-C(89)-C(90)	117.56(16)	C(102)-C(101)-C(106)	118.69(16)
C(94)-C(89)-S(9)	123.2(2)	C(102)-C(101)-S(11)	119.91(19)

C(106)-C(101)-S(11)	121.40(19)	C(114)-C(113)-H(113)	118.9
C(101)-C(102)-C(103)	122.21(19)	C(115)-C(114)-C(113)	119.73(19)
C(101)-C(102)-H(102)	118.9	C(115)-C(114)-H(114)	120.1
C(103)-C(102)-H(102)	118.9	C(113)-C(114)-H(114)	120.1
C(104)-C(103)-C(102)	120.3(2)	C(114)-C(115)-C(116)	117.31(18)
C(104)-C(103)-H(103)	119.9	C(114)-C(115)-H(115)	121.3
C(102)-C(103)-H(103)	119.9	C(116)-C(115)-H(115)	121.3
C(103)-C(104)-C(105)	118.25(18)	C(117)-C(116)-C(115)	120.83(18)
C(103)-C(104)-H(104)	120.9	C(117)-C(116)-H(116)	119.6
C(105)-C(104)-H(104)	120.9	C(115)-C(116)-H(116)	119.6
C(106)-C(105)-C(104)	120.94(19)	C(116)-C(117)-N(9)	122.20(17)
C(106)-C(105)-H(105)	119.5	C(116)-C(117)-C(118)	123.31(18)
C(104)-C(105)-H(105)	119.5	N(9)-C(117)-C(118)	114.28(17)
C(105)-C(106)-C(101)	119.53(18)	N(10)-C(118)-C(119)	121.69(15)
C(105)-C(106)-H(106)	120.2	N(10)-C(118)-C(117)	117.47(13)
C(101)-C(106)-H(106)	120.2	C(119)-C(118)-C(117)	120.83(17)
C(112)-C(107)-C(108)	117.50(16)	C(118)-C(119)-C(120)	120.09(18)
C(112)-C(107)-S(12)	120.48(19)	C(118)-C(119)-H(119)	120.0
C(108)-C(107)-S(12)	122.02(19)	C(120)-C(119)-H(119)	120.0
C(109)-C(108)-C(107)	119.70(18)	C(121)-C(120)-C(119)	117.24(18)
C(109)-C(108)-H(108)	120.2	C(121)-C(120)-H(120)	121.4
C(107)-C(108)-H(108)	120.2	C(119)-C(120)-H(120)	121.4
C(110)-C(109)-C(108)	122.1(2)	C(120)-C(121)-C(122)	119.13(19)
C(110)-C(109)-H(109)	118.9	C(120)-C(121)-H(121)	120.4
C(108)-C(109)-H(109)	118.9	C(122)-C(121)-H(121)	120.4
C(109)-C(110)-C(111)	118.9(2)	N(10)-C(122)-C(121)	126.04(19)
C(109)-C(110)-H(110)	120.6	N(10)-C(122)-H(122)	117.0
C(111)-C(110)-H(110)	120.6	C(121)-C(122)-H(122)	117.0
C(110)-C(111)-C(112)	120.1(2)	N(11)-C(123)-C(124)	126.50(19)
C(110)-C(111)-H(111)	119.9	N(11)-C(123)-H(123)	116.8
C(112)-C(111)-H(111)	119.9	C(124)-C(123)-H(123)	116.8
C(107)-C(112)-C(111)	121.50(19)	C(123)-C(124)-C(125)	116.58(19)
C(107)-C(112)-H(112)	119.2	C(123)-C(124)-H(124)	121.7
C(111)-C(112)-H(112)	119.2	C(125)-C(124)-H(124)	121.7
N(9)-C(113)-C(114)	122.18(18)	C(126)-C(125)-C(124)	120.76(19)
N(9)-C(113)-H(113)	118.9	C(126)-C(125)-H(125)	119.6

C(124)-C(125)-H(125)	119.6	S(15)-Th(4)-S(16)	120.37(7)
C(125)-C(126)-C(127)	117.94(18)	N(13)-Th(4)-S(13)	63.01(6)
C(125)-C(126)-H(126)	121.0	N(16)-Th(4)-S(13)	87.51(6)
C(127)-C(126)-H(126)	121.0	N(15)-Th(4)-S(13)	144.67(7)
N(11)-C(127)-C(126)	122.64(16)	N(14)-Th(4)-S(13)	90.78(7)
N(11)-C(127)-C(128)	117.67(14)	S(15)-Th(4)-S(13)	142.45(7)
C(126)-C(127)-C(128)	119.56(19)	S(16)-Th(4)-S(13)	84.48(6)
C(129)-C(128)-N(12)	120.33(16)	N(13)-Th(4)-S(14)	87.16(6)
C(129)-C(128)-C(127)	125.38(18)	N(16)-Th(4)-S(14)	64.73(6)
N(12)-C(128)-C(127)	114.21(16)	N(15)-Th(4)-S(14)	90.77(7)
C(130)-C(129)-C(128)	123.53(19)	N(14)-Th(4)-S(14)	143.63(7)
C(130)-C(129)-H(129)	118.2	S(15)-Th(4)-S(14)	83.86(6)
C(128)-C(129)-H(129)	118.2	S(16)-Th(4)-S(14)	143.61(7)
C(129)-C(130)-C(131)	115.56(18)	S(13)-Th(4)-S(14)	90.93(7)
C(129)-C(130)-H(130)	122.2	C(133)-S(13)-Th(4)	122.69(18)
C(131)-C(130)-H(130)	122.2	C(139)-S(14)-Th(4)	119.76(17)
C(132)-C(131)-C(130)	119.88(19)	C(145)-S(15)-Th(4)	112.33(16)
C(132)-C(131)-H(131)	120.1	C(151)-S(16)-Th(4)	113.04(16)
C(130)-C(131)-H(131)	120.1	C(157)-N(13)-C(161)	117.07(15)
N(12)-C(132)-C(131)	123.73(19)	C(157)-N(13)-Th(4)	120.16(15)
N(12)-C(132)-H(132)	118.1	C(161)-N(13)-Th(4)	122.44(13)
C(131)-C(132)-H(132)	118.1	C(166)-N(14)-C(162)	117.31(17)
N(13)-Th(4)-N(16)	139.37(7)	C(166)-N(14)-Th(4)	120.46(15)
N(13)-Th(4)-N(15)	152.31(8)	C(162)-N(14)-Th(4)	121.85(11)
N(16)-Th(4)-N(15)	61.66(5)	C(167)-N(15)-C(171)	117.77(15)
N(13)-Th(4)-N(14)	61.66(5)	C(167)-N(15)-Th(4)	120.86(14)
N(16)-Th(4)-N(14)	151.63(8)	C(171)-N(15)-Th(4)	121.36(10)
N(15)-Th(4)-N(14)	108.03(7)	C(172)-N(16)-C(176)	116.41(15)
N(13)-Th(4)-S(15)	79.57(6)	C(172)-N(16)-Th(4)	122.54(12)
N(16)-Th(4)-S(15)	122.54(7)	C(176)-N(16)-Th(4)	120.95(14)
N(15)-Th(4)-S(15)	72.75(6)	C(138)-C(133)-C(134)	118.48(16)
N(14)-Th(4)-S(15)	73.04(6)	C(138)-C(133)-S(13)	124.8(2)
N(13)-Th(4)-S(16)	121.63(7)	C(134)-C(133)-S(13)	116.54(18)
N(16)-Th(4)-S(16)	78.99(6)	C(135)-C(134)-C(133)	120.03(18)
N(15)-Th(4)-S(16)	73.61(6)	C(135)-C(134)-H(134)	120.0
N(14)-Th(4)-S(16)	72.66(6)	C(133)-C(134)-H(134)	120.0

C(134)-C(135)-C(136)	119.88(19)	C(148)-C(147)-C(146)	117.16(19)
C(134)-C(135)-H(135)	120.1	C(148)-C(147)-H(147)	121.4
C(136)-C(135)-H(135)	120.1	C(146)-C(147)-H(147)	121.4
C(137)-C(136)-C(135)	118.10(19)	C(149)-C(148)-C(147)	121.9(2)
C(137)-C(136)-H(136)	120.9	C(149)-C(148)-H(148)	119.1
C(135)-C(136)-H(136)	120.9	C(147)-C(148)-H(148)	119.1
C(136)-C(137)-C(138)	122.0(2)	C(148)-C(149)-C(150)	122.8(2)
C(136)-C(137)-H(137)	119.0	C(148)-C(149)-H(149)	118.6
C(138)-C(137)-H(137)	119.0	C(150)-C(149)-H(149)	118.6
C(133)-C(138)-C(137)	121.40(19)	C(145)-C(150)-C(149)	117.41(18)
C(133)-C(138)-H(138)	119.3	C(145)-C(150)-H(150)	121.3
C(137)-C(138)-H(138)	119.3	C(149)-C(150)-H(150)	121.3
C(144)-C(139)-C(140)	114.61(17)	C(156)-C(151)-C(152)	120.29(16)
C(144)-C(139)-S(14)	125.5(2)	C(156)-C(151)-S(16)	121.11(19)
C(140)-C(139)-S(14)	119.42(19)	C(152)-C(151)-S(16)	118.60(18)
C(141)-C(140)-C(139)	123.11(19)	C(153)-C(152)-C(151)	119.10(18)
C(141)-C(140)-H(140)	118.4	C(153)-C(152)-H(152)	120.5
C(139)-C(140)-H(140)	118.4	C(151)-C(152)-H(152)	120.5
C(140)-C(141)-C(142)	120.84(19)	C(154)-C(153)-C(152)	120.72(19)
C(140)-C(141)-H(141)	119.6	C(154)-C(153)-H(153)	119.6
C(142)-C(141)-H(141)	119.6	C(152)-C(153)-H(153)	119.6
C(141)-C(142)-C(143)	116.87(18)	C(155)-C(154)-C(153)	120.26(19)
C(141)-C(142)-H(142)	121.6	C(155)-C(154)-H(154)	119.9
C(143)-C(142)-H(142)	121.6	C(153)-C(154)-H(154)	119.9
C(144)-C(143)-C(142)	119.19(19)	C(154)-C(155)-C(156)	120.27(19)
C(144)-C(143)-H(143)	120.4	C(154)-C(155)-H(155)	119.9
C(142)-C(143)-H(143)	120.4	C(156)-C(155)-H(155)	119.9
C(143)-C(144)-C(139)	125.32(19)	C(151)-C(156)-C(155)	119.33(18)
C(143)-C(144)-H(144)	117.3	C(151)-C(156)-H(156)	120.3
C(139)-C(144)-H(144)	117.3	C(155)-C(156)-H(156)	120.3
C(146)-C(145)-C(150)	118.73(16)	N(13)-C(157)-C(158)	123.28(19)
C(146)-C(145)-S(15)	120.41(19)	N(13)-C(157)-H(157)	118.4
C(150)-C(145)-S(15)	120.83(19)	C(158)-C(157)-H(157)	118.4
C(147)-C(146)-C(145)	121.91(18)	C(159)-C(158)-C(157)	117.65(19)
C(147)-C(146)-H(146)	119.0	C(159)-C(158)-H(158)	121.2
C(145)-C(146)-H(146)	119.0	C(157)-C(158)-H(158)	121.2

C(160)-C(159)-C(158)	120.91(19)	N(15)-C(171)-C(170)	120.65(17)
C(160)-C(159)-H(159)	119.5	N(15)-C(171)-C(172)	116.73(15)
C(158)-C(159)-H(159)	119.5	C(170)-C(171)-C(172)	122.1(2)
C(159)-C(160)-C(161)	119.25(19)	N(16)-C(172)-C(173)	121.27(16)
C(159)-C(160)-H(160)	120.4	N(16)-C(172)-C(171)	117.10(14)
C(161)-C(160)-H(160)	120.4	C(173)-C(172)-C(171)	121.62(17)
N(13)-C(161)-C(160)	121.79(16)	C(174)-C(173)-C(172)	118.77(18)
N(13)-C(161)-C(162)	115.80(18)	C(174)-C(173)-H(173)	120.6
C(160)-C(161)-C(162)	122.20(18)	C(172)-C(173)-H(173)	120.6
N(14)-C(162)-C(163)	120.05(16)	C(175)-C(174)-C(173)	117.96(19)
N(14)-C(162)-C(161)	117.07(14)	C(175)-C(174)-H(174)	121.0
C(163)-C(162)-C(161)	122.88(17)	C(173)-C(174)-H(174)	121.0
C(164)-C(163)-C(162)	120.65(18)	C(174)-C(175)-C(176)	122.1(2)
C(164)-C(163)-H(163)	119.7	C(174)-C(175)-H(175)	119.0
C(162)-C(163)-H(163)	119.7	C(176)-C(175)-H(175)	119.0
C(165)-C(164)-C(163)	117.65(18)	N(16)-C(176)-C(175)	123.41(19)
C(165)-C(164)-H(164)	121.2	N(16)-C(176)-H(176)	118.3
C(163)-C(164)-H(164)	121.2	C(175)-C(176)-H(176)	118.3
C(166)-C(165)-C(164)	118.11(19)	N(4B)-Th(1B)-N(1B)	140.0
C(166)-C(165)-H(165)	120.9	N(4B)-Th(1B)-N(2B)	151.2
C(164)-C(165)-H(165)	120.9	N(1B)-Th(1B)-N(2B)	61.4
N(14)-C(166)-C(165)	125.99(19)	N(4B)-Th(1B)-N(3B)	61.4
N(14)-C(166)-H(166)	117.0	N(1B)-Th(1B)-N(3B)	151.5
C(165)-C(166)-H(166)	117.0	N(2B)-Th(1B)-N(3B)	108.8
N(15)-C(167)-C(168)	125.42(18)	N(4B)-Th(1B)-S(3B)	121.5
N(15)-C(167)-H(167)	117.3	N(1B)-Th(1B)-S(3B)	79.3
C(168)-C(167)-H(167)	117.3	N(2B)-Th(1B)-S(3B)	75.0
C(167)-C(168)-C(169)	115.24(18)	N(3B)-Th(1B)-S(3B)	72.2
C(167)-C(168)-H(168)	122.4	N(4B)-Th(1B)-S(4B)	80.4
C(169)-C(168)-H(168)	122.4	N(1B)-Th(1B)-S(4B)	120.9
C(170)-C(169)-C(168)	122.53(19)	N(2B)-Th(1B)-S(4B)	70.8
C(170)-C(169)-H(169)	118.7	N(3B)-Th(1B)-S(4B)	74.4
C(168)-C(169)-H(169)	118.7	S(3B)-Th(1B)-S(4B)	120.1
C(169)-C(170)-C(171)	118.34(18)	N(4B)-Th(1B)-S(1B)	86.9
C(169)-C(170)-H(170)	120.8	N(1B)-Th(1B)-S(1B)	64.3
C(171)-C(170)-H(170)	120.8	N(2B)-Th(1B)-S(1B)	90.6

N(3B)-Th(1B)-S(1B)	144.2	C(205)-C(204)-H(204)	119.4
S(3B)-Th(1B)-S(1B)	143.3	C(203)-C(204)-H(204)	119.4
S(4B)-Th(1B)-S(1B)	84.6	C(204)-C(205)-C(206)	120.9
N(4B)-Th(1B)-S(2B)	64.1	C(204)-C(205)-H(205)	119.6
N(1B)-Th(1B)-S(2B)	87.1	C(206)-C(205)-H(205)	119.6
N(2B)-Th(1B)-S(2B)	144.7	C(201)-C(206)-C(205)	120.0
N(3B)-Th(1B)-S(2B)	91.2	C(201)-C(206)-H(206)	120.0
S(3B)-Th(1B)-S(2B)	84.4	C(205)-C(206)-H(206)	120.0
S(4B)-Th(1B)-S(2B)	144.2	C(212)-C(207)-C(208)	119.0
S(1B)-Th(1B)-S(2B)	89.2	C(212)-C(207)-S(2B)	123.5
C(201)-S(1B)-Th(1B)	120.9	C(208)-C(207)-S(2B)	117.3
C(207)-S(2B)-Th(1B)	122.8	C(209)-C(208)-C(207)	118.5
C(213)-S(3B)-Th(1B)	115.3	C(209)-C(208)-H(208)	120.8
C(219)-S(4B)-Th(1B)	113.2	C(207)-C(208)-H(208)	120.8
C(229)-N(1B)-C(225)	117.7	C(210)-C(209)-C(208)	121.7
C(229)-N(1B)-Th(1B)	122.5	C(210)-C(209)-H(209)	119.1
C(225)-N(1B)-Th(1B)	119.4	C(208)-C(209)-H(209)	119.1
C(234)-N(2B)-C(230)	117.7	C(209)-C(210)-C(211)	120.0
C(234)-N(2B)-Th(1B)	119.1	C(209)-C(210)-H(210)	120.0
C(230)-N(2B)-Th(1B)	122.8	C(211)-C(210)-H(210)	120.0
C(235)-N(3B)-C(239)	120.3	C(212)-C(211)-C(210)	118.5
C(235)-N(3B)-Th(1B)	119.3	C(212)-C(211)-H(211)	120.7
C(239)-N(3B)-Th(1B)	120.0	C(210)-C(211)-H(211)	120.7
C(244)-N(4B)-C(240)	117.8	C(211)-C(212)-C(207)	122.2
C(244)-N(4B)-Th(1B)	119.4	C(211)-C(212)-H(212)	118.9
C(240)-N(4B)-Th(1B)	122.3	C(207)-C(212)-H(212)	118.9
C(202)-C(201)-C(206)	117.8	C(214)-C(213)-C(218)	117.6
C(202)-C(201)-S(1B)	118.7	C(214)-C(213)-S(3B)	122.6
C(206)-C(201)-S(1B)	123.0	C(218)-C(213)-S(3B)	119.8
C(203)-C(202)-C(201)	122.1	C(213)-C(214)-C(215)	121.2
C(203)-C(202)-H(202)	119.0	C(213)-C(214)-H(214)	119.4
C(201)-C(202)-H(202)	119.0	C(215)-C(214)-H(214)	119.4
C(202)-C(203)-C(204)	117.5	C(216)-C(215)-C(214)	120.6
C(202)-C(203)-H(203)	121.3	C(216)-C(215)-H(215)	119.7
C(204)-C(203)-H(203)	121.3	C(214)-C(215)-H(215)	119.7
C(205)-C(204)-C(203)	121.3	C(215)-C(216)-C(217)	119.5

C(215)-C(216)-H(216)	120.2	C(229)-C(228)-H(228)	122.1
C(217)-C(216)-H(216)	120.2	C(227)-C(228)-H(228)	122.1
C(216)-C(217)-C(218)	120.9	N(1B)-C(229)-C(228)	123.1
C(216)-C(217)-H(217)	119.5	N(1B)-C(229)-C(230)	118.3
C(218)-C(217)-H(217)	119.5	C(228)-C(229)-C(230)	118.4
C(217)-C(218)-C(213)	120.0	N(2B)-C(230)-C(231)	121.9
C(217)-C(218)-H(218)	120.0	N(2B)-C(230)-C(229)	114.3
C(213)-C(218)-H(218)	120.0	C(231)-C(230)-C(229)	123.5
C(220)-C(219)-C(224)	118.8	C(230)-C(231)-C(232)	118.8
C(220)-C(219)-S(4B)	119.0	C(230)-C(231)-H(231)	120.6
C(224)-C(219)-S(4B)	122.0	C(232)-C(231)-H(231)	120.6
C(219)-C(220)-C(221)	119.5	C(233)-C(232)-C(231)	120.4
C(219)-C(220)-H(220)	120.3	C(233)-C(232)-H(232)	119.8
C(221)-C(220)-H(220)	120.3	C(231)-C(232)-H(232)	119.8
C(222)-C(221)-C(220)	120.5	C(232)-C(233)-C(234)	118.3
C(222)-C(221)-H(221)	119.8	C(232)-C(233)-H(233)	120.9
C(220)-C(221)-H(221)	119.8	C(234)-C(233)-H(233)	120.9
C(221)-C(222)-C(223)	121.3	N(2B)-C(234)-C(233)	122.6
C(221)-C(222)-H(222)	119.4	N(2B)-C(234)-H(234)	118.7
C(223)-C(222)-H(222)	119.4	C(233)-C(234)-H(234)	118.7
C(224)-C(223)-C(222)	118.2	N(3B)-C(235)-C(236)	122.0
C(224)-C(223)-H(223)	120.9	N(3B)-C(235)-H(235)	119.0
C(222)-C(223)-H(223)	120.9	C(236)-C(235)-H(235)	119.0
C(223)-C(224)-C(219)	121.3	C(237)-C(236)-C(235)	119.1
C(223)-C(224)-H(224)	119.4	C(237)-C(236)-H(236)	120.5
C(219)-C(224)-H(224)	119.4	C(235)-C(236)-H(236)	120.5
C(226)-C(225)-N(1B)	123.0	C(236)-C(237)-C(238)	119.6
C(226)-C(225)-H(225)	118.5	C(236)-C(237)-H(237)	120.2
N(1B)-C(225)-H(225)	118.5	C(238)-C(237)-H(237)	120.2
C(225)-C(226)-C(227)	121.2	C(237)-C(238)-C(239)	120.2
C(225)-C(226)-H(226)	119.4	C(237)-C(238)-H(238)	119.9
C(227)-C(226)-H(226)	119.4	C(239)-C(238)-H(238)	119.9
C(226)-C(227)-C(228)	118.9	N(3B)-C(239)-C(238)	118.6
C(226)-C(227)-H(227)	120.6	N(3B)-C(239)-C(240)	117.7
C(228)-C(227)-H(227)	120.6	C(238)-C(239)-C(240)	123.7
C(229)-C(228)-C(227)	115.7	N(4B)-C(240)-C(241)	122.2

N(4B)-C(240)-C(239)	118.0	N(8B)-Th(2B)-S(6B)	63.7
C(241)-C(240)-C(239)	119.9	N(7B)-Th(2B)-S(6B)	91.0
C(242)-C(241)-C(240)	117.3	N(6B)-Th(2B)-S(6B)	143.9
C(242)-C(241)-H(241)	121.3	S(7B)-Th(2B)-S(6B)	84.4
C(240)-C(241)-H(241)	121.3	S(8B)-Th(2B)-S(6B)	143.9
C(241)-C(242)-C(243)	120.7	S(5B)-Th(2B)-S(6B)	89.4
C(241)-C(242)-H(242)	119.7	C(245)-S(5B)-Th(2B)	120.6
C(243)-C(242)-H(242)	119.7	C(251)-S(6B)-Th(2B)	120.9
C(244)-C(243)-C(242)	116.4	C(257)-S(7B)-Th(2B)	115.6
C(244)-C(243)-H(243)	121.8	C(263)-S(8B)-Th(2B)	111.4
C(242)-C(243)-H(243)	121.8	C(273)-N(5B)-C(269)	117.2
N(4B)-C(244)-C(243)	125.4	C(273)-N(5B)-Th(2B)	122.7
N(4B)-C(244)-H(244)	117.3	C(269)-N(5B)-Th(2B)	119.5
C(243)-C(244)-H(244)	117.3	C(274)-N(6B)-C(278)	118.1
N(5B)-Th(2B)-N(8B)	139.9	C(274)-N(6B)-Th(2B)	121.8
N(5B)-Th(2B)-N(7B)	151.7	C(278)-N(6B)-Th(2B)	119.6
N(8B)-Th(2B)-N(7B)	61.3	C(279)-N(7B)-C(283)	117.7
N(5B)-Th(2B)-N(6B)	60.9	C(279)-N(7B)-Th(2B)	119.1
N(8B)-Th(2B)-N(6B)	152.5	C(283)-N(7B)-Th(2B)	123.0
N(7B)-Th(2B)-N(6B)	108.4	C(288)-N(8B)-C(284)	118.1
N(5B)-Th(2B)-S(7B)	78.9	C(288)-N(8B)-Th(2B)	119.3
N(8B)-Th(2B)-S(7B)	121.8	C(284)-N(8B)-Th(2B)	121.9
N(7B)-Th(2B)-S(7B)	72.9	C(250)-C(245)-C(246)	117.1
N(6B)-Th(2B)-S(7B)	73.2	C(250)-C(245)-S(5B)	123.2
N(5B)-Th(2B)-S(8B)	121.1	C(246)-C(245)-S(5B)	119.1
N(8B)-Th(2B)-S(8B)	80.5	C(247)-C(246)-C(245)	119.4
N(7B)-Th(2B)-S(8B)	73.8	C(247)-C(246)-H(246)	120.3
N(6B)-Th(2B)-S(8B)	72.0	C(245)-C(246)-H(246)	120.3
S(7B)-Th(2B)-S(8B)	120.0	C(248)-C(247)-C(246)	121.6
N(5B)-Th(2B)-S(5B)	65.3	C(248)-C(247)-H(247)	119.2
N(8B)-Th(2B)-S(5B)	86.1	C(246)-C(247)-H(247)	119.2
N(7B)-Th(2B)-S(5B)	143.0	C(249)-C(248)-C(247)	119.3
N(6B)-Th(2B)-S(5B)	92.3	C(249)-C(248)-H(248)	120.4
S(7B)-Th(2B)-S(5B)	143.9	C(247)-C(248)-H(248)	120.4
S(8B)-Th(2B)-S(5B)	84.4	C(248)-C(249)-C(250)	122.0
N(5B)-Th(2B)-S(6B)	87.5	C(248)-C(249)-H(249)	119.0

C(250)-C(249)-H(249)	119.0	C(262)-C(261)-H(261)	120.5
C(249)-C(250)-C(245)	120.4	C(261)-C(262)-C(257)	121.7
C(249)-C(250)-H(250)	119.8	C(261)-C(262)-H(262)	119.1
C(245)-C(250)-H(250)	119.8	C(257)-C(262)-H(262)	119.1
C(256)-C(251)-C(252)	119.7	C(268)-C(263)-C(264)	118.7
C(256)-C(251)-S(6B)	122.3	C(268)-C(263)-S(8B)	122.6
C(252)-C(251)-S(6B)	117.8	C(264)-C(263)-S(8B)	118.6
C(253)-C(252)-C(251)	120.0	C(263)-C(264)-C(265)	120.6
C(253)-C(252)-H(252)	120.0	C(263)-C(264)-H(264)	119.7
C(251)-C(252)-H(252)	120.0	C(265)-C(264)-H(264)	119.7
C(254)-C(253)-C(252)	120.5	C(266)-C(265)-C(264)	119.6
C(254)-C(253)-H(253)	119.7	C(266)-C(265)-H(265)	120.2
C(252)-C(253)-H(253)	119.7	C(264)-C(265)-H(265)	120.2
C(253)-C(254)-C(255)	121.0	C(265)-C(266)-C(267)	118.4
C(253)-C(254)-H(254)	119.5	C(265)-C(266)-H(266)	120.8
C(255)-C(254)-H(254)	119.5	C(267)-C(266)-H(266)	120.8
C(254)-C(255)-C(256)	118.8	C(268)-C(267)-C(266)	122.5
C(254)-C(255)-H(255)	120.6	C(268)-C(267)-H(267)	118.8
C(256)-C(255)-H(255)	120.6	C(266)-C(267)-H(267)	118.8
C(251)-C(256)-C(255)	119.8	C(267)-C(268)-C(263)	119.9
C(251)-C(256)-H(256)	120.1	C(267)-C(268)-H(268)	120.0
C(255)-C(256)-H(256)	120.1	C(263)-C(268)-H(268)	120.0
C(262)-C(257)-C(258)	118.1	C(270)-C(269)-N(5B)	123.9
C(262)-C(257)-S(7B)	122.2	C(270)-C(269)-H(269)	118.0
C(258)-C(257)-S(7B)	119.4	N(5B)-C(269)-H(269)	118.0
C(259)-C(258)-C(257)	119.1	C(269)-C(270)-C(271)	118.9
C(259)-C(258)-H(258)	120.5	C(269)-C(270)-H(270)	120.5
C(257)-C(258)-H(258)	120.5	C(271)-C(270)-H(270)	120.5
C(260)-C(259)-C(258)	121.0	C(272)-C(271)-C(270)	118.8
C(260)-C(259)-H(259)	119.5	C(272)-C(271)-H(271)	120.6
C(258)-C(259)-H(259)	119.5	C(270)-C(271)-H(271)	120.6
C(259)-C(260)-C(261)	121.0	C(271)-C(272)-C(273)	121.0
C(259)-C(260)-H(260)	119.5	C(271)-C(272)-H(272)	119.5
C(261)-C(260)-H(260)	119.5	C(273)-C(272)-H(272)	119.5
C(260)-C(261)-C(262)	119.0	N(5B)-C(273)-C(272)	120.0
C(260)-C(261)-H(261)	120.5	N(5B)-C(273)-C(274)	115.8

C(272)-C(273)-C(274)	124.1	C(284)-C(285)-H(285)	120.6
N(6B)-C(274)-C(275)	121.4	C(285)-C(286)-C(287)	120.3
N(6B)-C(274)-C(273)	118.0	C(285)-C(286)-H(286)	119.8
C(275)-C(274)-C(273)	120.6	C(287)-C(286)-H(286)	119.8
C(274)-C(275)-C(276)	120.4	C(288)-C(287)-C(286)	115.9
C(274)-C(275)-H(275)	119.8	C(288)-C(287)-H(287)	122.1
C(276)-C(275)-H(275)	119.8	C(286)-C(287)-H(287)	122.1
C(275)-C(276)-C(277)	119.3	N(8B)-C(288)-C(287)	124.7
C(275)-C(276)-H(276)	120.3	N(8B)-C(288)-H(288)	117.6
C(277)-C(276)-H(276)	120.3	C(287)-C(288)-H(288)	117.6
C(278)-C(277)-C(276)	116.4	N(10B)-Th(3B)-N(12B)	150.6
C(278)-C(277)-H(277)	121.8	N(10B)-Th(3B)-N(9B)	61.3
C(276)-C(277)-H(277)	121.8	N(12B)-Th(3B)-N(9B)	141.6
C(277)-C(278)-N(6B)	124.1	N(10B)-Th(3B)-N(11B)	106.3
C(277)-C(278)-H(278)	118.0	N(12B)-Th(3B)-N(11B)	61.0
N(6B)-C(278)-H(278)	118.0	N(9B)-Th(3B)-N(11B)	152.1
N(7B)-C(279)-C(280)	123.5	N(10B)-Th(3B)-S(12B)	72.1
N(7B)-C(279)-H(279)	118.3	N(12B)-Th(3B)-S(12B)	78.6
C(280)-C(279)-H(279)	118.3	N(9B)-Th(3B)-S(12B)	120.8
C(279)-C(280)-C(281)	119.3	N(11B)-Th(3B)-S(12B)	72.5
C(279)-C(280)-H(280)	120.4	N(10B)-Th(3B)-S(11B)	73.1
C(281)-C(280)-H(280)	120.4	N(12B)-Th(3B)-S(11B)	121.4
C(282)-C(281)-C(280)	116.4	N(9B)-Th(3B)-S(11B)	79.6
C(282)-C(281)-H(281)	121.8	N(11B)-Th(3B)-S(11B)	72.7
C(280)-C(281)-H(281)	121.8	S(12B)-Th(3B)-S(11B)	120.1
C(283)-C(282)-C(281)	122.9	N(10B)-Th(3B)-S(10B)	145.1
C(283)-C(282)-H(282)	118.5	N(12B)-Th(3B)-S(10B)	64.3
C(281)-C(282)-H(282)	118.5	N(9B)-Th(3B)-S(10B)	88.8
C(282)-C(283)-N(7B)	120.0	N(11B)-Th(3B)-S(10B)	91.9
C(282)-C(283)-C(284)	124.6	S(12B)-Th(3B)-S(10B)	142.7
N(7B)-C(283)-C(284)	115.4	S(11B)-Th(3B)-S(10B)	84.9
N(8B)-C(284)-C(285)	121.9	N(10B)-Th(3B)-S(9B)	92.3
N(8B)-C(284)-C(283)	117.3	N(12B)-Th(3B)-S(9B)	87.8
C(285)-C(284)-C(283)	120.8	N(9B)-Th(3B)-S(9B)	63.8
C(286)-C(285)-C(284)	118.9	N(11B)-Th(3B)-S(9B)	144.1
C(286)-C(285)-H(285)	120.6	S(12B)-Th(3B)-S(9B)	85.0

S(11B)-Th(3B)-S(9B)	143.1	C(296)-C(295)-C(300)	118.4
S(10B)-Th(3B)-S(9B)	89.5	C(296)-C(295)-S(10B)	120.8
C(289)-S(9B)-Th(3B)	121.8	C(300)-C(295)-S(10B)	120.7
C(295)-S(10B)-Th(3B)	121.0	C(295)-C(296)-C(297)	124.1
C(301)-S(11B)-Th(3B)	114.8	C(295)-C(296)-H(296)	118.0
C(307)-S(12B)-Th(3B)	113.0	C(297)-C(296)-H(296)	118.0
C(313)-N(9B)-C(317)	117.7	C(298)-C(297)-C(296)	119.0
C(313)-N(9B)-Th(3B)	118.0	C(298)-C(297)-H(297)	120.5
C(317)-N(9B)-Th(3B)	123.6	C(296)-C(297)-H(297)	120.5
C(322)-N(10B)-C(318)	115.8	C(299)-C(298)-C(297)	119.6
C(322)-N(10B)-Th(3B)	122.0	C(299)-C(298)-H(298)	120.2
C(318)-N(10B)-Th(3B)	122.2	C(297)-C(298)-H(298)	120.2
C(323)-N(11B)-C(327)	115.6	C(298)-C(299)-C(300)	122.9
C(323)-N(11B)-Th(3B)	121.6	C(298)-C(299)-H(299)	118.5
C(327)-N(11B)-Th(3B)	122.8	C(300)-C(299)-H(299)	118.5
C(332)-N(12B)-C(328)	116.8	C(299)-C(300)-C(295)	115.9
C(332)-N(12B)-Th(3B)	119.1	C(299)-C(300)-H(300)	122.1
C(328)-N(12B)-Th(3B)	123.5	C(295)-C(300)-H(300)	122.1
C(294)-C(289)-C(290)	117.5	C(302)-C(301)-C(306)	118.7
C(294)-C(289)-S(9B)	123.1	C(302)-C(301)-S(11B)	119.9
C(290)-C(289)-S(9B)	119.1	C(306)-C(301)-S(11B)	121.4
C(291)-C(290)-C(289)	122.3	C(301)-C(302)-C(303)	122.2
C(291)-C(290)-H(290)	118.9	C(301)-C(302)-H(302)	118.9
C(289)-C(290)-H(290)	118.9	C(303)-C(302)-H(302)	118.9
C(290)-C(291)-C(292)	119.3	C(304)-C(303)-C(302)	120.3
C(290)-C(291)-H(291)	120.4	C(304)-C(303)-H(303)	119.9
C(292)-C(291)-H(291)	120.4	C(302)-C(303)-H(303)	119.9
C(291)-C(292)-C(293)	120.3	C(303)-C(304)-C(305)	118.2
C(291)-C(292)-H(292)	119.8	C(303)-C(304)-H(304)	120.9
C(293)-C(292)-H(292)	119.8	C(305)-C(304)-H(304)	120.9
C(294)-C(293)-C(292)	119.6	C(306)-C(305)-C(304)	120.9
C(294)-C(293)-H(293)	120.2	C(306)-C(305)-H(305)	119.5
C(292)-C(293)-H(293)	120.2	C(304)-C(305)-H(305)	119.5
C(293)-C(294)-C(289)	120.7	C(305)-C(306)-C(301)	119.5
C(293)-C(294)-H(294)	119.7	C(305)-C(306)-H(306)	120.2
C(289)-C(294)-H(294)	119.7	C(301)-C(306)-H(306)	120.2

C(312)-C(307)-C(308)	117.5	C(318)-C(319)-C(320)	120.1
C(312)-C(307)-S(12B)	120.5	C(318)-C(319)-H(319)	120.0
C(308)-C(307)-S(12B)	122.0	C(320)-C(319)-H(319)	120.0
C(309)-C(308)-C(307)	119.7	C(321)-C(320)-C(319)	117.2
C(309)-C(308)-H(308)	120.2	C(321)-C(320)-H(320)	121.4
C(307)-C(308)-H(308)	120.2	C(319)-C(320)-H(320)	121.4
C(310)-C(309)-C(308)	122.1	C(320)-C(321)-C(322)	119.1
C(310)-C(309)-H(309)	118.9	C(320)-C(321)-H(321)	120.4
C(308)-C(309)-H(309)	118.9	C(322)-C(321)-H(321)	120.4
C(309)-C(310)-C(311)	118.9	N(10B)-C(322)-C(321)	126.0
C(309)-C(310)-H(310)	120.6	N(10B)-C(322)-H(322)	117.0
C(311)-C(310)-H(310)	120.6	C(321)-C(322)-H(322)	117.0
C(310)-C(311)-C(312)	120.1	N(11B)-C(323)-C(324)	126.5
C(310)-C(311)-H(311)	119.9	N(11B)-C(323)-H(323)	116.8
C(312)-C(311)-H(311)	119.9	C(324)-C(323)-H(323)	116.8
C(307)-C(312)-C(311)	121.5	C(323)-C(324)-C(325)	116.6
C(307)-C(312)-H(312)	119.3	C(323)-C(324)-H(324)	121.7
C(311)-C(312)-H(312)	119.3	C(325)-C(324)-H(324)	121.7
N(9B)-C(313)-C(314)	122.2	C(326)-C(325)-C(324)	120.7
N(9B)-C(313)-H(313)	118.9	C(326)-C(325)-H(325)	119.6
C(314)-C(313)-H(313)	118.9	C(324)-C(325)-H(325)	119.6
C(315)-C(314)-C(313)	119.7	C(325)-C(326)-C(327)	117.9
C(315)-C(314)-H(314)	120.1	C(325)-C(326)-H(326)	121.0
C(313)-C(314)-H(314)	120.1	C(327)-C(326)-H(326)	121.0
C(314)-C(315)-C(316)	117.3	N(11B)-C(327)-C(326)	122.6
C(314)-C(315)-H(315)	121.4	N(11B)-C(327)-C(328)	117.6
C(316)-C(315)-H(315)	121.4	C(326)-C(327)-C(328)	119.6
C(317)-C(316)-C(315)	120.8	C(329)-C(328)-N(12B)	120.3
C(317)-C(316)-H(316)	119.6	C(329)-C(328)-C(327)	125.4
C(315)-C(316)-H(316)	119.6	N(12B)-C(328)-C(327)	114.2
C(316)-C(317)-N(9B)	122.2	C(330)-C(329)-C(328)	123.5
C(316)-C(317)-C(318)	123.3	C(330)-C(329)-H(329)	118.3
N(9B)-C(317)-C(318)	114.2	C(328)-C(329)-H(329)	118.3
N(10B)-C(318)-C(319)	121.7	C(329)-C(330)-C(331)	115.5
N(10B)-C(318)-C(317)	117.5	C(329)-C(330)-H(330)	122.2
C(319)-C(318)-C(317)	120.8	C(331)-C(330)-H(330)	122.2

C(332)-C(331)-C(330)	119.8	C(345)-S(15B)-Th(4B)	112.3
C(332)-C(331)-H(331)	120.1	C(351)-S(16B)-Th(4B)	113.0
C(330)-C(331)-H(331)	120.1	C(357)-N(13B)-C(361)	117.1
N(12B)-C(332)-C(331)	123.7	C(357)-N(13B)-Th(4B)	120.2
N(12B)-C(332)-H(332)	118.2	C(361)-N(13B)-Th(4B)	122.5
C(331)-C(332)-H(332)	118.2	C(366)-N(14B)-C(362)	117.3
N(13B)-Th(4B)-N(16B)	139.4	C(366)-N(14B)-Th(4B)	120.5
N(13B)-Th(4B)-N(15B)	152.3	C(362)-N(14B)-Th(4B)	121.9
N(16B)-Th(4B)-N(15B)	61.7	C(367)-N(15B)-C(371)	117.7
N(13B)-Th(4B)-N(14B)	61.7	C(367)-N(15B)-Th(4B)	120.9
N(16B)-Th(4B)-N(14B)	151.6	C(371)-N(15B)-Th(4B)	121.3
N(15B)-Th(4B)-N(14B)	108.0	C(372)-N(16B)-C(376)	116.4
N(13B)-Th(4B)-S(15B)	79.6	C(372)-N(16B)-Th(4B)	122.5
N(16B)-Th(4B)-S(15B)	122.5	C(376)-N(16B)-Th(4B)	120.9
N(15B)-Th(4B)-S(15B)	72.7	C(338)-C(333)-C(334)	118.5
N(14B)-Th(4B)-S(15B)	73.0	C(338)-C(333)-S(13B)	124.8
N(13B)-Th(4B)-S(16B)	121.6	C(334)-C(333)-S(13B)	116.6
N(16B)-Th(4B)-S(16B)	79.0	C(335)-C(334)-C(333)	120.0
N(15B)-Th(4B)-S(16B)	73.6	C(335)-C(334)-H(334)	120.0
N(14B)-Th(4B)-S(16B)	72.7	C(333)-C(334)-H(334)	120.0
S(15B)-Th(4B)-S(16B)	120.4	C(334)-C(335)-C(336)	119.9
N(13B)-Th(4B)-S(13B)	63.0	C(334)-C(335)-H(335)	120.1
N(16B)-Th(4B)-S(13B)	87.5	C(336)-C(335)-H(335)	120.1
N(15B)-Th(4B)-S(13B)	144.7	C(337)-C(336)-C(335)	118.1
N(14B)-Th(4B)-S(13B)	90.8	C(337)-C(336)-H(336)	120.9
S(15B)-Th(4B)-S(13B)	142.5	C(335)-C(336)-H(336)	120.9
S(16B)-Th(4B)-S(13B)	84.5	C(336)-C(337)-C(338)	122.0
N(13B)-Th(4B)-S(14B)	87.2	C(336)-C(337)-H(337)	119.0
N(16B)-Th(4B)-S(14B)	64.7	C(338)-C(337)-H(337)	119.0
N(15B)-Th(4B)-S(14B)	90.8	C(333)-C(338)-C(337)	121.4
N(14B)-Th(4B)-S(14B)	143.6	C(333)-C(338)-H(338)	119.3
S(15B)-Th(4B)-S(14B)	83.9	C(337)-C(338)-H(338)	119.3
S(16B)-Th(4B)-S(14B)	143.6	C(344)-C(339)-C(340)	114.6
S(13B)-Th(4B)-S(14B)	90.9	C(344)-C(339)-S(14B)	125.5
C(333)-S(13B)-Th(4B)	122.7	C(340)-C(339)-S(14B)	119.4
C(339)-S(14B)-Th(4B)	119.8	C(341)-C(340)-C(339)	123.1

C(341)-C(340)-H(340)	118.5	C(353)-C(352)-H(352)	120.5
C(339)-C(340)-H(340)	118.5	C(351)-C(352)-H(352)	120.5
C(340)-C(341)-C(342)	120.8	C(354)-C(353)-C(352)	120.7
C(340)-C(341)-H(341)	119.6	C(354)-C(353)-H(353)	119.6
C(342)-C(341)-H(341)	119.6	C(352)-C(353)-H(353)	119.7
C(341)-C(342)-C(343)	116.9	C(355)-C(354)-C(353)	120.2
C(341)-C(342)-H(342)	121.6	C(355)-C(354)-H(354)	119.9
C(343)-C(342)-H(342)	121.6	C(353)-C(354)-H(354)	119.9
C(344)-C(343)-C(342)	119.2	C(354)-C(355)-C(356)	120.3
C(344)-C(343)-H(343)	120.4	C(354)-C(355)-H(355)	119.9
C(342)-C(343)-H(343)	120.4	C(356)-C(355)-H(355)	119.9
C(343)-C(344)-C(339)	125.3	C(351)-C(356)-C(355)	119.3
C(343)-C(344)-H(344)	117.3	C(351)-C(356)-H(356)	120.3
C(339)-C(344)-H(344)	117.3	C(355)-C(356)-H(356)	120.3
C(346)-C(345)-C(350)	118.7	N(13B)-C(357)-C(358)	123.3
C(346)-C(345)-S(15B)	120.4	N(13B)-C(357)-H(357)	118.4
C(350)-C(345)-S(15B)	120.8	C(358)-C(357)-H(357)	118.4
C(347)-C(346)-C(345)	121.9	C(359)-C(358)-C(357)	117.6
C(347)-C(346)-H(346)	119.1	C(359)-C(358)-H(358)	121.2
C(345)-C(346)-H(346)	119.1	C(357)-C(358)-H(358)	121.2
C(348)-C(347)-C(346)	117.1	C(360)-C(359)-C(358)	120.9
C(348)-C(347)-H(347)	121.4	C(360)-C(359)-H(359)	119.6
C(346)-C(347)-H(347)	121.4	C(358)-C(359)-H(359)	119.6
C(349)-C(348)-C(347)	121.9	C(359)-C(360)-C(361)	119.2
C(349)-C(348)-H(348)	119.1	C(359)-C(360)-H(360)	120.4
C(347)-C(348)-H(348)	119.1	C(361)-C(360)-H(360)	120.4
C(348)-C(349)-C(350)	122.8	N(13B)-C(361)-C(360)	121.7
C(348)-C(349)-H(349)	118.6	N(13B)-C(361)-C(362)	115.8
C(350)-C(349)-H(349)	118.6	C(360)-C(361)-C(362)	122.1
C(345)-C(350)-C(349)	117.4	N(14B)-C(362)-C(363)	120.1
C(345)-C(350)-H(350)	121.3	N(14B)-C(362)-C(361)	117.1
C(349)-C(350)-H(350)	121.3	C(363)-C(362)-C(361)	122.9
C(356)-C(351)-C(352)	120.2	C(364)-C(363)-C(362)	120.6
C(356)-C(351)-S(16B)	121.1	C(364)-C(363)-H(363)	119.7
C(352)-C(351)-S(16B)	118.6	C(362)-C(363)-H(363)	119.7
C(353)-C(352)-C(351)	119.1	C(365)-C(364)-C(363)	117.6

C(365)-C(364)-H(364)	121.2	C(371)-C(370)-H(370)	120.8
C(363)-C(364)-H(364)	121.2	N(15B)-C(371)-C(370)	120.6
C(366)-C(365)-C(364)	118.1	N(15B)-C(371)-C(372)	116.7
C(366)-C(365)-H(365)	121.0	C(370)-C(371)-C(372)	122.1
C(364)-C(365)-H(365)	121.0	N(16B)-C(372)-C(373)	121.2
N(14B)-C(366)-C(365)	126.0	N(16B)-C(372)-C(371)	117.1
N(14B)-C(366)-H(366)	117.0	C(373)-C(372)-C(371)	121.6
C(365)-C(366)-H(366)	117.0	C(374)-C(373)-C(372)	118.7
N(15B)-C(367)-C(368)	125.4	C(374)-C(373)-H(373)	120.6
N(15B)-C(367)-H(367)	117.3	C(372)-C(373)-H(373)	120.6
C(368)-C(367)-H(367)	117.3	C(375)-C(374)-C(373)	117.9
C(367)-C(368)-C(369)	115.2	C(375)-C(374)-H(374)	121.0
C(367)-C(368)-H(368)	122.4	C(373)-C(374)-H(374)	121.0
C(369)-C(368)-H(368)	122.4	C(374)-C(375)-C(376)	122.0
C(370)-C(369)-C(368)	122.5	C(374)-C(375)-H(375)	119.0
C(370)-C(369)-H(369)	118.7	C(376)-C(375)-H(375)	119.0
C(368)-C(369)-H(369)	118.7	N(16B)-C(376)-C(375)	123.4
C(369)-C(370)-C(371)	118.3	N(16B)-C(376)-H(376)	118.3
C(369)-C(370)-H(370)	120.8	C(375)-C(376)-H(376)	118.3

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	12(1)	12(1)	18(1)	-2(1)	3(1)	0(1)
S(1)	16(3)	17(3)	23(3)	0(2)	2(3)	3(2)
S(2)	21(3)	15(3)	22(3)	-1(2)	0(2)	-1(2)
S(3)	23(4)	16(3)	23(3)	-1(3)	-1(3)	3(3)
S(4)	21(3)	19(3)	25(3)	2(3)	8(3)	4(3)
N(1)	16(7)	15(6)	15(6)	-5(5)	-5(5)	4(5)
N(2)	19(7)	15(6)	17(6)	-5(6)	1(5)	-2(6)
N(3)	17(6)	13(6)	13(6)	0(5)	-4(6)	3(6)
N(4)	13(6)	22(7)	19(7)	0(6)	4(6)	-3(5)
C(1)	20(8)	17(7)	21(7)	1(6)	0(6)	6(6)
C(2)	30(8)	22(7)	31(7)	1(7)	-4(7)	0(7)
C(3)	33(8)	28(7)	33(7)	-6(7)	-3(7)	4(7)
C(4)	34(8)	30(8)	24(7)	-6(6)	-1(7)	11(7)
C(5)	25(8)	26(7)	23(7)	3(6)	3(7)	9(7)
C(6)	19(8)	21(7)	23(7)	2(6)	0(6)	6(6)
C(7)	15(7)	20(7)	24(7)	3(6)	4(6)	3(6)
C(8)	19(7)	16(7)	23(7)	5(6)	2(6)	0(6)
C(9)	19(7)	15(7)	27(7)	3(6)	10(6)	1(6)
C(10)	26(8)	23(8)	27(7)	0(7)	5(6)	3(7)
C(11)	21(7)	24(8)	27(7)	-4(7)	1(6)	1(7)
C(12)	21(7)	22(8)	26(7)	0(7)	4(6)	4(6)
C(13)	25(8)	24(7)	21(7)	0(6)	-5(6)	5(7)
C(14)	33(8)	27(7)	31(8)	-1(7)	3(7)	3(7)
C(15)	32(8)	25(7)	34(8)	-8(6)	-2(7)	3(7)
C(16)	32(8)	33(7)	29(7)	-9(7)	2(7)	9(7)
C(17)	27(8)	32(7)	29(7)	1(7)	-4(6)	7(7)
C(18)	25(8)	26(7)	27(7)	-2(6)	-1(6)	2(7)
C(19)	25(7)	19(7)	20(7)	5(6)	2(6)	0(7)
C(20)	23(7)	22(7)	26(7)	3(6)	4(6)	2(6)
C(21)	27(7)	28(8)	33(8)	-3(7)	4(6)	4(7)
C(22)	25(8)	30(8)	28(8)	-1(6)	4(7)	6(7)
C(23)	28(7)	26(8)	28(8)	-3(6)	6(7)	4(7)

C(24)	23(7)	22(7)	20(7)	0(6)	3(6)	2(6)
C(25)	21(7)	20(7)	26(7)	0(6)	-1(6)	-1(6)
C(26)	23(7)	26(7)	28(8)	3(7)	-4(6)	-1(7)
C(27)	18(7)	29(7)	23(7)	-2(7)	7(6)	3(6)
C(28)	21(7)	22(7)	25(8)	-4(6)	2(6)	4(6)
C(29)	19(6)	14(6)	18(7)	-3(6)	0(5)	4(5)
C(30)	17(6)	16(6)	19(7)	-5(6)	-2(5)	2(6)
C(31)	23(7)	14(6)	21(7)	-7(6)	-1(6)	3(6)
C(32)	30(8)	16(7)	28(8)	-3(7)	-1(6)	2(6)
C(33)	25(7)	20(7)	24(7)	-2(7)	0(6)	-4(6)
C(34)	20(7)	16(7)	21(7)	-4(6)	-1(6)	-3(6)
C(35)	17(7)	20(7)	13(7)	1(6)	-1(6)	3(6)
C(36)	20(7)	23(7)	17(7)	4(6)	0(6)	-4(6)
C(37)	19(7)	23(7)	20(7)	7(6)	4(6)	-3(6)
C(38)	21(6)	16(7)	20(7)	2(6)	-2(6)	5(6)
C(39)	18(6)	10(6)	21(7)	4(5)	-4(6)	3(6)
C(40)	19(6)	17(6)	18(7)	-3(5)	0(6)	-2(6)
C(41)	24(7)	14(7)	23(7)	2(6)	10(6)	-3(6)
C(42)	27(7)	13(7)	22(7)	0(6)	2(7)	-2(6)
C(43)	27(7)	17(7)	26(8)	2(6)	-1(7)	-1(7)
C(44)	20(7)	18(7)	23(7)	-2(6)	-7(6)	0(6)
Th(2)	14(1)	13(1)	18(1)	-1(1)	2(1)	1(1)
S(5)	15(3)	20(3)	22(3)	2(2)	2(2)	2(2)
S(6)	18(3)	17(3)	19(3)	-1(2)	2(2)	1(2)
S(7)	24(4)	19(3)	24(3)	-2(3)	-1(3)	-2(3)
S(8)	20(3)	21(3)	25(3)	4(3)	3(3)	1(3)
N(5)	12(6)	18(6)	16(6)	2(6)	-3(5)	-1(5)
N(6)	17(7)	23(7)	18(7)	4(6)	-1(5)	-1(6)
N(7)	23(7)	14(7)	20(7)	-4(6)	-3(6)	2(6)
N(8)	19(6)	14(6)	16(6)	1(5)	-1(6)	-1(5)
C(45)	16(7)	25(7)	18(7)	-4(6)	-3(6)	4(6)
C(46)	19(8)	22(7)	21(7)	-5(6)	-2(6)	4(6)
C(47)	29(8)	31(7)	22(7)	-2(6)	-4(7)	2(7)
C(48)	25(8)	34(8)	16(7)	-1(6)	-4(7)	7(7)
C(49)	22(8)	31(7)	25(7)	6(6)	-2(7)	8(7)
C(50)	17(7)	25(7)	24(7)	2(6)	-4(6)	2(6)

C(51)	19(7)	14(7)	26(7)	-1(6)	2(6)	3(6)
C(52)	17(7)	19(7)	25(7)	7(6)	1(6)	3(6)
C(53)	29(8)	32(8)	29(7)	6(7)	7(6)	1(7)
C(54)	35(8)	30(8)	24(7)	3(7)	3(6)	3(7)
C(55)	34(8)	28(8)	31(7)	-2(7)	-6(7)	-4(7)
C(56)	26(7)	15(7)	30(7)	0(7)	1(6)	2(6)
C(57)	20(8)	25(7)	17(7)	-4(6)	-4(6)	3(7)
C(58)	20(7)	18(7)	23(7)	0(6)	-1(6)	3(6)
C(59)	20(8)	20(7)	24(7)	0(6)	1(6)	7(6)
C(60)	22(8)	30(7)	22(7)	-1(6)	2(6)	3(7)
C(61)	23(8)	35(7)	25(7)	2(7)	2(6)	-1(7)
C(62)	27(8)	29(7)	24(7)	1(6)	-5(6)	-4(7)
C(63)	24(7)	21(7)	13(7)	2(6)	1(6)	5(7)
C(64)	22(7)	22(7)	11(7)	1(6)	-3(6)	4(6)
C(65)	21(7)	25(8)	22(7)	-3(6)	6(6)	5(6)
C(66)	26(7)	24(8)	21(7)	-4(6)	8(6)	5(7)
C(67)	27(7)	24(8)	19(7)	-2(6)	4(6)	1(7)
C(68)	23(7)	26(7)	18(7)	0(6)	4(6)	-1(6)
C(69)	23(7)	18(6)	21(7)	1(6)	4(6)	-3(6)
C(70)	21(7)	24(7)	23(7)	5(7)	5(6)	3(6)
C(71)	19(7)	27(7)	22(7)	7(7)	7(6)	7(6)
C(72)	20(7)	24(7)	25(8)	2(6)	4(6)	3(6)
C(73)	14(6)	21(6)	22(7)	2(6)	-1(5)	-4(6)
C(74)	18(7)	23(6)	21(7)	3(6)	1(6)	-2(6)
C(75)	24(7)	22(6)	24(7)	3(6)	-1(6)	2(6)
C(76)	25(7)	24(7)	24(7)	2(6)	-2(6)	-1(6)
C(77)	18(7)	26(7)	26(8)	1(7)	-5(6)	-1(6)
C(78)	18(7)	27(7)	27(7)	5(7)	-3(6)	-2(6)
C(79)	26(7)	19(7)	17(7)	-2(6)	0(6)	4(6)
C(80)	25(7)	24(7)	19(7)	-1(6)	4(7)	-1(7)
C(81)	22(7)	23(7)	21(7)	4(6)	4(6)	-1(6)
C(82)	21(7)	19(7)	18(7)	1(6)	2(6)	2(6)
C(83)	21(6)	15(6)	18(7)	1(5)	0(6)	2(6)
C(84)	20(6)	19(6)	21(7)	-1(6)	2(6)	0(6)
C(85)	21(7)	21(7)	25(7)	-2(6)	1(6)	5(6)
C(86)	30(7)	18(7)	24(8)	-2(6)	-2(7)	5(6)

C(87)	24(7)	17(7)	19(7)	-2(6)	-1(7)	1(6)
C(88)	23(7)	19(7)	20(7)	-2(6)	-3(6)	-1(6)
Th(3)	14(1)	12(1)	17(1)	-2(1)	2(1)	1(1)
S(9)	18(3)	23(3)	16(3)	-3(2)	1(2)	-2(3)
S(10)	21(3)	16(3)	20(3)	3(2)	1(2)	2(2)
S(11)	19(3)	27(3)	16(3)	-5(3)	-1(2)	1(3)
S(12)	23(3)	16(3)	17(3)	-4(2)	1(2)	0(3)
N(9)	19(7)	19(6)	18(7)	-3(6)	3(6)	-1(6)
N(10)	14(6)	17(6)	16(6)	-2(6)	1(5)	2(5)
N(11)	26(7)	19(7)	22(7)	-6(6)	11(6)	-4(6)
N(12)	19(6)	16(6)	19(7)	-3(6)	3(6)	0(5)
C(89)	16(8)	20(7)	23(7)	0(6)	-1(6)	4(6)
C(90)	23(8)	21(7)	29(7)	0(7)	-2(7)	2(6)
C(91)	32(8)	31(8)	34(7)	-3(7)	-8(7)	2(7)
C(92)	30(8)	35(8)	28(7)	-7(7)	-2(7)	2(7)
C(93)	23(8)	34(8)	26(7)	6(7)	3(7)	3(7)
C(94)	21(8)	29(7)	29(7)	3(6)	2(7)	2(7)
C(95)	18(7)	19(7)	19(7)	-2(6)	0(6)	-3(6)
C(96)	24(7)	28(8)	27(7)	1(7)	3(6)	-5(7)
C(97)	24(8)	31(8)	27(7)	-1(7)	7(6)	-4(7)
C(98)	27(8)	26(8)	27(7)	-1(7)	9(6)	-2(7)
C(99)	25(8)	24(8)	23(7)	-1(7)	0(6)	2(7)
C(100)	21(7)	24(8)	22(7)	0(6)	1(6)	-2(6)
C(101)	21(7)	22(7)	13(7)	0(6)	-6(6)	1(7)
C(102)	28(8)	25(7)	22(7)	2(6)	1(6)	-3(7)
C(103)	29(8)	28(7)	26(8)	-5(6)	1(7)	-3(7)
C(104)	30(8)	35(7)	21(7)	-5(7)	2(6)	4(7)
C(105)	25(8)	32(8)	22(7)	1(7)	1(6)	1(7)
C(106)	21(7)	26(7)	21(7)	-1(6)	-2(6)	-3(6)
C(107)	27(7)	21(7)	23(7)	4(6)	0(6)	5(7)
C(108)	23(7)	25(7)	27(7)	2(6)	-2(7)	1(7)
C(109)	24(7)	25(8)	38(8)	3(7)	7(6)	4(7)
C(110)	35(8)	22(8)	31(8)	-1(7)	2(7)	8(7)
C(111)	32(7)	23(7)	21(7)	3(6)	-6(6)	6(7)
C(112)	26(7)	21(7)	18(7)	4(6)	0(6)	2(6)
C(113)	16(7)	23(7)	25(7)	-6(6)	5(6)	0(6)

C(114)	15(7)	26(7)	18(7)	2(7)	2(6)	2(6)
C(115)	21(7)	29(7)	23(7)	-2(7)	5(6)	1(6)
C(116)	24(7)	24(7)	22(7)	0(6)	3(6)	4(6)
C(117)	18(6)	20(6)	15(7)	-4(6)	-2(5)	1(6)
C(118)	12(6)	18(6)	17(6)	-2(6)	-3(5)	3(6)
C(119)	20(7)	16(6)	26(7)	-5(6)	0(6)	1(6)
C(120)	24(7)	18(7)	26(7)	-6(7)	2(6)	-2(6)
C(121)	23(7)	20(7)	22(7)	-3(7)	3(6)	-1(6)
C(122)	17(7)	19(7)	16(7)	-2(6)	0(6)	2(6)
C(123)	23(7)	19(7)	24(7)	4(6)	2(6)	-2(6)
C(124)	26(7)	18(7)	26(8)	7(6)	3(7)	-6(7)
C(125)	25(7)	22(7)	31(8)	6(6)	5(7)	-1(6)
C(126)	24(7)	22(7)	30(8)	0(6)	7(7)	3(6)
C(127)	21(6)	18(6)	21(7)	-2(6)	9(6)	0(6)
C(128)	22(6)	16(6)	18(7)	0(5)	4(6)	3(6)
C(129)	20(7)	16(7)	21(7)	2(6)	1(6)	4(6)
C(130)	28(7)	23(7)	24(8)	-6(6)	1(7)	4(6)
C(131)	24(7)	25(7)	17(7)	-7(6)	1(7)	-3(7)
C(132)	19(7)	18(7)	16(7)	1(6)	5(6)	-1(6)
Th(4)	12(1)	12(1)	19(1)	-1(1)	2(1)	1(1)
S(13)	13(3)	18(3)	22(3)	-2(2)	-1(2)	-3(2)
S(14)	21(3)	16(3)	19(3)	0(2)	0(2)	-1(2)
S(15)	17(3)	19(3)	17(3)	-4(2)	3(2)	2(3)
S(16)	18(3)	21(3)	21(3)	4(2)	7(2)	0(3)
N(13)	16(6)	21(6)	17(6)	2(6)	1(5)	7(5)
N(14)	19(7)	18(7)	26(7)	0(6)	4(6)	2(6)
N(15)	17(6)	18(7)	15(7)	-7(6)	4(6)	-5(6)
N(16)	15(6)	16(6)	18(7)	4(5)	1(6)	-4(5)
C(133)	17(6)	22(5)	22(5)	-3(5)	-2(5)	0(5)
C(134)	17(6)	18(5)	17(5)	-1(5)	-1(5)	0(5)
C(135)	22(5)	21(5)	21(5)	-4(5)	1(5)	-2(5)
C(136)	19(6)	21(5)	19(5)	1(5)	-2(5)	3(5)
C(137)	22(6)	24(6)	24(5)	0(5)	-2(5)	0(5)
C(138)	18(6)	23(5)	23(5)	0(5)	-1(5)	-2(5)
C(139)	21(5)	23(6)	20(5)	1(5)	3(5)	3(5)
C(140)	21(5)	20(5)	25(5)	1(5)	1(5)	5(5)

C(141)	24(5)	25(5)	27(5)	3(5)	3(5)	-1(5)
C(142)	27(6)	23(6)	23(5)	0(5)	2(5)	5(5)
C(143)	20(6)	20(6)	25(6)	-2(6)	-1(5)	7(5)
C(144)	23(6)	19(6)	24(6)	3(5)	-2(5)	2(5)
C(145)	19(7)	27(7)	19(7)	-3(6)	-2(6)	1(7)
C(146)	25(8)	29(7)	29(8)	-7(7)	-1(6)	-4(7)
C(147)	31(8)	31(7)	28(8)	-6(7)	-5(7)	3(7)
C(148)	29(8)	40(8)	24(8)	-1(7)	3(6)	7(7)
C(149)	21(8)	41(7)	17(7)	1(7)	5(6)	7(7)
C(150)	22(8)	27(7)	20(7)	1(6)	-3(6)	1(6)
C(151)	19(7)	15(7)	12(7)	9(6)	-1(6)	1(6)
C(152)	22(7)	18(7)	23(7)	3(6)	0(6)	1(6)
C(153)	24(7)	19(7)	29(8)	0(6)	3(6)	-3(6)
C(154)	27(7)	22(7)	27(8)	-2(6)	6(7)	1(7)
C(155)	28(7)	22(7)	21(7)	-6(6)	-1(6)	3(7)
C(156)	22(7)	22(7)	15(7)	3(6)	-4(6)	0(6)
C(157)	21(6)	19(6)	22(6)	-1(5)	1(5)	0(5)
C(158)	23(6)	22(5)	22(6)	2(5)	1(5)	-1(5)
C(159)	20(6)	25(6)	21(6)	2(5)	9(5)	1(5)
C(160)	21(7)	21(7)	19(7)	2(6)	5(6)	3(6)
C(161)	17(6)	19(6)	16(6)	0(6)	-1(5)	0(6)
C(162)	16(6)	21(6)	23(7)	-2(6)	-1(5)	1(6)
C(163)	18(7)	17(6)	26(7)	0(6)	0(6)	4(6)
C(164)	26(7)	13(6)	30(8)	3(6)	0(6)	6(6)
C(165)	21(7)	19(7)	26(8)	-4(7)	2(6)	-2(6)
C(166)	16(7)	16(7)	30(8)	-2(6)	0(6)	1(6)
C(167)	16(7)	19(7)	20(7)	-3(6)	4(6)	-8(6)
C(168)	17(7)	27(7)	26(8)	6(6)	2(7)	-7(7)
C(169)	16(7)	30(8)	25(8)	8(6)	3(6)	-1(6)
C(170)	16(6)	27(7)	18(7)	3(6)	2(6)	4(6)
C(171)	17(6)	15(6)	20(7)	0(5)	-2(6)	3(6)
C(172)	20(6)	16(6)	19(7)	0(5)	-4(6)	0(6)
C(173)	20(7)	15(7)	25(7)	1(6)	8(6)	2(6)
C(174)	25(6)	19(6)	24(6)	-5(5)	2(6)	3(5)
C(175)	22(5)	23(5)	23(6)	1(5)	2(5)	2(5)
C(176)	18(6)	22(6)	23(6)	1(5)	1(5)	0(5)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	-4503	3036	-1004	33
H(3)	-4783	2920	-1923	38
H(4)	-4512	3559	-2589	35
H(5)	-4156	4336	-2314	30
H(6)	-3836	4442	-1400	25
H(8)	-3841	2365	1006	23
H(9)	-3967	2124	1921	24
H(10)	-3349	2325	2597	30
H(11)	-2583	2794	2373	29
H(12)	-2444	3021	1460	28
H(14)	-2359	5205	1309	36
H(15)	-2724	5663	2047	37
H(16)	-3228	5223	2686	37
H(17)	-3359	4314	2605	35
H(18)	-3050	3856	1845	31
H(20)	-1756	4608	-1361	28
H(21)	-1296	4166	-2050	35
H(22)	-1716	3557	-2601	33
H(23)	-2563	3255	-2386	33
H(24)	-3040	3722	-1736	26
H(25)	-3887	3442	884	27
H(26)	-4583	3613	1406	31
H(27)	-4892	4471	1511	28
H(28)	-4384	5189	1149	27
H(31)	-3814	5758	955	23
H(32)	-3234	6373	582	29
H(33)	-2521	6083	73	28
H(34)	-2444	5183	-122	23
H(35)	-1681	4418	153	20
H(36)	-799	4354	-101	24
H(37)	-540	3669	-648	25

H(38)	-1165	3047	-960	23
H(41)	-1734	2483	-1158	24
H(42)	-2435	1959	-1497	25
H(43)	-3314	2209	-1326	28
H(44)	-3449	2950	-794	24
H(46)	-1939	5518	-1105	25
H(47)	-2164	5468	-2041	33
H(48)	-1977	6157	-2635	30
H(49)	-1642	6931	-2292	31
H(50)	-1383	7010	-1379	26
H(52)	-1340	4874	1040	25
H(53)	-1466	4662	1962	36
H(54)	-837	4865	2613	36
H(55)	-76	5343	2374	37
H(56)	62	5557	1436	28
H(58)	172	7698	1343	24
H(59)	-214	8171	2057	26
H(60)	-777	7762	2651	30
H(61)	-975	6873	2559	33
H(62)	-636	6400	1829	32
H(64)	771	7056	-1274	22
H(65)	1280	6581	-1905	27
H(66)	876	5951	-2474	28
H(67)	-3	5744	-2338	28
H(68)	-516	6232	-1753	27
H(69)	-1452	5935	839	25
H(70)	-2164	6107	1371	27
H(71)	-2421	6993	1515	27
H(72)	-1896	7670	1184	28
H(75)	-1324	8219	990	28
H(76)	-716	8850	699	29
H(77)	-2	8576	129	28
H(78)	48	7692	-99	29
H(79)	782	6932	171	25
H(80)	1662	6885	-47	27
H(81)	1970	6157	-575	26

H(82)	1348	5528	-868	23
H(85)	780	4964	-1099	27
H(86)	110	4446	-1465	29
H(87)	-789	4720	-1368	24
H(88)	-945	5440	-792	25
H(90)	1958	3210	997	29
H(91)	2218	3348	1888	39
H(92)	1971	2758	2556	37
H(93)	1507	1979	2312	33
H(94)	1310	1808	1400	31
H(96)	1338	3844	-954	32
H(97)	1559	4090	-1837	33
H(98)	1022	3832	-2577	32
H(99)	270	3353	-2423	29
H(100)	3	3124	-1517	27
H(102)	-276	1052	-1315	30
H(103)	75	507	-1984	33
H(104)	741	818	-2546	34
H(105)	1026	1706	-2443	31
H(106)	617	2270	-1819	27
H(108)	-854	1801	1311	30
H(109)	-1241	2295	2003	35
H(110)	-757	2887	2534	35
H(111)	152	2937	2425	30
H(112)	549	2484	1703	26
H(113)	1378	2769	-849	25
H(114)	2114	2577	-1385	23
H(115)	2353	1701	-1533	29
H(116)	1810	1029	-1166	28
H(119)	1288	466	-905	25
H(120)	665	-157	-576	27
H(121)	-36	167	-62	26
H(122)	-109	1055	90	21
H(123)	-848	1817	-199	27
H(124)	-1714	1840	39	28
H(125)	-1999	2551	585	31

H(126)	-1399	3173	906	30
H(129)	-816	3732	1128	23
H(130)	-158	4242	1535	30
H(131)	726	3995	1351	27
H(132)	891	3272	811	21
H(134)	4528	5698	977	21
H(135)	4802	5881	1882	26
H(136)	4611	5269	2592	24
H(137)	4067	4557	2389	28
H(138)	3799	4378	1504	26
H(140)	3749	6251	-1138	26
H(141)	3810	6434	-2049	30
H(142)	3105	6236	-2665	29
H(143)	2320	5862	-2282	26
H(144)	2298	5673	-1371	26
H(146)	2384	3491	-1264	33
H(147)	2839	3012	-1942	36
H(148)	3464	3469	-2470	37
H(149)	3576	4343	-2390	32
H(150)	3127	4852	-1726	28
H(152)	1652	4182	1263	25
H(153)	1101	4652	1850	29
H(154)	1441	5297	2428	30
H(155)	2326	5504	2414	28
H(156)	2899	5028	1835	23
H(157)	3866	5264	-812	24
H(158)	4619	5067	-1330	27
H(159)	4839	4186	-1467	26
H(160)	4366	3528	-1061	24
H(163)	3800	2950	-839	24
H(164)	3173	2342	-530	28
H(165)	2453	2671	-39	27
H(166)	2438	3550	187	25
H(167)	1679	4295	-109	22
H(168)	785	4373	67	28
H(169)	518	5115	585	28

H(170)	1122	5719	925	24
H(173)	1700	6264	1182	24
H(174)	2400	6769	1562	27
H(175)	3238	6501	1409	27
H(176)	3417	5780	888	25
H(202)	4543	613	956	24
H(203)	4854	641	1872	24
H(204)	4472	44	2520	24
H(205)	3980	-646	2224	24
H(206)	3640	-663	1310	24
H(208)	3781	1458	-1062	24
H(209)	3929	1703	-1972	24
H(210)	3345	1471	-2670	24
H(211)	2645	891	-2488	24
H(212)	2509	619	-1588	24
H(214)	2319	-1482	-1357	24
H(215)	2751	-2005	-2002	24
H(216)	3266	-1618	-2668	24
H(217)	3425	-711	-2640	24
H(218)	2989	-174	-2017	24
H(220)	1683	-855	1219	24
H(221)	1209	-386	1879	24
H(222)	1631	203	2451	24
H(223)	2501	466	2280	24
H(224)	2985	-20	1652	24
H(225)	3868	297	-964	24
H(226)	4613	128	-1409	24
H(227)	4846	-731	-1635	24
H(228)	4298	-1447	-1335	24
H(231)	3756	-2012	-1099	24
H(232)	3097	-2602	-843	24
H(233)	2456	-2336	-226	24
H(234)	2457	-1463	82	24
H(235)	1640	-666	-314	24
H(236)	769	-648	-15	24
H(237)	492	46	511	24

H(238)	1106	682	819	24
H(241)	1672	1235	1051	24
H(242)	2362	1800	1337	24
H(243)	3246	1549	1190	24
H(244)	3394	770	723	24
H(246)	7136	3183	1128	24
H(247)	7398	3143	2054	24
H(248)	7053	2513	2638	24
H(249)	6509	1870	2292	24
H(250)	6272	1843	1370	24
H(252)	6298	4002	-1036	24
H(253)	6460	4124	-1968	24
H(254)	5889	3797	-2621	24
H(255)	5159	3279	-2368	24
H(256)	5004	3127	-1420	24
H(258)	4803	1094	-1226	24
H(259)	5108	591	-1962	24
H(260)	5634	964	-2615	24
H(261)	5935	1824	-2519	24
H(262)	5631	2342	-1804	24
H(264)	4295	1715	1396	24
H(265)	3781	2201	2013	24
H(266)	4142	2941	2456	24
H(267)	5030	3125	2344	24
H(268)	5528	2680	1712	24
H(269)	6461	2884	-819	24
H(270)	7137	2710	-1397	24
H(271)	7354	1823	-1598	24
H(272)	6888	1148	-1177	24
H(275)	6322	600	-963	24
H(276)	5753	-38	-609	24
H(277)	5025	245	-61	24
H(278)	4973	1133	153	24
H(279)	4234	1882	-101	24
H(280)	3352	1945	106	24
H(281)	3064	2641	692	24

H(282)	3680	3298	926	24
H(285)	4250	3865	1142	24
H(286)	4924	4393	1483	24
H(287)	5822	4120	1374	24
H(288)	5970	3397	800	24
H(290)	3050	5522	-1014	24
H(291)	2723	5377	-1880	24
H(292)	2845	6004	-2553	24
H(293)	3382	6751	-2372	24
H(294)	3729	6883	-1500	24
H(296)	3706	4948	939	24
H(297)	3545	4655	1822	24
H(298)	4093	4932	2546	24
H(299)	4826	5433	2367	24
H(300)	5024	5724	1459	24
H(302)	5192	7783	1155	24
H(303)	4808	8328	1804	24
H(304)	4332	7960	2521	24
H(305)	4149	7040	2499	24
H(306)	4482	6507	1801	24
H(308)	5867	6862	-1309	24
H(309)	6260	6403	-2021	24
H(310)	5769	5902	-2641	24
H(311)	4858	5853	-2545	24
H(312)	4439	6389	-1901	24
H(313)	3638	6029	785	24
H(314)	2923	6229	1349	24
H(315)	2703	7108	1509	24
H(316)	3190	7771	1052	24
H(319)	3751	8327	839	24
H(320)	4343	8950	453	24
H(321)	5020	8623	-93	24
H(322)	5107	7731	-209	24
H(323)	5859	6974	108	24
H(324)	6733	6920	-90	24
H(325)	7001	6252	-702	24

H(326)	6404	5618	-1001	24
H(329)	5831	5005	-1124	24
H(330)	5177	4414	-1393	24
H(331)	4291	4699	-1288	24
H(332)	4122	5498	-881	24
H(334)	-4653	-1854	-1005	24
H(335)	-4911	-2016	-1918	24
H(336)	-4541	-1506	-2636	24
H(337)	-4025	-782	-2402	24
H(338)	-3793	-606	-1506	24
H(340)	-3760	-2594	1087	24
H(341)	-3780	-2867	1976	24
H(342)	-3129	-2581	2619	24
H(343)	-2482	-1960	2303	24
H(344)	-2478	-1724	1402	24
H(346)	-2339	292	1250	24
H(347)	-2724	797	1955	24
H(348)	-3320	369	2543	24
H(349)	-3601	-455	2372	24
H(350)	-3263	-972	1645	24
H(352)	-1727	-382	-1371	24
H(353)	-1193	-902	-1930	24
H(354)	-1535	-1637	-2377	24
H(355)	-2424	-1823	-2336	24
H(356)	-2982	-1290	-1795	24
H(357)	-3928	-1486	781	24
H(358)	-4632	-1288	1370	24
H(359)	-4856	-407	1501	24
H(360)	-4411	249	1058	24
H(363)	-3804	818	892	24
H(364)	-3237	1440	497	24
H(365)	-2540	1119	-34	24
H(366)	-2484	228	-193	24
H(367)	-1723	-544	141	24
H(368)	-826	-628	-25	24
H(369)	-571	-1320	-619	24

H(370)	-1170	-1941	-934	24
H(373)	-1749	-2481	-1201	24
H(374)	-2446	-3046	-1482	24
H(375)	-3286	-2769	-1350	24
H(376)	-3465	-1997	-911	24

Table S7. Torsion angles [°] for **1**.

Th(1)-S(1)-C(1)-C(2)	120.8(11)	C(19)-C(20)-C(21)-C(22)	3(3)
Th(1)-S(1)-C(1)-C(6)	-66.3(11)	C(20)-C(21)-C(22)-C(23)	-5(3)
C(6)-C(1)-C(2)-C(3)	1(3)	C(21)-C(22)-C(23)-C(24)	7(3)
S(1)-C(1)-C(2)-C(3)	174.0(16)	C(22)-C(23)-C(24)-C(19)	-7(3)
C(1)-C(2)-C(3)-C(4)	2(3)	C(20)-C(19)-C(24)-C(23)	6(2)
C(2)-C(3)-C(4)-C(5)	-6(3)	S(4)-C(19)-C(24)-C(23)	179.2(14)
C(3)-C(4)-C(5)-C(6)	8(3)	C(29)-N(1)-C(25)-C(26)	1(2)
C(2)-C(1)-C(6)-C(5)	1(2)	Th(1)-N(1)-C(25)-C(26)	-171.3(16)
S(1)-C(1)-C(6)-C(5)	-172.2(13)	N(1)-C(25)-C(26)-C(27)	4(3)
C(4)-C(5)-C(6)-C(1)	-5(3)	C(25)-C(26)-C(27)-C(28)	-4(3)
Th(1)-S(2)-C(7)-C(12)	-66.0(12)	C(26)-C(27)-C(28)-C(29)	1(3)
Th(1)-S(2)-C(7)-C(8)	118.8(10)	C(25)-N(1)-C(29)-C(28)	-5(2)
C(12)-C(7)-C(8)-C(9)	1(2)	Th(1)-N(1)-C(29)-C(28)	167.5(13)
S(2)-C(7)-C(8)-C(9)	176.2(13)	C(25)-N(1)-C(29)-C(30)	178.1(13)
C(7)-C(8)-C(9)-C(10)	0(3)	Th(1)-N(1)-C(29)-C(30)	-9.7(15)
C(8)-C(9)-C(10)-C(11)	0(3)	C(27)-C(28)-C(29)-N(1)	4(3)
C(9)-C(10)-C(11)-C(12)	-1(3)	C(27)-C(28)-C(29)-C(30)	-179.2(16)
C(10)-C(11)-C(12)-C(7)	2(3)	C(34)-N(2)-C(30)-C(31)	4(2)
C(8)-C(7)-C(12)-C(11)	-2(3)	Th(1)-N(2)-C(30)-C(31)	176.4(12)
S(2)-C(7)-C(12)-C(11)	-176.6(15)	C(34)-N(2)-C(30)-C(29)	-171.5(13)
Th(1)-S(3)-C(13)-C(14)	-98.6(12)	Th(1)-N(2)-C(30)-C(29)	1.3(15)
Th(1)-S(3)-C(13)-C(18)	86.1(10)	N(1)-C(29)-C(30)-N(2)	5.3(18)
C(18)-C(13)-C(14)-C(15)	1(3)	C(28)-C(29)-C(30)-N(2)	-172.0(15)
S(3)-C(13)-C(14)-C(15)	-174.3(16)	N(1)-C(29)-C(30)-C(31)	-169.7(16)
C(13)-C(14)-C(15)-C(16)	0(3)	C(28)-C(29)-C(30)-C(31)	13(2)
C(14)-C(15)-C(16)-C(17)	0(4)	N(2)-C(30)-C(31)-C(32)	1(3)
C(15)-C(16)-C(17)-C(18)	-3(3)	C(29)-C(30)-C(31)-C(32)	175.6(17)
C(16)-C(17)-C(18)-C(13)	4(3)	C(30)-C(31)-C(32)-C(33)	-4(3)
C(14)-C(13)-C(18)-C(17)	-3(2)	C(31)-C(32)-C(33)-C(34)	3(3)
S(3)-C(13)-C(18)-C(17)	172.2(14)	C(30)-N(2)-C(34)-C(33)	-5(2)
Th(1)-S(4)-C(19)-C(20)	-109.7(10)	Th(1)-N(2)-C(34)-C(33)	-178.0(15)
Th(1)-S(4)-C(19)-C(24)	76.6(11)	C(32)-C(33)-C(34)-N(2)	2(3)
C(24)-C(19)-C(20)-C(21)	-4(2)	C(39)-N(3)-C(35)-C(36)	-4(2)
S(4)-C(19)-C(20)-C(21)	-177.4(14)	Th(1)-N(3)-C(35)-C(36)	-175.2(14)

N(3)-C(35)-C(36)-C(37)	1(3)	C(56)-C(51)-C(52)-C(53)	1(2)
C(35)-C(36)-C(37)-C(38)	1(3)	S(6)-C(51)-C(52)-C(53)	176.2(15)
C(36)-C(37)-C(38)-C(39)	0(3)	C(51)-C(52)-C(53)-C(54)	-2(3)
C(35)-N(3)-C(39)-C(38)	5(2)	C(52)-C(53)-C(54)-C(55)	2(4)
Th(1)-N(3)-C(39)-C(38)	176.2(12)	C(53)-C(54)-C(55)-C(56)	-2(3)
C(35)-N(3)-C(39)-C(40)	-174.5(13)	C(52)-C(51)-C(56)-C(55)	-2(2)
Th(1)-N(3)-C(39)-C(40)	-3.0(16)	S(6)-C(51)-C(56)-C(55)	-176.2(15)
C(37)-C(38)-C(39)-N(3)	-3(3)	C(54)-C(55)-C(56)-C(51)	2(3)
C(37)-C(38)-C(39)-C(40)	176.1(17)	Th(2)-S(7)-C(57)-C(62)	82.7(11)
C(44)-N(4)-C(40)-C(41)	-1(2)	Th(2)-S(7)-C(57)-C(58)	-104.0(10)
Th(1)-N(4)-C(40)-C(41)	170.5(12)	C(62)-C(57)-C(58)-C(59)	-2(2)
C(44)-N(4)-C(40)-C(39)	177.8(13)	S(7)-C(57)-C(58)-C(59)	-175.2(14)
Th(1)-N(4)-C(40)-C(39)	-10.3(17)	C(57)-C(58)-C(59)-C(60)	2(3)
N(3)-C(39)-C(40)-N(4)	9(2)	C(58)-C(59)-C(60)-C(61)	0(3)
C(38)-C(39)-C(40)-N(4)	-170.6(16)	C(59)-C(60)-C(61)-C(62)	-2(3)
N(3)-C(39)-C(40)-C(41)	-172.2(15)	C(60)-C(61)-C(62)-C(57)	2(3)
C(38)-C(39)-C(40)-C(41)	9(2)	C(58)-C(57)-C(62)-C(61)	0(2)
N(4)-C(40)-C(41)-C(42)	1(3)	S(7)-C(57)-C(62)-C(61)	173.3(15)
C(39)-C(40)-C(41)-C(42)	-177.8(17)	Th(2)-S(8)-C(63)-C(68)	79.4(11)
C(40)-C(41)-C(42)-C(43)	0(3)	Th(2)-S(8)-C(63)-C(64)	-104.2(10)
C(41)-C(42)-C(43)-C(44)	-1(3)	C(68)-C(63)-C(64)-C(65)	-3(2)
C(40)-N(4)-C(44)-C(43)	0(2)	S(8)-C(63)-C(64)-C(65)	-179.9(14)
Th(1)-N(4)-C(44)-C(43)	-172.3(15)	C(63)-C(64)-C(65)-C(66)	2(3)
C(42)-C(43)-C(44)-N(4)	1(3)	C(64)-C(65)-C(66)-C(67)	-3(3)
Th(2)-S(5)-C(45)-C(50)	-69.8(11)	C(65)-C(66)-C(67)-C(68)	4(3)
Th(2)-S(5)-C(45)-C(46)	118.4(10)	C(66)-C(67)-C(68)-C(63)	-6(3)
C(50)-C(45)-C(46)-C(47)	2(2)	C(64)-C(63)-C(68)-C(67)	5(2)
S(5)-C(45)-C(46)-C(47)	174.2(14)	S(8)-C(63)-C(68)-C(67)	-178.7(14)
C(45)-C(46)-C(47)-C(48)	0(3)	C(73)-N(5)-C(69)-C(70)	-1(2)
C(46)-C(47)-C(48)-C(49)	-3(3)	Th(2)-N(5)-C(69)-C(70)	-172.6(16)
C(47)-C(48)-C(49)-C(50)	4(3)	N(5)-C(69)-C(70)-C(71)	3(3)
C(48)-C(49)-C(50)-C(45)	-2(3)	C(69)-C(70)-C(71)-C(72)	-3(3)
C(46)-C(45)-C(50)-C(49)	-1(2)	C(70)-C(71)-C(72)-C(73)	1(3)
S(5)-C(45)-C(50)-C(49)	-173.0(14)	C(69)-N(5)-C(73)-C(72)	-1(2)
Th(2)-S(6)-C(51)-C(56)	-65.7(12)	Th(2)-N(5)-C(73)-C(72)	170.0(13)
Th(2)-S(6)-C(51)-C(52)	119.6(10)	C(69)-N(5)-C(73)-C(74)	178.1(13)

Th(2)-N(5)-C(73)-C(74)	-10.5(16)	N(7)-C(83)-C(84)-C(85)	-174.2(15)
C(71)-C(72)-C(73)-N(5)	1(3)	N(8)-C(84)-C(85)-C(86)	2(3)
C(71)-C(72)-C(73)-C(74)	-178.2(18)	C(83)-C(84)-C(85)-C(86)	-175.7(18)
C(78)-N(6)-C(74)-C(75)	4(2)	C(84)-C(85)-C(86)-C(87)	1(3)
Th(2)-N(6)-C(74)-C(75)	175.5(13)	C(85)-C(86)-C(87)-C(88)	-4(3)
C(78)-N(6)-C(74)-C(73)	-173.4(14)	C(84)-N(8)-C(88)-C(87)	-3(2)
Th(2)-N(6)-C(74)-C(73)	-2.1(17)	Th(2)-N(8)-C(88)-C(87)	-174.5(14)
N(5)-C(73)-C(74)-N(6)	8.0(19)	C(86)-C(87)-C(88)-N(8)	6(3)
C(72)-C(73)-C(74)-N(6)	-172.5(17)	Th(3)-S(9)-C(89)-C(94)	65.1(13)
N(5)-C(73)-C(74)-C(75)	-169.6(16)	Th(3)-S(9)-C(89)-C(90)	-117.9(11)
C(72)-C(73)-C(74)-C(75)	10(3)	C(94)-C(89)-C(90)-C(91)	1(3)
N(6)-C(74)-C(75)-C(76)	-2(3)	S(9)-C(89)-C(90)-C(91)	-175.9(17)
C(73)-C(74)-C(75)-C(76)	175.6(17)	C(89)-C(90)-C(91)-C(92)	-3(3)
C(74)-C(75)-C(76)-C(77)	0(3)	C(90)-C(91)-C(92)-C(93)	2(4)
C(75)-C(76)-C(77)-C(78)	0(3)	C(91)-C(92)-C(93)-C(94)	0(4)
C(76)-C(77)-C(78)-N(6)	2(3)	C(92)-C(93)-C(94)-C(89)	-2(3)
C(74)-N(6)-C(78)-C(77)	-4(2)	C(90)-C(89)-C(94)-C(93)	2(3)
Th(2)-N(6)-C(78)-C(77)	-175.8(16)	S(9)-C(89)-C(94)-C(93)	178.7(16)
C(83)-N(7)-C(79)-C(80)	-1(3)	Th(3)-S(10)-C(95)-C(96)	-116.9(12)
Th(2)-N(7)-C(79)-C(80)	-177.1(16)	Th(3)-S(10)-C(95)-C(100)	63.6(11)
N(7)-C(79)-C(80)-C(81)	-1(3)	C(100)-C(95)-C(96)-C(97)	4(3)
C(79)-C(80)-C(81)-C(82)	1(3)	S(10)-C(95)-C(96)-C(97)	-175.9(17)
C(80)-C(81)-C(82)-C(83)	1(3)	C(95)-C(96)-C(97)-C(98)	-3(3)
C(81)-C(82)-C(83)-N(7)	-4(3)	C(96)-C(97)-C(98)-C(99)	0(3)
C(81)-C(82)-C(83)-C(84)	175.6(18)	C(97)-C(98)-C(99)-C(100)	1(3)
C(79)-N(7)-C(83)-C(82)	4(2)	C(98)-C(99)-C(100)-C(95)	0(3)
Th(2)-N(7)-C(83)-C(82)	179.4(12)	C(96)-C(95)-C(100)-C(99)	-2(2)
C(79)-N(7)-C(83)-C(84)	-175.7(14)	S(10)-C(95)-C(100)-C(99)	177.6(13)
Th(2)-N(7)-C(83)-C(84)	-0.2(17)	Th(3)-S(11)-C(101)-C(102)	102.3(11)
C(88)-N(8)-C(84)-C(85)	-1(2)	Th(3)-S(11)-C(101)-C(106)	-78.0(11)
Th(2)-N(8)-C(84)-C(85)	170.0(13)	C(106)-C(101)-C(102)-C(103)	-2(3)
C(88)-N(8)-C(84)-C(83)	177.0(13)	S(11)-C(101)-C(102)-C(103)	177.4(16)
Th(2)-N(8)-C(84)-C(83)	-12.3(16)	C(101)-C(102)-C(103)-C(104)	3(3)
C(82)-C(83)-C(84)-N(8)	-171.6(17)	C(102)-C(103)-C(104)-C(105)	-1(3)
N(7)-C(83)-C(84)-N(8)	8.0(19)	C(103)-C(104)-C(105)-C(106)	-2(3)
C(82)-C(83)-C(84)-C(85)	6(3)	C(104)-C(105)-C(106)-C(101)	3(3)

C(102)-C(101)-C(106)-C(105)	-1(2)	Th(3)-N(10)-C(122)-C(121)	-177.9(16)
S(11)-C(101)-C(106)-C(105)	179.6(14)	C(120)-C(121)-C(122)-N(10)	-1(3)
Th(3)-S(12)-C(107)-C(112)	-78.3(10)	C(127)-N(11)-C(123)-C(124)	-1(3)
Th(3)-S(12)-C(107)-C(108)	101.2(11)	Th(3)-N(11)-C(123)-C(124)	175.5(16)
C(112)-C(107)-C(108)-C(109)	-1(2)	N(11)-C(123)-C(124)-C(125)	2(3)
S(12)-C(107)-C(108)-C(109)	179.5(14)	C(123)-C(124)-C(125)-C(126)	-2(3)
C(107)-C(108)-C(109)-C(110)	1(3)	C(124)-C(125)-C(126)-C(127)	1(3)
C(108)-C(109)-C(110)-C(111)	-2(3)	C(123)-N(11)-C(127)-C(126)	0(2)
C(109)-C(110)-C(111)-C(112)	4(3)	Th(3)-N(11)-C(127)-C(126)	-176.8(13)
C(108)-C(107)-C(112)-C(111)	3(2)	C(123)-N(11)-C(127)-C(128)	175.8(14)
S(12)-C(107)-C(112)-C(111)	-177.6(14)	Th(3)-N(11)-C(127)-C(128)	-1.1(17)
C(110)-C(111)-C(112)-C(107)	-5(3)	C(125)-C(126)-C(127)-N(11)	0(3)
C(117)-N(9)-C(113)-C(114)	2(2)	C(125)-C(126)-C(127)-C(128)	-175.4(18)
Th(3)-N(9)-C(113)-C(114)	173.1(14)	C(132)-N(12)-C(128)-C(129)	0(2)
N(9)-C(113)-C(114)-C(115)	-2(3)	Th(3)-N(12)-C(128)-C(129)	-171.9(12)
C(113)-C(114)-C(115)-C(116)	1(3)	C(132)-N(12)-C(128)-C(127)	-176.8(13)
C(114)-C(115)-C(116)-C(117)	-1(3)	Th(3)-N(12)-C(128)-C(127)	11.2(15)
C(115)-C(116)-C(117)-N(9)	2(3)	N(11)-C(127)-C(128)-C(129)	177.0(16)
C(115)-C(116)-C(117)-C(118)	176.3(18)	C(126)-C(127)-C(128)-C(129)	-7(3)
C(113)-N(9)-C(117)-C(116)	-2(2)	N(11)-C(127)-C(128)-N(12)	-6.3(19)
Th(3)-N(9)-C(117)-C(116)	-172.6(14)	C(126)-C(127)-C(128)-N(12)	169.6(16)
C(113)-N(9)-C(117)-C(118)	-177.1(13)	N(12)-C(128)-C(129)-C(130)	-1(3)
Th(3)-N(9)-C(117)-C(118)	12.5(16)	C(127)-C(128)-C(129)-C(130)	175.1(18)
C(122)-N(10)-C(118)-C(119)	-2(2)	C(128)-C(129)-C(130)-C(131)	2(3)
Th(3)-N(10)-C(118)-C(119)	178.2(14)	C(129)-C(130)-C(131)-C(132)	-1(3)
C(122)-N(10)-C(118)-C(117)	177.0(14)	C(128)-N(12)-C(132)-C(131)	1(2)
Th(3)-N(10)-C(118)-C(117)	-3.1(17)	Th(3)-N(12)-C(132)-C(131)	173.2(15)
C(116)-C(117)-C(118)-N(10)	179.3(16)	C(130)-C(131)-C(132)-N(12)	-1(3)
N(9)-C(117)-C(118)-N(10)	-5.9(19)	Th(4)-S(13)-C(133)-C(138)	62.9(12)
C(116)-C(117)-C(118)-C(119)	-2(3)	Th(4)-S(13)-C(133)-C(134)	-122.1(10)
N(9)-C(117)-C(118)-C(119)	172.9(16)	C(138)-C(133)-C(134)-C(135)	0(2)
N(10)-C(118)-C(119)-C(120)	1(3)	S(13)-C(133)-C(134)-C(135)	-175.2(14)
C(117)-C(118)-C(119)-C(120)	-177.8(17)	C(133)-C(134)-C(135)-C(136)	2(3)
C(118)-C(119)-C(120)-C(121)	0(3)	C(134)-C(135)-C(136)-C(137)	-4(3)
C(119)-C(120)-C(121)-C(122)	0(3)	C(135)-C(136)-C(137)-C(138)	4(3)
C(118)-N(10)-C(122)-C(121)	2(2)	C(134)-C(133)-C(138)-C(137)	0(3)

S(13)-C(133)-C(138)-C(137)	174.7(15)	C(158)-C(159)-C(160)-C(161)	2(3)
C(136)-C(137)-C(138)-C(133)	-2(3)	C(157)-N(13)-C(161)-C(160)	1.5(19)
Th(4)-S(14)-C(139)-C(144)	70.3(12)	Th(4)-N(13)-C(161)-C(160)	-172.0(12)
Th(4)-S(14)-C(139)-C(140)	-117.8(10)	C(157)-N(13)-C(161)-C(162)	-173.3(13)
C(144)-C(139)-C(140)-C(141)	-2(2)	Th(4)-N(13)-C(161)-C(162)	13.2(15)
S(14)-C(139)-C(140)-C(141)	-175.0(15)	C(159)-C(160)-C(161)-N(13)	-2(3)
C(139)-C(140)-C(141)-C(142)	1(3)	C(159)-C(160)-C(161)-C(162)	172.3(17)
C(140)-C(141)-C(142)-C(143)	1(3)	C(166)-N(14)-C(162)-C(163)	-5(2)
C(141)-C(142)-C(143)-C(144)	-2(3)	Th(4)-N(14)-C(162)-C(163)	-177.9(12)
C(142)-C(143)-C(144)-C(139)	1(3)	C(166)-N(14)-C(162)-C(161)	175.6(14)
C(140)-C(139)-C(144)-C(143)	1(3)	Th(4)-N(14)-C(162)-C(161)	2.6(17)
S(14)-C(139)-C(144)-C(143)	173.6(15)	N(13)-C(161)-C(162)-N(14)	-10.0(19)
Th(4)-S(15)-C(145)-C(146)	102.8(11)	C(160)-C(161)-C(162)-N(14)	175.2(15)
Th(4)-S(15)-C(145)-C(150)	-79.0(10)	N(13)-C(161)-C(162)-C(163)	170.5(16)
C(150)-C(145)-C(146)-C(147)	-1(3)	C(160)-C(161)-C(162)-C(163)	-4(3)
S(15)-C(145)-C(146)-C(147)	177.7(15)	N(14)-C(162)-C(163)-C(164)	4(3)
C(145)-C(146)-C(147)-C(148)	2(3)	C(161)-C(162)-C(163)-C(164)	-176.5(17)
C(146)-C(147)-C(148)-C(149)	-3(3)	C(162)-C(163)-C(164)-C(165)	0(3)
C(147)-C(148)-C(149)-C(150)	2(4)	C(163)-C(164)-C(165)-C(166)	-3(3)
C(146)-C(145)-C(150)-C(149)	0(2)	C(162)-N(14)-C(166)-C(165)	2(3)
S(15)-C(145)-C(150)-C(149)	-178.2(13)	Th(4)-N(14)-C(166)-C(165)	174.8(16)
C(148)-C(149)-C(150)-C(145)	-1(3)	C(164)-C(165)-C(166)-N(14)	3(3)
Th(4)-S(16)-C(151)-C(156)	-82.1(10)	C(171)-N(15)-C(167)-C(168)	1(3)
Th(4)-S(16)-C(151)-C(152)	97.5(10)	Th(4)-N(15)-C(167)-C(168)	179.7(16)
C(156)-C(151)-C(152)-C(153)	1(2)	N(15)-C(167)-C(168)-C(169)	-1(3)
S(16)-C(151)-C(152)-C(153)	-178.3(14)	C(167)-C(168)-C(169)-C(170)	-1(3)
C(151)-C(152)-C(153)-C(154)	-1(3)	C(168)-C(169)-C(170)-C(171)	3(3)
C(152)-C(153)-C(154)-C(155)	1(3)	C(167)-N(15)-C(171)-C(170)	0.8(19)
C(153)-C(154)-C(155)-C(156)	-1(3)	Th(4)-N(15)-C(171)-C(170)	-178.1(11)
C(152)-C(151)-C(156)-C(155)	-2(2)	C(167)-N(15)-C(171)-C(172)	172.4(14)
S(16)-C(151)-C(156)-C(155)	177.7(13)	Th(4)-N(15)-C(171)-C(172)	-6.5(15)
C(154)-C(155)-C(156)-C(151)	2(3)	C(169)-C(170)-C(171)-N(15)	-2(2)
C(161)-N(13)-C(157)-C(158)	-1(2)	C(169)-C(170)-C(171)-C(172)	-173.6(18)
Th(4)-N(13)-C(157)-C(158)	172.7(15)	C(176)-N(16)-C(172)-C(173)	3(2)
N(13)-C(157)-C(158)-C(159)	1(3)	Th(4)-N(16)-C(172)-C(173)	-173.0(12)
C(157)-C(158)-C(159)-C(160)	-2(3)	C(176)-N(16)-C(172)-C(171)	-177.5(14)

Th(4)-N(16)-C(172)-C(171)	6.1(17)	C(213)-C(214)-C(215)-C(216)	-2.8
N(15)-C(171)-C(172)-N(16)	0.3(19)	C(214)-C(215)-C(216)-C(217)	2.7
C(170)-C(171)-C(172)-N(16)	171.7(15)	C(215)-C(216)-C(217)-C(218)	-3.4
N(15)-C(171)-C(172)-C(173)	179.4(15)	C(216)-C(217)-C(218)-C(213)	4.1
C(170)-C(171)-C(172)-C(173)	-9(2)	C(214)-C(213)-C(218)-C(217)	-4.0
N(16)-C(172)-C(173)-C(174)	-2(3)	S(3B)-C(213)-C(218)-C(217)	178.7
C(171)-C(172)-C(173)-C(174)	178.6(17)	Th(1B)-S(4B)-C(219)-C(220)	107.4
C(172)-C(173)-C(174)-C(175)	0(3)	Th(1B)-S(4B)-C(219)-C(224)	-77.7
C(173)-C(174)-C(175)-C(176)	1(3)	C(224)-C(219)-C(220)-C(221)	4.7
C(172)-N(16)-C(176)-C(175)	-2(2)	S(4B)-C(219)-C(220)-C(221)	179.7
Th(4)-N(16)-C(176)-C(175)	174.1(15)	C(219)-C(220)-C(221)-C(222)	-4.3
C(174)-C(175)-C(176)-N(16)	0(3)	C(220)-C(221)-C(222)-C(223)	5.1
Th(1B)-S(1B)-C(201)-C(202)	-131.5	C(221)-C(222)-C(223)-C(224)	-6.4
Th(1B)-S(1B)-C(201)-C(206)	56.2	C(222)-C(223)-C(224)-C(219)	6.9
C(206)-C(201)-C(202)-C(203)	2.7	C(220)-C(219)-C(224)-C(223)	-6.2
S(1B)-C(201)-C(202)-C(203)	-170.0	S(4B)-C(219)-C(224)-C(223)	178.9
C(201)-C(202)-C(203)-C(204)	-4.0	C(229)-N(1B)-C(225)-C(226)	-3.1
C(202)-C(203)-C(204)-C(205)	6.7	Th(1B)-N(1B)-C(225)-C(226)	169.8
C(203)-C(204)-C(205)-C(206)	-8.1	N(1B)-C(225)-C(226)-C(227)	5.2
C(202)-C(201)-C(206)-C(205)	-3.7	C(225)-C(226)-C(227)-C(228)	-1.8
S(1B)-C(201)-C(206)-C(205)	168.6	C(226)-C(227)-C(228)-C(229)	-3.2
C(204)-C(205)-C(206)-C(201)	6.6	C(225)-N(1B)-C(229)-C(228)	-2.4
Th(1B)-S(2B)-C(207)-C(212)	58.7	Th(1B)-N(1B)-C(229)-C(228)	-175.1
Th(1B)-S(2B)-C(207)-C(208)	-125.7	C(225)-N(1B)-C(229)-C(230)	-177.2
C(212)-C(207)-C(208)-C(209)	0.5	Th(1B)-N(1B)-C(229)-C(230)	10.2
S(2B)-C(207)-C(208)-C(209)	-175.4	C(227)-C(228)-C(229)-N(1B)	5.4
C(207)-C(208)-C(209)-C(210)	2.4	C(227)-C(228)-C(229)-C(230)	-179.9
C(208)-C(209)-C(210)-C(211)	-4.0	C(234)-N(2B)-C(230)-C(231)	2.3
C(209)-C(210)-C(211)-C(212)	2.7	Th(1B)-N(2B)-C(230)-C(231)	-171.4
C(210)-C(211)-C(212)-C(207)	0.2	C(234)-N(2B)-C(230)-C(229)	176.4
C(208)-C(207)-C(212)-C(211)	-1.7	Th(1B)-N(2B)-C(230)-C(229)	2.7
S(2B)-C(207)-C(212)-C(211)	173.8	N(1B)-C(229)-C(230)-N(2B)	-8.2
Th(1B)-S(3B)-C(213)-C(214)	92.5	C(228)-C(229)-C(230)-N(2B)	176.8
Th(1B)-S(3B)-C(213)-C(218)	-90.4	N(1B)-C(229)-C(230)-C(231)	165.8
C(218)-C(213)-C(214)-C(215)	3.3	C(228)-C(229)-C(230)-C(231)	-9.2
S(3B)-C(213)-C(214)-C(215)	-179.5	N(2B)-C(230)-C(231)-C(232)	1.9

C(229)-C(230)-C(231)-C(232)	-171.6	C(245)-C(246)-C(247)-C(248)	-2.3
C(230)-C(231)-C(232)-C(233)	-4.2	C(246)-C(247)-C(248)-C(249)	3.3
C(231)-C(232)-C(233)-C(234)	2.2	C(247)-C(248)-C(249)-C(250)	-1.0
C(230)-N(2B)-C(234)-C(233)	-4.5	C(248)-C(249)-C(250)-C(245)	-2.3
Th(1B)-N(2B)-C(234)-C(233)	169.5	C(246)-C(245)-C(250)-C(249)	3.1
C(232)-C(233)-C(234)-N(2B)	2.3	S(5B)-C(245)-C(250)-C(249)	175.0
C(239)-N(3B)-C(235)-C(236)	-0.3	Th(2B)-S(6B)-C(251)-C(256)	52.9
Th(1B)-N(3B)-C(235)-C(236)	171.4	Th(2B)-S(6B)-C(251)-C(252)	-121.5
N(3B)-C(235)-C(236)-C(237)	4.1	C(256)-C(251)-C(252)-C(253)	2.1
C(235)-C(236)-C(237)-C(238)	-3.5	S(6B)-C(251)-C(252)-C(253)	176.7
C(236)-C(237)-C(238)-C(239)	-0.5	C(251)-C(252)-C(253)-C(254)	0.8
C(235)-N(3B)-C(239)-C(238)	-3.8	C(252)-C(253)-C(254)-C(255)	-2.5
Th(1B)-N(3B)-C(239)-C(238)	-175.4	C(253)-C(254)-C(255)-C(256)	1.4
C(235)-N(3B)-C(239)-C(240)	174.9	C(252)-C(251)-C(256)-C(255)	-3.2
Th(1B)-N(3B)-C(239)-C(240)	3.3	S(6B)-C(251)-C(256)-C(255)	-177.5
C(237)-C(238)-C(239)-N(3B)	4.2	C(254)-C(255)-C(256)-C(251)	1.5
C(237)-C(238)-C(239)-C(240)	-174.4	Th(2B)-S(7B)-C(257)-C(262)	-83.8
C(244)-N(4B)-C(240)-C(241)	1.4	Th(2B)-S(7B)-C(257)-C(258)	103.0
Th(1B)-N(4B)-C(240)-C(241)	-170.3	C(262)-C(257)-C(258)-C(259)	-2.3
C(244)-N(4B)-C(240)-C(239)	-178.1	S(7B)-C(257)-C(258)-C(259)	171.1
Th(1B)-N(4B)-C(240)-C(239)	10.2	C(257)-C(258)-C(259)-C(260)	0.1
N(3B)-C(239)-C(240)-N(4B)	-8.7	C(258)-C(259)-C(260)-C(261)	2.8
C(238)-C(239)-C(240)-N(4B)	169.9	C(259)-C(260)-C(261)-C(262)	-3.4
N(3B)-C(239)-C(240)-C(241)	171.8	C(260)-C(261)-C(262)-C(257)	1.0
C(238)-C(239)-C(240)-C(241)	-9.6	C(258)-C(257)-C(262)-C(261)	1.8
N(4B)-C(240)-C(241)-C(242)	2.4	S(7B)-C(257)-C(262)-C(261)	-171.5
C(239)-C(240)-C(241)-C(242)	-178.2	Th(2B)-S(8B)-C(263)-C(268)	-73.2
C(240)-C(241)-C(242)-C(243)	-4.0	Th(2B)-S(8B)-C(263)-C(264)	109.6
C(241)-C(242)-C(243)-C(244)	1.9	C(268)-C(263)-C(264)-C(265)	4.5
C(240)-N(4B)-C(244)-C(243)	-3.8	S(8B)-C(263)-C(264)-C(265)	-178.2
Th(1B)-N(4B)-C(244)-C(243)	168.1	C(263)-C(264)-C(265)-C(266)	-1.3
C(242)-C(243)-C(244)-N(4B)	2.2	C(264)-C(265)-C(266)-C(267)	-3.4
Th(2B)-S(5B)-C(245)-C(250)	54.3	C(265)-C(266)-C(267)-C(268)	5.2
Th(2B)-S(5B)-C(245)-C(246)	-133.9	C(266)-C(267)-C(268)-C(263)	-2.0
C(250)-C(245)-C(246)-C(247)	-0.9	C(264)-C(263)-C(268)-C(267)	-2.9
S(5B)-C(245)-C(246)-C(247)	-173.1	S(8B)-C(263)-C(268)-C(267)	179.9

C(273)-N(5B)-C(269)-C(270)	4.1	Th(2B)-N(7B)-C(283)-C(284)	0.1
Th(2B)-N(5B)-C(269)-C(270)	175.7	C(288)-N(8B)-C(284)-C(285)	0.1
N(5B)-C(269)-C(270)-C(271)	-3.0	Th(2B)-N(8B)-C(284)-C(285)	-170.5
C(269)-C(270)-C(271)-C(272)	-1.2	C(288)-N(8B)-C(284)-C(283)	-177.0
C(270)-C(271)-C(272)-C(273)	4.1	Th(2B)-N(8B)-C(284)-C(283)	12.4
C(269)-N(5B)-C(273)-C(272)	-1.1	C(282)-C(283)-C(284)-N(8B)	170.4
Th(2B)-N(5B)-C(273)-C(272)	-172.4	N(7B)-C(283)-C(284)-N(8B)	-8.0
C(269)-N(5B)-C(273)-C(274)	-178.3	C(282)-C(283)-C(284)-C(285)	-6.7
Th(2B)-N(5B)-C(273)-C(274)	10.4	N(7B)-C(283)-C(284)-C(285)	174.9
C(271)-C(272)-C(273)-N(5B)	-2.9	N(8B)-C(284)-C(285)-C(286)	-1.2
C(271)-C(272)-C(273)-C(274)	174.0	C(283)-C(284)-C(285)-C(286)	175.8
C(278)-N(6B)-C(274)-C(275)	-4.3	C(284)-C(285)-C(286)-C(287)	-1.4
Th(2B)-N(6B)-C(274)-C(275)	-175.7	C(285)-C(286)-C(287)-C(288)	4.8
C(278)-N(6B)-C(274)-C(273)	173.5	C(284)-N(8B)-C(288)-C(287)	3.9
Th(2B)-N(6B)-C(274)-C(273)	2.1	Th(2B)-N(8B)-C(288)-C(287)	174.7
N(5B)-C(273)-C(274)-N(6B)	-7.9	C(286)-C(287)-C(288)-N(8B)	-6.2
C(272)-C(273)-C(274)-N(6B)	175.0	Th(3B)-S(9B)-C(289)-C(294)	-65.9
N(5B)-C(273)-C(274)-C(275)	169.9	Th(3B)-S(9B)-C(289)-C(290)	120.1
C(272)-C(273)-C(274)-C(275)	-7.2	C(294)-C(289)-C(290)-C(291)	-5.0
N(6B)-C(274)-C(275)-C(276)	-0.1	S(9B)-C(289)-C(290)-C(291)	169.3
C(273)-C(274)-C(275)-C(276)	-177.8	C(289)-C(290)-C(291)-C(292)	0.2
C(274)-C(275)-C(276)-C(277)	3.9	C(290)-C(291)-C(292)-C(293)	3.7
C(275)-C(276)-C(277)-C(278)	-3.2	C(291)-C(292)-C(293)-C(294)	-2.9
C(276)-C(277)-C(278)-N(6B)	-1.2	C(292)-C(293)-C(294)-C(289)	-2.0
C(274)-N(6B)-C(278)-C(277)	5.0	C(290)-C(289)-C(294)-C(293)	5.8
Th(2B)-N(6B)-C(278)-C(277)	176.6	S(9B)-C(289)-C(294)-C(293)	-168.3
C(283)-N(7B)-C(279)-C(280)	2.3	Th(3B)-S(10B)-C(295)-C(296)	120.1
Th(2B)-N(7B)-C(279)-C(280)	177.9	Th(3B)-S(10B)-C(295)-C(300)	-64.1
N(7B)-C(279)-C(280)-C(281)	-2.9	C(300)-C(295)-C(296)-C(297)	-5.4
C(279)-C(280)-C(281)-C(282)	4.0	S(10B)-C(295)-C(296)-C(297)	170.5
C(280)-C(281)-C(282)-C(283)	-4.9	C(295)-C(296)-C(297)-C(298)	4.3
C(281)-C(282)-C(283)-N(7B)	4.6	C(296)-C(297)-C(298)-C(299)	-2.0
C(281)-C(282)-C(283)-C(284)	-173.7	C(297)-C(298)-C(299)-C(300)	1.2
C(279)-N(7B)-C(283)-C(282)	-3.0	C(298)-C(299)-C(300)-C(295)	-2.2
Th(2B)-N(7B)-C(283)-C(282)	-178.4	C(296)-C(295)-C(300)-C(299)	4.1
C(279)-N(7B)-C(283)-C(284)	175.4	S(10B)-C(295)-C(300)-C(299)	-171.8

Th(3B)-S(11B)-C(301)-C(302)	-96.0	N(9B)-C(317)-C(318)-N(10B)	7.0
Th(3B)-S(11B)-C(301)-C(306)	86.1	C(316)-C(317)-C(318)-C(319)	4.8
C(306)-C(301)-C(302)-C(303)	1.1	N(9B)-C(317)-C(318)-C(319)	-169.5
S(11B)-C(301)-C(302)-C(303)	-176.9	N(10B)-C(318)-C(319)-C(320)	3.6
C(301)-C(302)-C(303)-C(304)	3.2	C(317)-C(318)-C(319)-C(320)	180.0
C(302)-C(303)-C(304)-C(305)	-4.7	C(318)-C(319)-C(320)-C(321)	-2.3
C(303)-C(304)-C(305)-C(306)	2.0	C(319)-C(320)-C(321)-C(322)	-1.1
C(304)-C(305)-C(306)-C(301)	2.3	C(318)-N(10B)-C(322)-C(321)	-2.6
C(302)-C(301)-C(306)-C(305)	-3.8	Th(3B)-N(10B)-C(322)-C(321)	177.9
S(11B)-C(301)-C(306)-C(305)	174.2	C(320)-C(321)-C(322)-N(10B)	3.8
Th(3B)-S(12B)-C(307)-C(312)	90.7	C(327)-N(11B)-C(323)-C(324)	0.9
Th(3B)-S(12B)-C(307)-C(308)	-92.0	Th(3B)-N(11B)-C(323)-C(324)	-177.8
C(312)-C(307)-C(308)-C(309)	0.9	N(11B)-C(323)-C(324)-C(325)	2.5
S(12B)-C(307)-C(308)-C(309)	-176.5	C(323)-C(324)-C(325)-C(326)	-3.8
C(307)-C(308)-C(309)-C(310)	-2.6	C(324)-C(325)-C(326)-C(327)	1.9
C(308)-C(309)-C(310)-C(311)	0.1	C(323)-N(11B)-C(327)-C(326)	-3.0
C(309)-C(310)-C(311)-C(312)	3.9	Th(3B)-N(11B)-C(327)-C(326)	175.7
C(308)-C(307)-C(312)-C(311)	3.1	C(323)-N(11B)-C(327)-C(328)	-178.2
S(12B)-C(307)-C(312)-C(311)	-179.4	Th(3B)-N(11B)-C(327)-C(328)	0.4
C(310)-C(311)-C(312)-C(307)	-5.6	C(325)-C(326)-C(327)-N(11B)	1.7
C(317)-N(9B)-C(313)-C(314)	-4.4	C(325)-C(326)-C(327)-C(328)	176.8
Th(3B)-N(9B)-C(313)-C(314)	-175.0	C(332)-N(12B)-C(328)-C(329)	-6.0
N(9B)-C(313)-C(314)-C(315)	2.2	Th(3B)-N(12B)-C(328)-C(329)	164.6
C(313)-C(314)-C(315)-C(316)	1.9	C(332)-N(12B)-C(328)-C(327)	177.9
C(314)-C(315)-C(316)-C(317)	-3.7	Th(3B)-N(12B)-C(328)-C(327)	-11.5
C(315)-C(316)-C(317)-N(9B)	1.6	N(11B)-C(327)-C(328)-C(329)	-168.9
C(315)-C(316)-C(317)-C(318)	-172.3	C(326)-C(327)-C(328)-C(329)	15.7
C(313)-N(9B)-C(317)-C(316)	2.4	N(11B)-C(327)-C(328)-N(12B)	6.9
Th(3B)-N(9B)-C(317)-C(316)	172.5	C(326)-C(327)-C(328)-N(12B)	-168.4
C(313)-N(9B)-C(317)-C(318)	176.8	N(12B)-C(328)-C(329)-C(330)	1.5
Th(3B)-N(9B)-C(317)-C(318)	-13.1	C(327)-C(328)-C(329)-C(330)	177.1
C(322)-N(10B)-C(318)-C(319)	-1.2	C(328)-C(329)-C(330)-C(331)	2.9
Th(3B)-N(10B)-C(318)-C(319)	178.4	C(329)-C(330)-C(331)-C(332)	-2.8
C(322)-N(10B)-C(318)-C(317)	-177.7	C(328)-N(12B)-C(332)-C(331)	6.2
Th(3B)-N(10B)-C(318)-C(317)	1.9	Th(3B)-N(12B)-C(332)-C(331)	-164.8
C(316)-C(317)-C(318)-N(10B)	-178.7	C(330)-C(331)-C(332)-N(12B)	-1.8

Th(4B)-S(13B)-C(333)-C(338)	-55.4	C(353)-C(354)-C(355)-C(356)	-2.0
Th(4B)-S(13B)-C(333)-C(334)	128.0	C(352)-C(351)-C(356)-C(355)	4.0
C(338)-C(333)-C(334)-C(335)	1.5	S(16B)-C(351)-C(356)-C(355)	-172.5
S(13B)-C(333)-C(334)-C(335)	178.3	C(354)-C(355)-C(356)-C(351)	-1.6
C(333)-C(334)-C(335)-C(336)	2.1	C(361)-N(13B)-C(357)-C(358)	-2.6
C(334)-C(335)-C(336)-C(337)	-4.6	Th(4B)-N(13B)-C(357)-C(358)	-177.0
C(335)-C(336)-C(337)-C(338)	3.6	N(13B)-C(357)-C(358)-C(359)	2.9
C(334)-C(333)-C(338)-C(337)	-2.7	C(357)-C(358)-C(359)-C(360)	0.4
S(13B)-C(333)-C(338)-C(337)	-179.2	C(358)-C(359)-C(360)-C(361)	-3.6
C(336)-C(337)-C(338)-C(333)	0.1	C(357)-N(13B)-C(361)-C(360)	-0.7
Th(4B)-S(14B)-C(339)-C(344)	-59.4	Th(4B)-N(13B)-C(361)-C(360)	173.5
Th(4B)-S(14B)-C(339)-C(340)	129.5	C(357)-N(13B)-C(361)-C(362)	172.8
C(344)-C(339)-C(340)-C(341)	-4.2	Th(4B)-N(13B)-C(361)-C(362)	-12.9
S(14B)-C(339)-C(340)-C(341)	167.8	C(359)-C(360)-C(361)-N(13B)	3.9
C(339)-C(340)-C(341)-C(342)	1.6	C(359)-C(360)-C(361)-C(362)	-169.3
C(340)-C(341)-C(342)-C(343)	2.0	C(366)-N(14B)-C(362)-C(363)	1.8
C(341)-C(342)-C(343)-C(344)	-2.9	Th(4B)-N(14B)-C(362)-C(363)	174.9
C(342)-C(343)-C(344)-C(339)	0.1	C(366)-N(14B)-C(362)-C(361)	-176.7
C(340)-C(339)-C(344)-C(343)	3.3	Th(4B)-N(14B)-C(362)-C(361)	-3.6
S(14B)-C(339)-C(344)-C(343)	-168.1	N(13B)-C(361)-C(362)-N(14B)	10.5
Th(4B)-S(15B)-C(345)-C(346)	-109.2	C(360)-C(361)-C(362)-N(14B)	-176.0
Th(4B)-S(15B)-C(345)-C(350)	75.9	N(13B)-C(361)-C(362)-C(363)	-168.0
C(350)-C(345)-C(346)-C(347)	3.7	C(360)-C(361)-C(362)-C(363)	5.5
S(15B)-C(345)-C(346)-C(347)	-171.3	N(14B)-C(362)-C(363)-C(364)	3.4
C(345)-C(346)-C(347)-C(348)	1.2	C(361)-C(362)-C(363)-C(364)	-178.2
C(346)-C(347)-C(348)-C(349)	-4.7	C(362)-C(363)-C(364)-C(365)	-5.5
C(347)-C(348)-C(349)-C(350)	3.1	C(363)-C(364)-C(365)-C(366)	2.6
C(346)-C(345)-C(350)-C(349)	-5.3	C(362)-N(14B)-C(366)-C(365)	-5.0
S(15B)-C(345)-C(350)-C(349)	169.7	Th(4B)-N(14B)-C(366)-C(365)	-178.3
C(348)-C(349)-C(350)-C(345)	2.1	C(364)-C(365)-C(366)-N(14B)	2.8
Th(4B)-S(16B)-C(351)-C(356)	74.4	C(371)-N(15B)-C(367)-C(368)	2.8
Th(4B)-S(16B)-C(351)-C(352)	-102.2	Th(4B)-N(15B)-C(367)-C(368)	179.9
C(356)-C(351)-C(352)-C(353)	-2.9	N(15B)-C(367)-C(368)-C(369)	1.4
S(16B)-C(351)-C(352)-C(353)	173.6	C(367)-C(368)-C(369)-C(370)	-4.0
C(351)-C(352)-C(353)-C(354)	-0.6	C(368)-C(369)-C(370)-C(371)	2.3
C(352)-C(353)-C(354)-C(355)	3.0	C(367)-N(15B)-C(371)-C(370)	-4.7

Th(4B)-N(15B)-C(371)-C(370)	178.2
C(367)-N(15B)-C(371)-C(372)	-176.2
Th(4B)-N(15B)-C(371)-C(372)	6.8
C(369)-C(370)-C(371)-N(15B)	2.3
C(369)-C(370)-C(371)-C(372)	173.3
C(376)-N(16B)-C(372)-C(373)	-3.5
Th(4B)-N(16B)-C(372)-C(373)	171.1
C(376)-N(16B)-C(372)-C(371)	179.2
Th(4B)-N(16B)-C(372)-C(371)	-6.1
N(15B)-C(371)-C(372)-N(16B)	-0.5
C(370)-C(371)-C(372)-N(16B)	-171.8
N(15B)-C(371)-C(372)-C(373)	-177.7
C(370)-C(371)-C(372)-C(373)	11.0
N(16B)-C(372)-C(373)-C(374)	-1.9
C(371)-C(372)-C(373)-C(374)	175.2
C(372)-C(373)-C(374)-C(375)	4.9
C(373)-C(374)-C(375)-C(376)	-2.5
C(372)-N(16B)-C(376)-C(375)	6.3
Th(4B)-N(16B)-C(376)-C(375)	-168.5
C(374)-C(375)-C(376)-N(16B)	-3.4

Table S8. Hydrogen bonds [Å and °] for **1**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6)...S(4)	0.95	2.89	3.574(14)	129.5
C(25)-H(25)...S(2)	0.95	2.86	3.621(5)	138.0
C(33)-H(33)...S(5)	0.95	2.92	3.783(7)	151.7
C(34)-H(34)...S(4)	0.95	2.71	3.163(12)	109.9
C(35)-H(35)...S(3)	0.95	2.74	3.235(11)	113.1
C(36)-H(36)...S(6)	0.95	2.95	3.809(7)	151.4
C(44)-H(44)...S(1)	0.95	2.84	3.611(5)	138.5
C(50)-H(50)...S(8)	0.95	2.97	3.561(15)	121.3
C(56)-H(56)...S(7)	0.95	2.91	3.553(14)	126.3
C(69)-H(69)...S(6)	0.95	2.92	3.659(5)	136.0
C(77)-H(77)...S(1)#1	0.95	2.93	3.795(6)	152.6
C(78)-H(78)...S(8)	0.95	2.76	3.237(12)	111.7
C(79)-H(79)...S(7)	0.95	2.73	3.223(12)	112.8
C(80)-H(80)...S(2)#1	0.95	2.86	3.751(6)	157.0
C(88)-H(88)...S(5)	0.95	2.82	3.585(5)	137.9
C(100)-H(100)...S(11)	0.95	2.87	3.579(14)	132.4
C(113)-H(113)...S(10)	0.95	2.90	3.661(5)	137.9
C(121)-H(121)...S(13)#2	0.95	2.90	3.787(6)	155.6
C(122)-H(122)...S(12)	0.95	2.75	3.202(12)	110.3
C(123)-H(123)...S(11)	0.95	2.72	3.239(12)	115.0
C(124)-H(124)...S(14)#2	0.95	2.87	3.756(6)	156.0
C(132)-H(132)...S(9)	0.95	2.89	3.648(5)	137.9
C(138)-H(138)...S(16)	0.95	2.94	3.649(13)	132.8
C(144)-H(144)...S(15)	0.95	2.98	3.543(15)	119.4
C(157)-H(157)...S(14)	0.95	2.85	3.611(5)	137.7
C(165)-H(165)...S(9)	0.95	2.82	3.720(6)	157.6
C(166)-H(166)...S(16)	0.95	2.76	3.261(12)	114.1
C(167)-H(167)...S(15)	0.95	2.72	3.204(13)	112.5
C(168)-H(168)...S(10)	0.95	2.92	3.799(6)	153.6
C(176)-H(176)...S(13)	0.95	2.90	3.644(5)	136.5

Symmetry transformations used to generate equivalent atoms: #1 x+1/2,y+1/2,z #2 x-1

Table S9. Crystal data and structure refinement for **2**.

Identification code	ThSePh4bipy2_P21c	
Empirical formula	C49 H41 N5 Se4 Th	
Formula weight	1247.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 20.895(2) Å	α= 90°.
	b = 9.4734(11) Å	β= 100.9157(14)°.
	c = 22.815(3) Å	γ = 90°.
Volume	4434.5(9) $Å^3$	
Z	4	
Density (calculated)	1.869 Mg/m^3	
Absorption coefficient	6.686 mm^{-1}	
F(000)	2384	
Crystal size	0.350 x 0.060 x 0.050 mm^3	
Theta range for data collection	1.818 to 27.482°.	
Index ranges	-27<=h<=26, -12<=k<=12, -29<=l<=29	
Reflections collected	38078	
Independent reflections	10171 [R(int) = 0.0586]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2636 and 0.1461	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10171 / 0 / 520	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0879	
R indices (all data)	R1 = 0.0572, wR2 = 0.0952	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.415 and -1.591 $e.Å^{-3}$	

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	-2169(1)	3544(1)	-2094(1)	20(1)
Se(1)	-1164(1)	1303(1)	-2014(1)	25(1)
Se(2)	-2945(1)	5476(1)	-1486(1)	25(1)
Se(3)	-3210(1)	2720(1)	-3101(1)	29(1)
Se(4)	-1656(1)	3083(1)	-3228(1)	27(1)
N(1)	-2671(2)	1597(5)	-1495(2)	24(1)
N(2)	-1703(2)	3275(5)	-934(2)	22(1)
N(3)	-2405(2)	6040(5)	-2592(2)	25(1)
N(4)	-1189(2)	5291(5)	-2056(2)	22(1)
C(1)	-1100(3)	3(6)	-1359(2)	25(1)
C(2)	-508(3)	-85(7)	-948(3)	30(1)
C(3)	-412(3)	-1104(7)	-518(3)	36(2)
C(4)	-903(3)	-2051(7)	-472(3)	37(2)
C(5)	-1499(3)	-1966(7)	-870(3)	35(2)
C(6)	-1585(3)	-960(7)	-1309(3)	28(1)
C(7)	-3081(3)	4654(7)	-751(3)	30(1)
C(8)	-2699(3)	5092(8)	-212(3)	37(2)
C(9)	-2787(4)	4507(9)	320(3)	49(2)
C(10)	-3261(4)	3500(9)	322(3)	51(2)
C(11)	-3656(4)	3083(8)	-210(3)	44(2)
C(12)	-3565(3)	3679(7)	-741(3)	37(2)
C(13)	-4088(3)	2503(6)	-2957(2)	26(1)
C(14)	-4336(3)	3230(7)	-2527(3)	34(2)
C(15)	-4974(3)	3018(8)	-2462(3)	37(2)
C(16)	-5373(3)	2105(7)	-2835(3)	41(2)
C(17)	-5140(3)	1427(8)	-3278(4)	50(2)
C(18)	-4496(3)	1611(7)	-3342(3)	44(2)
C(19)	-1636(3)	4877(7)	-3606(2)	27(1)
C(20)	-2199(3)	5496(7)	-3934(2)	30(1)
C(21)	-2176(3)	6778(7)	-4206(3)	36(2)
C(22)	-1593(3)	7510(8)	-4156(3)	37(2)

C(23)	-1031(3)	6920(7)	-3835(3)	36(2)
C(24)	-1045(3)	5619(7)	-3563(3)	32(1)
C(25)	-2450(3)	1352(6)	-902(3)	27(1)
C(26)	-3163(3)	779(7)	-1773(3)	32(1)
C(27)	-3454(3)	-252(8)	-1483(3)	42(2)
C(28)	-3232(3)	-466(8)	-891(3)	49(2)
C(29)	-2733(3)	353(7)	-597(3)	37(2)
C(30)	-1905(3)	2248(6)	-603(2)	24(1)
C(31)	-1236(3)	4151(7)	-657(3)	28(1)
C(32)	-940(3)	4029(7)	-61(3)	34(1)
C(33)	-1132(3)	2929(8)	260(3)	37(2)
C(34)	-1622(3)	2047(7)	-6(2)	30(1)
C(35)	-1936(3)	7026(6)	-2574(2)	23(1)
C(36)	-3016(3)	6390(7)	-2849(3)	31(1)
C(37)	-3184(3)	7715(8)	-3085(3)	40(2)
C(38)	-2703(3)	8721(7)	-3056(3)	35(2)
C(39)	-2065(3)	8363(6)	-2805(3)	29(1)
C(40)	-1262(3)	6611(6)	-2292(2)	20(1)
C(41)	-573(3)	4865(6)	-1832(2)	26(1)
C(42)	-29(3)	5669(7)	-1824(3)	30(1)
C(43)	-113(3)	7042(7)	-2045(3)	29(1)
C(44)	-733(3)	7492(7)	-2278(3)	29(1)
N(5)	-3892(3)	-1471(10)	292(3)	106(3)
C(45)	-4184(3)	-2780(8)	322(3)	88(3)
C(46)	-4651(3)	-2958(6)	677(3)	87(4)
C(47)	-4826(3)	-1825(9)	1000(3)	82(3)
C(48)	-4534(4)	-516(7)	970(3)	87(3)
C(49)	-4067(4)	-338(7)	616(4)	103(4)

Table S11. Bond lengths [Å] and angles [°] for **2**.

Th(1)-N(4)	2.620(4)	C(8)-H(8)	0.9500
Th(1)-N(3)	2.629(5)	C(9)-C(10)	1.376(11)
Th(1)-N(1)	2.630(5)	C(9)-H(9)	0.9500
Th(1)-N(2)	2.653(4)	C(10)-C(11)	1.388(10)
Th(1)-Se(3)	2.9544(6)	C(10)-H(10)	0.9500
Th(1)-Se(2)	2.9575(6)	C(11)-C(12)	1.383(9)
Th(1)-Se(1)	2.9676(6)	C(11)-H(11)	0.9500
Th(1)-Se(4)	3.0154(6)	C(12)-H(12)	0.9500
Se(1)-C(1)	1.922(6)	C(13)-C(14)	1.377(8)
Se(2)-C(7)	1.919(6)	C(13)-C(18)	1.389(8)
Se(3)-C(13)	1.935(5)	C(14)-C(15)	1.384(8)
Se(4)-C(19)	1.910(6)	C(14)-H(14)	0.9500
N(1)-C(26)	1.347(7)	C(15)-C(16)	1.377(9)
N(1)-C(25)	1.364(7)	C(15)-H(15)	0.9500
N(2)-C(31)	1.345(7)	C(16)-C(17)	1.364(10)
N(2)-C(30)	1.347(7)	C(16)-H(16)	0.9500
N(3)-C(36)	1.341(7)	C(17)-C(18)	1.392(9)
N(3)-C(35)	1.350(7)	C(17)-H(17)	0.9500
N(4)-C(41)	1.354(7)	C(18)-H(18)	0.9500
N(4)-C(40)	1.359(7)	C(19)-C(20)	1.398(8)
C(1)-C(6)	1.384(8)	C(19)-C(24)	1.409(8)
C(1)-C(2)	1.406(8)	C(20)-C(21)	1.368(9)
C(2)-C(3)	1.364(9)	C(20)-H(20)	0.9500
C(2)-H(2)	0.9500	C(21)-C(22)	1.387(9)
C(3)-C(4)	1.382(9)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(23)	1.380(9)
C(4)-C(5)	1.398(8)	C(22)-H(22)	0.9500
C(4)-H(4)	0.9500	C(23)-C(24)	1.383(9)
C(5)-C(6)	1.370(8)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(24)-H(24)	0.9500
C(6)-H(6)	0.9500	C(25)-C(29)	1.373(8)
C(7)-C(12)	1.372(9)	C(25)-C(30)	1.480(8)
C(7)-C(8)	1.397(8)	C(26)-C(27)	1.383(8)
C(8)-C(9)	1.377(9)	C(26)-H(26)	0.9500

C(27)-C(28)	1.357(9)	C(39)-H(39)	0.9500
C(27)-H(27)	0.9500	C(40)-C(44)	1.381(8)
C(28)-C(29)	1.369(9)	C(41)-C(42)	1.366(8)
C(28)-H(28)	0.9500	C(41)-H(41)	0.9500
C(29)-H(29)	0.9500	C(42)-C(43)	1.394(9)
C(30)-C(34)	1.392(8)	C(42)-H(42)	0.9500
C(31)-C(32)	1.389(8)	C(43)-C(44)	1.371(8)
C(31)-H(31)	0.9500	C(43)-H(43)	0.9500
C(32)-C(33)	1.378(9)	C(44)-H(44)	0.9500
C(32)-H(32)	0.9500	N(5)-C(45)	1.3900
C(33)-C(34)	1.370(9)	N(5)-C(49)	1.3900
C(33)-H(33)	0.9500	C(45)-C(46)	1.3900
C(34)-H(34)	0.9500	C(45)-H(45)	0.9500
C(35)-C(39)	1.379(8)	C(46)-C(47)	1.3900
C(35)-C(40)	1.486(7)	C(46)-H(46)	0.9500
C(36)-C(37)	1.384(9)	C(47)-C(48)	1.3900
C(36)-H(36)	0.9500	C(47)-H(47)	0.9500
C(37)-C(38)	1.377(10)	C(48)-C(49)	1.3900
C(37)-H(37)	0.9500	C(48)-H(48)	0.9500
C(38)-C(39)	1.390(8)	C(49)-H(49)	0.9500
C(38)-H(38)	0.9500		

N(4)-Th(1)-N(3)	61.84(14)	Se(3)-Th(1)-Se(2)	98.030(18)
N(4)-Th(1)-N(1)	144.25(13)	N(4)-Th(1)-Se(1)	84.89(10)
N(3)-Th(1)-N(1)	142.67(14)	N(3)-Th(1)-Se(1)	137.95(10)
N(4)-Th(1)-N(2)	83.76(14)	N(1)-Th(1)-Se(1)	79.22(10)
N(3)-Th(1)-N(2)	121.44(14)	N(2)-Th(1)-Se(1)	75.43(10)
N(1)-Th(1)-N(2)	61.37(14)	Se(3)-Th(1)-Se(1)	105.466(19)
N(4)-Th(1)-Se(3)	130.40(10)	Se(2)-Th(1)-Se(1)	149.119(17)
N(3)-Th(1)-Se(3)	81.42(10)	N(4)-Th(1)-Se(4)	73.61(10)
N(1)-Th(1)-Se(3)	84.93(10)	N(3)-Th(1)-Se(4)	80.04(10)
N(2)-Th(1)-Se(3)	145.80(10)	N(1)-Th(1)-Se(4)	125.87(10)
N(4)-Th(1)-Se(2)	95.03(10)	N(2)-Th(1)-Se(4)	136.02(9)
N(3)-Th(1)-Se(2)	64.66(10)	Se(3)-Th(1)-Se(4)	67.846(18)
N(1)-Th(1)-Se(2)	83.26(10)	Se(2)-Th(1)-Se(4)	143.849(18)
N(2)-Th(1)-Se(2)	73.88(10)	Se(1)-Th(1)-Se(4)	65.575(17)

C(1)-Se(1)-Th(1)	116.79(16)	C(8)-C(7)-Se(2)	119.6(5)
C(7)-Se(2)-Th(1)	110.12(18)	C(9)-C(8)-C(7)	120.5(7)
C(13)-Se(3)-Th(1)	118.57(17)	C(9)-C(8)-H(8)	119.8
C(19)-Se(4)-Th(1)	107.47(16)	C(7)-C(8)-H(8)	119.8
C(26)-N(1)-C(25)	117.0(5)	C(10)-C(9)-C(8)	119.8(7)
C(26)-N(1)-Th(1)	120.2(4)	C(10)-C(9)-H(9)	120.1
C(25)-N(1)-Th(1)	122.8(4)	C(8)-C(9)-H(9)	120.1
C(31)-N(2)-C(30)	117.3(5)	C(9)-C(10)-C(11)	120.3(6)
C(31)-N(2)-Th(1)	120.3(4)	C(9)-C(10)-H(10)	119.9
C(30)-N(2)-Th(1)	122.4(4)	C(11)-C(10)-H(10)	119.9
C(36)-N(3)-C(35)	117.9(5)	C(12)-C(11)-C(10)	119.5(7)
C(36)-N(3)-Th(1)	119.8(4)	C(12)-C(11)-H(11)	120.3
C(35)-N(3)-Th(1)	122.2(4)	C(10)-C(11)-H(11)	120.3
C(41)-N(4)-C(40)	116.8(5)	C(7)-C(12)-C(11)	120.9(6)
C(41)-N(4)-Th(1)	120.4(4)	C(7)-C(12)-H(12)	119.6
C(40)-N(4)-Th(1)	122.7(3)	C(11)-C(12)-H(12)	119.6
C(6)-C(1)-C(2)	118.2(5)	C(14)-C(13)-C(18)	119.1(6)
C(6)-C(1)-Se(1)	122.7(4)	C(14)-C(13)-Se(3)	124.4(4)
C(2)-C(1)-Se(1)	118.7(4)	C(18)-C(13)-Se(3)	116.5(5)
C(3)-C(2)-C(1)	120.8(6)	C(13)-C(14)-C(15)	120.2(6)
C(3)-C(2)-H(2)	119.6	C(13)-C(14)-H(14)	119.9
C(1)-C(2)-H(2)	119.6	C(15)-C(14)-H(14)	119.9
C(2)-C(3)-C(4)	120.2(6)	C(16)-C(15)-C(14)	120.6(6)
C(2)-C(3)-H(3)	119.9	C(16)-C(15)-H(15)	119.7
C(4)-C(3)-H(3)	119.9	C(14)-C(15)-H(15)	119.7
C(3)-C(4)-C(5)	119.8(6)	C(17)-C(16)-C(15)	119.5(6)
C(3)-C(4)-H(4)	120.1	C(17)-C(16)-H(16)	120.2
C(5)-C(4)-H(4)	120.1	C(15)-C(16)-H(16)	120.2
C(6)-C(5)-C(4)	119.6(6)	C(16)-C(17)-C(18)	120.5(7)
C(6)-C(5)-H(5)	120.2	C(16)-C(17)-H(17)	119.7
C(4)-C(5)-H(5)	120.2	C(18)-C(17)-H(17)	119.7
C(5)-C(6)-C(1)	121.4(5)	C(13)-C(18)-C(17)	120.0(7)
C(5)-C(6)-H(6)	119.3	C(13)-C(18)-H(18)	120.0
C(1)-C(6)-H(6)	119.3	C(17)-C(18)-H(18)	120.0
C(12)-C(7)-C(8)	119.0(6)	C(20)-C(19)-C(24)	117.8(6)
C(12)-C(7)-Se(2)	121.3(5)	C(20)-C(19)-Se(4)	121.8(4)

C(24)-C(19)-Se(4)	120.4(4)	C(32)-C(31)-H(31)	118.1
C(21)-C(20)-C(19)	121.2(6)	C(33)-C(32)-C(31)	117.7(6)
C(21)-C(20)-H(20)	119.4	C(33)-C(32)-H(32)	121.2
C(19)-C(20)-H(20)	119.4	C(31)-C(32)-H(32)	121.2
C(20)-C(21)-C(22)	120.7(6)	C(34)-C(33)-C(32)	119.6(6)
C(20)-C(21)-H(21)	119.6	C(34)-C(33)-H(33)	120.2
C(22)-C(21)-H(21)	119.6	C(32)-C(33)-H(33)	120.2
C(23)-C(22)-C(21)	119.2(7)	C(33)-C(34)-C(30)	119.6(6)
C(23)-C(22)-H(22)	120.4	C(33)-C(34)-H(34)	120.2
C(21)-C(22)-H(22)	120.4	C(30)-C(34)-H(34)	120.2
C(22)-C(23)-C(24)	120.7(6)	N(3)-C(35)-C(39)	122.4(5)
C(22)-C(23)-H(23)	119.6	N(3)-C(35)-C(40)	117.0(5)
C(24)-C(23)-H(23)	119.6	C(39)-C(35)-C(40)	120.7(5)
C(23)-C(24)-C(19)	120.4(6)	N(3)-C(36)-C(37)	123.0(6)
C(23)-C(24)-H(24)	119.8	N(3)-C(36)-H(36)	118.5
C(19)-C(24)-H(24)	119.8	C(37)-C(36)-H(36)	118.5
N(1)-C(25)-C(29)	121.5(6)	C(38)-C(37)-C(36)	118.7(6)
N(1)-C(25)-C(30)	116.5(5)	C(38)-C(37)-H(37)	120.7
C(29)-C(25)-C(30)	122.0(5)	C(36)-C(37)-H(37)	120.7
N(1)-C(26)-C(27)	123.1(6)	C(37)-C(38)-C(39)	119.0(6)
N(1)-C(26)-H(26)	118.4	C(37)-C(38)-H(38)	120.5
C(27)-C(26)-H(26)	118.4	C(39)-C(38)-H(38)	120.5
C(28)-C(27)-C(26)	118.9(6)	C(35)-C(39)-C(38)	119.0(6)
C(28)-C(27)-H(27)	120.5	C(35)-C(39)-H(39)	120.5
C(26)-C(27)-H(27)	120.5	C(38)-C(39)-H(39)	120.5
C(27)-C(28)-C(29)	119.2(6)	N(4)-C(40)-C(44)	121.3(5)
C(27)-C(28)-H(28)	120.4	N(4)-C(40)-C(35)	116.2(5)
C(29)-C(28)-H(28)	120.4	C(44)-C(40)-C(35)	122.6(5)
C(28)-C(29)-C(25)	120.2(6)	N(4)-C(41)-C(42)	124.7(6)
C(28)-C(29)-H(29)	119.9	N(4)-C(41)-H(41)	117.6
C(25)-C(29)-H(29)	119.9	C(42)-C(41)-H(41)	117.6
N(2)-C(30)-C(34)	121.9(5)	C(41)-C(42)-C(43)	117.8(5)
N(2)-C(30)-C(25)	116.8(5)	C(41)-C(42)-H(42)	121.1
C(34)-C(30)-C(25)	121.3(5)	C(43)-C(42)-H(42)	121.1
N(2)-C(31)-C(32)	123.9(6)	C(44)-C(43)-C(42)	118.4(5)
N(2)-C(31)-H(31)	118.1	C(44)-C(43)-H(43)	120.8

C(42)-C(43)-H(43)	120.8	C(47)-C(46)-H(46)	120.0
C(43)-C(44)-C(40)	120.9(6)	C(48)-C(47)-C(46)	120.0
C(43)-C(44)-H(44)	119.5	C(48)-C(47)-H(47)	120.0
C(40)-C(44)-H(44)	119.5	C(46)-C(47)-H(47)	120.0
C(45)-N(5)-C(49)	120.0	C(49)-C(48)-C(47)	120.0
C(46)-C(45)-N(5)	120.0	C(49)-C(48)-H(48)	120.0
C(46)-C(45)-H(45)	120.0	C(47)-C(48)-H(48)	120.0
N(5)-C(45)-H(45)	120.0	C(48)-C(49)-N(5)	120.0
C(45)-C(46)-C(47)	120.0	C(48)-C(49)-H(49)	120.0
C(45)-C(46)-H(46)	120.0	N(5)-C(49)-H(49)	120.0

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	12(1)	31(1)	16(1)	0(1)	3(1)	-1(1)
Se(1)	19(1)	33(1)	23(1)	-1(1)	8(1)	1(1)
Se(2)	17(1)	40(1)	18(1)	1(1)	4(1)	6(1)
Se(3)	19(1)	48(1)	19(1)	-2(1)	2(1)	-7(1)
Se(4)	20(1)	42(1)	20(1)	-3(1)	7(1)	-3(1)
N(1)	14(2)	35(3)	24(2)	-1(2)	3(2)	-2(2)
N(2)	17(2)	30(3)	20(2)	3(2)	7(2)	4(2)
N(3)	17(2)	37(3)	20(2)	0(2)	5(2)	0(2)
N(4)	18(2)	28(3)	20(2)	-3(2)	2(2)	0(2)
C(1)	23(3)	35(3)	18(3)	-4(2)	6(2)	2(2)
C(2)	21(3)	40(4)	29(3)	-3(3)	4(2)	3(3)
C(3)	27(3)	45(4)	34(4)	-6(3)	-3(3)	6(3)
C(4)	43(4)	47(4)	19(3)	5(3)	2(3)	6(3)
C(5)	35(4)	44(4)	27(3)	-3(3)	11(3)	1(3)
C(6)	19(3)	41(4)	22(3)	-2(3)	0(2)	1(3)
C(7)	21(3)	45(4)	23(3)	4(3)	7(2)	10(3)
C(8)	23(3)	63(5)	24(3)	1(3)	5(3)	7(3)
C(9)	42(4)	85(6)	19(3)	1(3)	6(3)	17(4)
C(10)	52(5)	79(6)	27(4)	17(4)	18(3)	17(4)
C(11)	52(4)	54(5)	33(4)	9(3)	19(3)	1(4)
C(12)	41(4)	47(4)	23(3)	5(3)	8(3)	1(3)
C(13)	17(3)	36(3)	24(3)	7(2)	1(2)	0(2)
C(14)	14(3)	54(4)	32(3)	-5(3)	1(2)	-8(3)
C(15)	21(3)	52(4)	39(4)	0(3)	7(3)	2(3)
C(16)	17(3)	37(4)	66(5)	3(3)	1(3)	-7(3)
C(17)	32(4)	39(4)	77(6)	-14(4)	8(4)	-14(3)
C(18)	25(3)	50(4)	55(4)	-9(4)	1(3)	-12(3)
C(19)	23(3)	44(4)	15(3)	-3(2)	8(2)	0(3)
C(20)	21(3)	54(4)	14(3)	-3(3)	5(2)	-2(3)
C(21)	33(3)	55(4)	20(3)	1(3)	6(3)	4(3)
C(22)	41(4)	50(4)	25(3)	1(3)	16(3)	1(3)

C(23)	29(3)	49(4)	34(4)	-1(3)	13(3)	-3(3)
C(24)	29(3)	48(4)	21(3)	-2(3)	15(3)	-8(3)
C(25)	22(3)	37(3)	24(3)	4(3)	7(2)	4(3)
C(26)	22(3)	41(4)	32(3)	5(3)	4(3)	-5(3)
C(27)	35(4)	54(5)	37(4)	2(3)	7(3)	-19(3)
C(28)	43(4)	64(5)	43(4)	13(4)	13(3)	-22(4)
C(29)	33(3)	50(4)	31(3)	10(3)	14(3)	-6(3)
C(30)	17(3)	32(3)	22(3)	1(2)	6(2)	5(2)
C(31)	25(3)	38(3)	23(3)	-4(3)	9(2)	-3(3)
C(32)	27(3)	47(4)	27(3)	-4(3)	5(3)	-1(3)
C(33)	30(3)	56(4)	22(3)	4(3)	1(3)	2(3)
C(34)	34(3)	41(4)	17(3)	2(3)	7(2)	-1(3)
C(35)	24(3)	31(3)	15(3)	1(2)	5(2)	2(2)
C(36)	21(3)	47(4)	25(3)	4(3)	4(2)	3(3)
C(37)	27(3)	67(5)	29(3)	14(3)	8(3)	17(3)
C(38)	40(4)	37(4)	27(3)	10(3)	5(3)	14(3)
C(39)	29(3)	33(3)	25(3)	0(3)	5(2)	7(3)
C(40)	21(3)	23(3)	18(3)	-2(2)	7(2)	3(2)
C(41)	22(3)	30(3)	27(3)	1(2)	4(2)	3(2)
C(42)	15(3)	39(4)	37(3)	-2(3)	5(2)	0(3)
C(43)	15(3)	41(4)	32(3)	-10(3)	9(2)	-7(2)
C(44)	27(3)	33(3)	30(3)	-1(3)	10(3)	-1(3)
N(5)	116(8)	139(10)	65(6)	18(6)	19(6)	-15(8)
C(45)	57(6)	95(9)	110(9)	-11(7)	9(6)	13(6)
C(46)	42(5)	84(8)	125(10)	26(7)	-9(6)	-24(5)
C(47)	64(6)	126(10)	59(6)	-7(6)	18(5)	-25(7)
C(48)	59(6)	93(8)	101(9)	-22(7)	-10(6)	-4(6)
C(49)	98(10)	116(11)	86(9)	34(8)	-7(7)	-26(8)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **2**.

	x	y	z	U(eq)
H(2)	-170	574	-970	36
H(3)	-6	-1164	-249	44
H(4)	-836	-2756	-170	44
H(5)	-1841	-2603	-837	42
H(6)	-1987	-922	-1586	33
H(8)	-2377	5799	-212	44
H(9)	-2521	4798	685	58
H(10)	-3319	3088	688	62
H(11)	-3986	2395	-208	53
H(12)	-3841	3410	-1104	44
H(14)	-4068	3879	-2274	41
H(15)	-5138	3506	-2158	45
H(16)	-5808	1948	-2783	49
H(17)	-5419	826	-3545	60
H(18)	-4335	1126	-3649	53
H(20)	-2604	5019	-3969	35
H(21)	-2564	7171	-4431	43
H(22)	-1582	8406	-4340	45
H(23)	-630	7414	-3800	43
H(24)	-653	5223	-3346	38
H(26)	-3318	917	-2188	38
H(27)	-3802	-802	-1695	50
H(28)	-3422	-1174	-684	59
H(29)	-2582	228	-181	45
H(31)	-1100	4898	-883	34
H(32)	-616	4681	119	40
H(33)	-926	2781	664	44
H(34)	-1768	1304	216	36
H(36)	-3348	5697	-2871	37
H(37)	-3622	7926	-3263	49

H(38)	-2806	9646	-3205	42
H(39)	-1723	9029	-2794	35
H(41)	-515	3940	-1670	32
H(42)	394	5305	-1672	36
H(43)	250	7651	-2035	34
H(44)	-799	8423	-2433	35
H(45)	-4065	-3554	101	106
H(46)	-4851	-3853	698	104
H(47)	-5145	-1947	1242	99
H(48)	-4654	258	1191	105
H(49)	-3868	557	595	124

Table S14. Torsion angles [°] for **2**.

C(6)-C(1)-C(2)-C(3)	0.9(9)	C(26)-N(1)-C(25)-C(30)	179.3(5)
Se(1)-C(1)-C(2)-C(3)	-172.1(5)	Th(1)-N(1)-C(25)-C(30)	-0.1(7)
C(1)-C(2)-C(3)-C(4)	-1.4(9)	C(25)-N(1)-C(26)-C(27)	1.4(9)
C(2)-C(3)-C(4)-C(5)	0.4(10)	Th(1)-N(1)-C(26)-C(27)	-179.2(5)
C(3)-C(4)-C(5)-C(6)	1.1(10)	N(1)-C(26)-C(27)-C(28)	-0.6(11)
C(4)-C(5)-C(6)-C(1)	-1.7(9)	C(26)-C(27)-C(28)-C(29)	0.6(12)
C(2)-C(1)-C(6)-C(5)	0.7(9)	C(27)-C(28)-C(29)-C(25)	-1.6(11)
Se(1)-C(1)-C(6)-C(5)	173.4(5)	N(1)-C(25)-C(29)-C(28)	2.5(10)
C(12)-C(7)-C(8)-C(9)	2.9(10)	C(30)-C(25)-C(29)-C(28)	-179.3(6)
Se(2)-C(7)-C(8)-C(9)	-179.5(5)	C(31)-N(2)-C(30)-C(34)	-3.1(8)
C(7)-C(8)-C(9)-C(10)	-1.1(11)	Th(1)-N(2)-C(30)-C(34)	174.9(4)
C(8)-C(9)-C(10)-C(11)	-0.7(11)	C(31)-N(2)-C(30)-C(25)	175.9(5)
C(9)-C(10)-C(11)-C(12)	0.6(11)	Th(1)-N(2)-C(30)-C(25)	-6.1(6)
C(8)-C(7)-C(12)-C(11)	-3.1(10)	N(1)-C(25)-C(30)-N(2)	3.9(8)
Se(2)-C(7)-C(12)-C(11)	179.4(5)	C(29)-C(25)-C(30)-N(2)	-174.4(5)
C(10)-C(11)-C(12)-C(7)	1.3(11)	N(1)-C(25)-C(30)-C(34)	-177.0(5)
C(18)-C(13)-C(14)-C(15)	3.1(10)	C(29)-C(25)-C(30)-C(34)	4.6(9)
Se(3)-C(13)-C(14)-C(15)	179.2(5)	C(30)-N(2)-C(31)-C(32)	2.0(8)
C(13)-C(14)-C(15)-C(16)	-1.5(10)	Th(1)-N(2)-C(31)-C(32)	-176.1(5)
C(14)-C(15)-C(16)-C(17)	-1.3(11)	N(2)-C(31)-C(32)-C(33)	1.1(9)
C(15)-C(16)-C(17)-C(18)	2.5(11)	C(31)-C(32)-C(33)-C(34)	-3.1(10)
C(14)-C(13)-C(18)-C(17)	-2.0(10)	C(32)-C(33)-C(34)-C(30)	2.1(10)
Se(3)-C(13)-C(18)-C(17)	-178.3(6)	N(2)-C(30)-C(34)-C(33)	1.1(9)
C(16)-C(17)-C(18)-C(13)	-0.8(12)	C(25)-C(30)-C(34)-C(33)	-177.8(6)
C(24)-C(19)-C(20)-C(21)	0.2(8)	C(36)-N(3)-C(35)-C(39)	0.4(8)
Se(4)-C(19)-C(20)-C(21)	-179.6(4)	Th(1)-N(3)-C(35)-C(39)	-176.2(4)
C(19)-C(20)-C(21)-C(22)	-0.9(9)	C(36)-N(3)-C(35)-C(40)	-179.6(5)
C(20)-C(21)-C(22)-C(23)	0.9(9)	Th(1)-N(3)-C(35)-C(40)	3.9(6)
C(21)-C(22)-C(23)-C(24)	-0.3(9)	C(35)-N(3)-C(36)-C(37)	-1.1(8)
C(22)-C(23)-C(24)-C(19)	-0.4(9)	Th(1)-N(3)-C(36)-C(37)	175.5(5)
C(20)-C(19)-C(24)-C(23)	0.5(8)	N(3)-C(36)-C(37)-C(38)	0.1(9)
Se(4)-C(19)-C(24)-C(23)	-179.7(5)	C(36)-C(37)-C(38)-C(39)	1.6(9)
C(26)-N(1)-C(25)-C(29)	-2.3(8)	N(3)-C(35)-C(39)-C(38)	1.3(9)
Th(1)-N(1)-C(25)-C(29)	178.3(4)	C(40)-C(35)-C(39)-C(38)	-178.7(5)

C(37)-C(38)-C(39)-C(35)	-2.3(9)	N(4)-C(41)-C(42)-C(43)	1.8(9)
C(41)-N(4)-C(40)-C(44)	-2.9(8)	C(41)-C(42)-C(43)-C(44)	-2.3(8)
Th(1)-N(4)-C(40)-C(44)	-178.2(4)	C(42)-C(43)-C(44)-C(40)	0.3(9)
C(41)-N(4)-C(40)-C(35)	175.7(5)	N(4)-C(40)-C(44)-C(43)	2.4(8)
Th(1)-N(4)-C(40)-C(35)	0.4(6)	C(35)-C(40)-C(44)-C(43)	-176.1(5)
N(3)-C(35)-C(40)-N(4)	-2.7(7)	C(49)-N(5)-C(45)-C(46)	0.0
C(39)-C(35)-C(40)-N(4)	177.3(5)	N(5)-C(45)-C(46)-C(47)	0.0
N(3)-C(35)-C(40)-C(44)	175.9(5)	C(45)-C(46)-C(47)-C(48)	0.0
C(39)-C(35)-C(40)-C(44)	-4.1(8)	C(46)-C(47)-C(48)-C(49)	0.0
C(40)-N(4)-C(41)-C(42)	0.8(8)	C(47)-C(48)-C(49)-N(5)	0.0
Th(1)-N(4)-C(41)-C(42)	176.2(5)	C(45)-N(5)-C(49)-C(48)	0.0

Table S15. Hydrogen bonds [Å and °] for **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(26)-H(26)...Se(3)	0.95	2.74	3.530(6)	141.5
C(36)-H(36)...Se(3)	0.95	2.89	3.534(7)	125.8
C(39)-H(39)...Se(1)#1	0.95	2.89	3.643(6)	136.5
C(41)-H(41)...Se(1)	0.95	2.88	3.591(6)	132.5

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

Table S16. Crystal data and structure refinement for **3**.

Identification code	ThSCF4bp4THF2_C2c	
Empirical formula	C52 H32 F20 N4 O2 S4 Th	
Formula weight	1485.09	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 26.2472(11) Å	α= 90°.
	b = 12.5980(5) Å	β= 114.1892(7)°.
	c = 17.2129(7) Å	γ = 90°.
Volume	5191.9(4) $Å^3$	
Z	4	
Density (calculated)	1.900 Mg/m^3	
Absorption coefficient	3.153 mm^{-1}	
F(000)	2888	
Crystal size	0.270 x 0.110 x 0.040 mm^3	
Theta range for data collection	1.701 to 30.537°.	
Index ranges	-37<=h<=37, -18<=k<=17, -24<=l<=24	
Reflections collected	32094	
Independent reflections	7926 [R(int) = 0.0412]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9025 and 0.6349	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7926 / 250 / 421	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0643	
R indices (all data)	R1 = 0.0350, wR2 = 0.0662	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.788 and -1.047 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	5000	1854(1)	7500	14(1)
S(1)	4155(1)	640(1)	7717(1)	19(1)
S(2)	5393(1)	2840(1)	6343(1)	22(1)
F(1)	4650(1)	-1544(1)	7882(1)	26(1)
F(2)	4271(1)	-3190(1)	6813(1)	32(1)
F(3)	3315(1)	-2999(1)	5364(1)	34(1)
F(4)	2760(1)	-1124(1)	4997(1)	30(1)
F(5)	3122(1)	525(1)	6066(1)	26(1)
F(6)	4752(1)	2022(1)	4562(1)	31(1)
F(7)	3926(1)	3001(2)	3268(1)	48(1)
F(8)	3589(1)	4970(2)	3474(1)	57(1)
F(9)	4087(1)	5968(2)	5008(1)	49(1)
F(10)	4900(1)	5001(1)	6319(1)	35(1)
N(1)	4379(1)	1068(2)	5990(1)	18(1)
N(2)	4129(1)	2967(2)	6508(1)	20(1)
C(1)	3915(1)	-429(2)	7006(2)	19(1)
C(2)	4188(1)	-1406(2)	7168(2)	21(1)
C(3)	3997(1)	-2264(2)	6624(2)	23(1)
C(4)	3514(1)	-2172(2)	5889(2)	24(1)
C(5)	3231(1)	-1220(2)	5711(2)	22(1)
C(6)	3426(1)	-376(2)	6261(2)	20(1)
C(7)	4850(1)	3464(2)	5493(2)	23(1)
C(8)	4598(1)	2996(2)	4699(2)	27(1)
C(9)	4173(1)	3493(3)	4025(2)	35(1)
C(10)	3999(1)	4494(3)	4130(2)	40(1)
C(11)	4249(1)	4988(3)	4904(2)	36(1)
C(12)	4665(1)	4477(2)	5569(2)	29(1)
C(13)	3907(1)	1565(2)	5454(2)	20(1)
C(14)	4527(1)	160(2)	5723(2)	21(1)
C(15)	4226(1)	-276(2)	4928(2)	25(1)
C(16)	3747(1)	239(3)	4385(2)	31(1)

C(17)	3586(1)	1167(3)	4648(2)	28(1)
C(18)	3760(1)	2578(2)	5754(2)	20(1)
C(19)	4021(1)	3924(2)	6760(2)	23(1)
C(20)	3544(1)	4505(2)	6295(2)	28(1)
C(21)	3161(1)	4077(2)	5548(2)	32(1)
C(22)	3266(1)	3112(2)	5271(2)	27(1)
O(1A)	2543(2)	1968(6)	3099(3)	59(2)
C(23A)	2044(4)	2539(10)	2684(5)	74(2)
C(24A)	2015(4)	2871(9)	1840(6)	78(2)
C(25A)	2498(5)	2358(12)	1761(7)	91(3)
C(26A)	2660(3)	1517(6)	2434(5)	49(2)
O(1B)	2459(2)	2459(3)	3260(3)	29(1)
C(23B)	2210(4)	1646(6)	2649(4)	49(2)
C(24B)	2365(5)	1855(7)	1913(6)	73(2)
C(25B)	2511(4)	3017(6)	1997(4)	47(2)
C(26B)	2446(3)	3378(5)	2775(4)	38(1)

Table S18. Bond lengths [Å] and angles [°] for **3**.

Th(1)-N(2)#1	2.628(2)	C(10)-C(11)	1.370(5)
Th(1)-N(2)	2.628(2)	C(11)-C(12)	1.376(4)
Th(1)-N(1)#1	2.631(2)	C(13)-C(17)	1.388(4)
Th(1)-N(1)	2.631(2)	C(13)-C(18)	1.486(4)
Th(1)-S(1)	2.8428(6)	C(14)-C(15)	1.382(3)
Th(1)-S(1)#1	2.8428(6)	C(14)-H(14)	0.9500
Th(1)-S(2)#1	2.8730(6)	C(15)-C(16)	1.383(4)
Th(1)-S(2)	2.8730(6)	C(15)-H(15)	0.9500
S(1)-C(1)	1.754(3)	C(16)-C(17)	1.381(4)
S(2)-C(7)	1.755(3)	C(16)-H(16)	0.9500
F(1)-C(2)	1.339(3)	C(17)-H(17)	0.9500
F(2)-C(3)	1.340(3)	C(18)-C(22)	1.392(4)
F(3)-C(4)	1.337(3)	C(19)-C(20)	1.385(4)
F(4)-C(5)	1.343(3)	C(19)-H(19)	0.9500
F(5)-C(6)	1.348(3)	C(20)-C(21)	1.377(4)
F(6)-C(8)	1.344(3)	C(20)-H(20)	0.9500
F(7)-C(9)	1.345(4)	C(21)-C(22)	1.375(4)
F(8)-C(10)	1.342(3)	C(21)-H(21)	0.9500
F(9)-C(11)	1.341(3)	C(22)-H(22)	0.9500
F(10)-C(12)	1.352(3)	O(1A)-C(23A)	1.406(6)
N(1)-C(14)	1.348(3)	O(1A)-C(26A)	1.419(6)
N(1)-C(13)	1.357(3)	C(23A)-C(24A)	1.484(8)
N(2)-C(19)	1.351(3)	C(23A)-H(23A)	0.9900
N(2)-C(18)	1.354(3)	C(23A)-H(23B)	0.9900
C(1)-C(2)	1.393(4)	C(24A)-C(25A)	1.478(9)
C(1)-C(6)	1.397(3)	C(24A)-H(24A)	0.9900
C(2)-C(3)	1.383(4)	C(24A)-H(24B)	0.9900
C(3)-C(4)	1.379(4)	C(25A)-C(26A)	1.497(8)
C(4)-C(5)	1.379(4)	C(25A)-H(25A)	0.9900
C(5)-C(6)	1.375(4)	C(25A)-H(25B)	0.9900
C(7)-C(8)	1.383(4)	C(26A)-H(26A)	0.9900
C(7)-C(12)	1.391(4)	C(26A)-H(26B)	0.9900
C(8)-C(9)	1.386(4)	O(1B)-C(26B)	1.420(6)
C(9)-C(10)	1.378(5)	O(1B)-C(23B)	1.420(6)

C(23B)-C(24B)	1.504(8)	C(25B)-C(26B)	1.488(7)
C(23B)-H(23C)	0.9900	C(25B)-H(25C)	0.9900
C(23B)-H(23D)	0.9900	C(25B)-H(25D)	0.9900
C(24B)-C(25B)	1.505(9)	C(26B)-H(26C)	0.9900
C(24B)-H(24C)	0.9900	C(26B)-H(26D)	0.9900
C(24B)-H(24D)	0.9900		

N(2)#1-Th(1)-N(2)	115.53(10)	C(7)-S(2)-Th(1)	111.81(9)
N(2)#1-Th(1)-N(1)#1	62.42(7)	C(14)-N(1)-C(13)	118.0(2)
N(2)-Th(1)-N(1)#1	149.80(6)	C(14)-N(1)-Th(1)	120.53(16)
N(2)#1-Th(1)-N(1)	149.80(6)	C(13)-N(1)-Th(1)	121.44(16)
N(2)-Th(1)-N(1)	62.42(7)	C(19)-N(2)-C(18)	117.9(2)
N(1)#1-Th(1)-N(1)	135.80(9)	C(19)-N(2)-Th(1)	120.61(17)
N(2)#1-Th(1)-S(1)	136.03(5)	C(18)-N(2)-Th(1)	121.37(16)
N(2)-Th(1)-S(1)	81.62(5)	C(2)-C(1)-C(6)	115.4(2)
N(1)#1-Th(1)-S(1)	82.45(5)	C(2)-C(1)-S(1)	122.09(19)
N(1)-Th(1)-S(1)	74.12(5)	C(6)-C(1)-S(1)	122.4(2)
N(2)#1-Th(1)-S(1)#1	81.63(5)	F(1)-C(2)-C(3)	117.5(2)
N(2)-Th(1)-S(1)#1	136.03(5)	F(1)-C(2)-C(1)	119.8(2)
N(1)#1-Th(1)-S(1)#1	74.13(5)	C(3)-C(2)-C(1)	122.8(2)
N(1)-Th(1)-S(1)#1	82.45(5)	F(2)-C(3)-C(4)	119.8(2)
S(1)-Th(1)-S(1)#1	114.89(3)	F(2)-C(3)-C(2)	120.4(2)
N(2)#1-Th(1)-S(2)#1	77.46(5)	C(4)-C(3)-C(2)	119.8(3)
N(2)-Th(1)-S(2)#1	75.88(5)	F(3)-C(4)-C(5)	120.1(2)
N(1)#1-Th(1)-S(2)#1	74.36(5)	F(3)-C(4)-C(3)	120.8(3)
N(1)-Th(1)-S(2)#1	126.48(5)	C(5)-C(4)-C(3)	119.1(2)
S(1)-Th(1)-S(2)#1	67.691(18)	F(4)-C(5)-C(6)	120.2(2)
S(1)#1-Th(1)-S(2)#1	147.633(18)	F(4)-C(5)-C(4)	119.5(2)
N(2)#1-Th(1)-S(2)	75.89(5)	C(6)-C(5)-C(4)	120.3(2)
N(2)-Th(1)-S(2)	77.46(5)	F(5)-C(6)-C(5)	117.7(2)
N(1)#1-Th(1)-S(2)	126.49(5)	F(5)-C(6)-C(1)	119.8(2)
N(1)-Th(1)-S(2)	74.37(5)	C(5)-C(6)-C(1)	122.6(2)
S(1)-Th(1)-S(2)	147.633(18)	C(8)-C(7)-C(12)	116.1(3)
S(1)#1-Th(1)-S(2)	67.691(18)	C(8)-C(7)-S(2)	121.9(2)
S(2)#1-Th(1)-S(2)	128.80(3)	C(12)-C(7)-S(2)	121.9(2)
C(1)-S(1)-Th(1)	113.42(8)	F(6)-C(8)-C(7)	120.4(2)

F(6)-C(8)-C(9)	117.6(3)	C(21)-C(20)-H(20)	120.8
C(7)-C(8)-C(9)	122.0(3)	C(19)-C(20)-H(20)	120.8
F(7)-C(9)-C(10)	119.7(3)	C(22)-C(21)-C(20)	119.7(3)
F(7)-C(9)-C(8)	120.4(3)	C(22)-C(21)-H(21)	120.2
C(10)-C(9)-C(8)	119.9(3)	C(20)-C(21)-H(21)	120.2
F(8)-C(10)-C(11)	121.0(3)	C(21)-C(22)-C(18)	119.4(3)
F(8)-C(10)-C(9)	119.6(3)	C(21)-C(22)-H(22)	120.3
C(11)-C(10)-C(9)	119.4(3)	C(18)-C(22)-H(22)	120.3
F(9)-C(11)-C(10)	119.8(3)	C(23A)-O(1A)-C(26A)	105.1(5)
F(9)-C(11)-C(12)	120.4(3)	O(1A)-C(23A)-C(24A)	107.8(5)
C(10)-C(11)-C(12)	119.8(3)	O(1A)-C(23A)-H(23A)	110.2
F(10)-C(12)-C(11)	117.5(3)	C(24A)-C(23A)-H(23A)	110.2
F(10)-C(12)-C(7)	119.8(3)	O(1A)-C(23A)-H(23B)	110.2
C(11)-C(12)-C(7)	122.7(3)	C(24A)-C(23A)-H(23B)	110.2
N(1)-C(13)-C(17)	121.6(2)	H(23A)-C(23A)-H(23B)	108.5
N(1)-C(13)-C(18)	117.1(2)	C(25A)-C(24A)-C(23A)	105.3(5)
C(17)-C(13)-C(18)	121.3(2)	C(25A)-C(24A)-H(24A)	110.7
N(1)-C(14)-C(15)	123.2(2)	C(23A)-C(24A)-H(24A)	110.7
N(1)-C(14)-H(14)	118.4	C(25A)-C(24A)-H(24B)	110.7
C(15)-C(14)-H(14)	118.4	C(23A)-C(24A)-H(24B)	110.7
C(14)-C(15)-C(16)	118.3(3)	H(24A)-C(24A)-H(24B)	108.8
C(14)-C(15)-H(15)	120.8	C(24A)-C(25A)-C(26A)	102.8(5)
C(16)-C(15)-H(15)	120.8	C(24A)-C(25A)-H(25A)	111.2
C(17)-C(16)-C(15)	119.4(3)	C(26A)-C(25A)-H(25A)	111.2
C(17)-C(16)-H(16)	120.3	C(24A)-C(25A)-H(25B)	111.2
C(15)-C(16)-H(16)	120.3	C(26A)-C(25A)-H(25B)	111.2
C(16)-C(17)-C(13)	119.4(2)	H(25A)-C(25A)-H(25B)	109.1
C(16)-C(17)-H(17)	120.3	O(1A)-C(26A)-C(25A)	104.7(6)
C(13)-C(17)-H(17)	120.3	O(1A)-C(26A)-H(26A)	110.8
N(2)-C(18)-C(22)	121.6(2)	C(25A)-C(26A)-H(26A)	110.8
N(2)-C(18)-C(13)	117.2(2)	O(1A)-C(26A)-H(26B)	110.8
C(22)-C(18)-C(13)	121.2(2)	C(25A)-C(26A)-H(26B)	110.8
N(2)-C(19)-C(20)	123.0(3)	H(26A)-C(26A)-H(26B)	108.9
N(2)-C(19)-H(19)	118.5	C(26B)-O(1B)-C(23B)	105.1(5)
C(20)-C(19)-H(19)	118.5	O(1B)-C(23B)-C(24B)	107.2(5)
C(21)-C(20)-C(19)	118.4(3)	O(1B)-C(23B)-H(23C)	110.3

C(24B)-C(23B)-H(23C)	110.3	C(26B)-C(25B)-H(25C)	110.7
O(1B)-C(23B)-H(23D)	110.3	C(24B)-C(25B)-H(25C)	110.7
C(24B)-C(23B)-H(23D)	110.3	C(26B)-C(25B)-H(25D)	110.7
H(23C)-C(23B)-H(23D)	108.5	C(24B)-C(25B)-H(25D)	110.7
C(23B)-C(24B)-C(25B)	103.6(5)	H(25C)-C(25B)-H(25D)	108.8
C(23B)-C(24B)-H(24C)	111.0	O(1B)-C(26B)-C(25B)	107.2(5)
C(25B)-C(24B)-H(24C)	111.0	O(1B)-C(26B)-H(26C)	110.3
C(23B)-C(24B)-H(24D)	111.0	C(25B)-C(26B)-H(26C)	110.3
C(25B)-C(24B)-H(24D)	111.0	O(1B)-C(26B)-H(26D)	110.3
H(24C)-C(24B)-H(24D)	109.0	C(25B)-C(26B)-H(26D)	110.3
C(26B)-C(25B)-C(24B)	105.4(5)	H(26C)-C(26B)-H(26D)	108.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	12(1)	21(1)	9(1)	0	3(1)	0
S(1)	17(1)	26(1)	14(1)	-4(1)	6(1)	-5(1)
S(2)	21(1)	29(1)	16(1)	6(1)	8(1)	2(1)
F(1)	20(1)	34(1)	17(1)	2(1)	2(1)	1(1)
F(2)	32(1)	26(1)	34(1)	-2(1)	9(1)	7(1)
F(3)	28(1)	33(1)	34(1)	-17(1)	6(1)	-3(1)
F(4)	19(1)	39(1)	23(1)	-10(1)	-2(1)	1(1)
F(5)	20(1)	28(1)	24(1)	-4(1)	4(1)	4(1)
F(6)	32(1)	40(1)	20(1)	-1(1)	10(1)	10(1)
F(7)	36(1)	86(2)	18(1)	7(1)	6(1)	21(1)
F(8)	46(1)	87(2)	40(1)	36(1)	20(1)	42(1)
F(9)	62(1)	42(1)	62(1)	24(1)	44(1)	31(1)
F(10)	43(1)	32(1)	36(1)	2(1)	24(1)	3(1)
N(1)	16(1)	27(1)	12(1)	0(1)	6(1)	1(1)
N(2)	17(1)	28(1)	14(1)	1(1)	7(1)	4(1)
C(1)	16(1)	27(1)	15(1)	-2(1)	6(1)	-3(1)
C(2)	16(1)	30(1)	14(1)	0(1)	4(1)	-2(1)
C(3)	23(1)	24(1)	24(1)	-2(1)	11(1)	2(1)
C(4)	22(1)	27(1)	23(1)	-9(1)	8(1)	-4(1)
C(5)	14(1)	34(2)	16(1)	-5(1)	2(1)	-1(1)
C(6)	16(1)	25(1)	19(1)	-3(1)	7(1)	1(1)
C(7)	24(1)	29(1)	21(1)	9(1)	14(1)	7(1)
C(8)	24(1)	38(2)	20(1)	8(1)	11(1)	11(1)
C(9)	28(2)	60(2)	18(1)	12(1)	10(1)	16(1)
C(10)	31(2)	60(2)	32(2)	28(2)	17(1)	25(2)
C(11)	40(2)	38(2)	41(2)	20(1)	29(2)	21(1)
C(12)	35(2)	33(2)	28(1)	9(1)	21(1)	6(1)
C(13)	15(1)	30(1)	13(1)	1(1)	5(1)	3(1)
C(14)	18(1)	30(1)	15(1)	-2(1)	5(1)	2(1)
C(15)	21(1)	36(2)	17(1)	-7(1)	7(1)	1(1)
C(16)	21(1)	53(2)	17(1)	-10(1)	5(1)	4(1)

C(17)	17(1)	47(2)	14(1)	-3(1)	1(1)	9(1)
C(18)	16(1)	29(1)	15(1)	4(1)	6(1)	1(1)
C(19)	21(1)	29(1)	20(1)	1(1)	10(1)	3(1)
C(20)	27(1)	28(1)	31(2)	3(1)	12(1)	8(1)
C(21)	23(1)	36(2)	34(2)	7(1)	7(1)	14(1)
C(22)	19(1)	34(2)	23(1)	1(1)	3(1)	3(1)
O(1A)	44(3)	106(5)	25(3)	15(3)	11(2)	39(3)
C(23A)	61(5)	116(6)	47(4)	6(4)	23(4)	45(5)
C(24A)	66(5)	114(6)	65(5)	51(4)	37(4)	38(4)
C(25A)	82(6)	143(8)	59(5)	40(6)	41(5)	36(6)
C(26A)	48(4)	46(4)	51(4)	-20(3)	20(3)	13(3)
O(1B)	25(2)	39(3)	17(2)	-1(2)	1(2)	5(2)
C(23B)	57(4)	62(4)	30(3)	-13(3)	18(3)	-26(4)
C(24B)	87(5)	84(5)	63(5)	-5(4)	47(4)	-35(4)
C(25B)	50(4)	67(5)	29(3)	11(3)	21(3)	6(4)
C(26B)	47(3)	39(3)	32(3)	10(3)	21(3)	14(3)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **3**.

	x	y	z	U(eq)
H(14)	4854	-198	6099	26
H(15)	4346	-913	4760	30
H(16)	3531	-43	3836	37
H(17)	3258	1530	4281	33
H(19)	4284	4213	7280	27
H(20)	3484	5180	6487	34
H(21)	2825	4448	5226	39
H(22)	3005	2812	4756	32
H(23A)	2039	3169	3025	89
H(23B)	1719	2087	2613	89
H(24A)	1661	2632	1379	94
H(24B)	2040	3653	1811	94
H(25A)	2806	2870	1871	109
H(25B)	2391	2044	1189	109
H(26A)	2439	864	2213	58
H(26B)	3062	1343	2638	58
H(23C)	1799	1657	2455	59
H(23D)	2350	941	2902	59
H(24C)	2048	1704	1363	87
H(24D)	2689	1417	1957	87
H(25C)	2899	3125	2059	57
H(25D)	2255	3413	1491	57
H(26C)	2754	3865	3110	45
H(26D)	2087	3758	2617	45

Table S21. Torsion angles [°] for **3**.

Th(1)-S(1)-C(1)-C(2)	84.6(2)	F(6)-C(8)-C(9)-C(10)	-179.8(3)
Th(1)-S(1)-C(1)-C(6)	-98.5(2)	C(7)-C(8)-C(9)-C(10)	1.5(5)
C(6)-C(1)-C(2)-F(1)	-177.7(2)	F(7)-C(9)-C(10)-F(8)	-0.6(5)
S(1)-C(1)-C(2)-F(1)	-0.6(3)	C(8)-C(9)-C(10)-F(8)	179.9(3)
C(6)-C(1)-C(2)-C(3)	1.4(4)	F(7)-C(9)-C(10)-C(11)	179.4(3)
S(1)-C(1)-C(2)-C(3)	178.5(2)	C(8)-C(9)-C(10)-C(11)	-0.1(5)
F(1)-C(2)-C(3)-F(2)	-0.2(4)	F(8)-C(10)-C(11)-F(9)	-0.9(5)
C(1)-C(2)-C(3)-F(2)	-179.3(2)	C(9)-C(10)-C(11)-F(9)	179.1(3)
F(1)-C(2)-C(3)-C(4)	178.4(2)	F(8)-C(10)-C(11)-C(12)	179.3(3)
C(1)-C(2)-C(3)-C(4)	-0.7(4)	C(9)-C(10)-C(11)-C(12)	-0.7(5)
F(2)-C(3)-C(4)-F(3)	0.3(4)	F(9)-C(11)-C(12)-F(10)	-0.2(4)
C(2)-C(3)-C(4)-F(3)	-178.4(2)	C(10)-C(11)-C(12)-F(10)	179.6(3)
F(2)-C(3)-C(4)-C(5)	178.7(2)	F(9)-C(11)-C(12)-C(7)	-179.7(3)
C(2)-C(3)-C(4)-C(5)	0.1(4)	C(10)-C(11)-C(12)-C(7)	0.1(5)
F(3)-C(4)-C(5)-F(4)	-1.5(4)	C(8)-C(7)-C(12)-F(10)	-178.3(2)
C(3)-C(4)-C(5)-F(4)	-179.9(2)	S(2)-C(7)-C(12)-F(10)	-1.1(4)
F(3)-C(4)-C(5)-C(6)	178.2(2)	C(8)-C(7)-C(12)-C(11)	1.2(4)
C(3)-C(4)-C(5)-C(6)	-0.3(4)	S(2)-C(7)-C(12)-C(11)	178.4(2)
F(4)-C(5)-C(6)-F(5)	1.5(4)	C(14)-N(1)-C(13)-C(17)	-0.9(4)
C(4)-C(5)-C(6)-F(5)	-178.2(2)	Th(1)-N(1)-C(13)-C(17)	178.3(2)
F(4)-C(5)-C(6)-C(1)	-179.3(2)	C(14)-N(1)-C(13)-C(18)	-178.6(2)
C(4)-C(5)-C(6)-C(1)	1.1(4)	Th(1)-N(1)-C(13)-C(18)	0.7(3)
C(2)-C(1)-C(6)-F(5)	177.7(2)	C(13)-N(1)-C(14)-C(15)	1.1(4)
S(1)-C(1)-C(6)-F(5)	0.6(3)	Th(1)-N(1)-C(14)-C(15)	-178.2(2)
C(2)-C(1)-C(6)-C(5)	-1.6(4)	N(1)-C(14)-C(15)-C(16)	-0.8(4)
S(1)-C(1)-C(6)-C(5)	-178.7(2)	C(14)-C(15)-C(16)-C(17)	0.3(4)
Th(1)-S(2)-C(7)-C(8)	-100.4(2)	C(15)-C(16)-C(17)-C(13)	-0.2(5)
Th(1)-S(2)-C(7)-C(12)	82.5(2)	N(1)-C(13)-C(17)-C(16)	0.5(4)
C(12)-C(7)-C(8)-F(6)	179.3(2)	C(18)-C(13)-C(17)-C(16)	178.0(3)
S(2)-C(7)-C(8)-F(6)	2.1(4)	C(19)-N(2)-C(18)-C(22)	-3.8(4)
C(12)-C(7)-C(8)-C(9)	-2.0(4)	Th(1)-N(2)-C(18)-C(22)	172.73(19)
S(2)-C(7)-C(8)-C(9)	-179.2(2)	C(19)-N(2)-C(18)-C(13)	175.3(2)
F(6)-C(8)-C(9)-F(7)	0.7(4)	Th(1)-N(2)-C(18)-C(13)	-8.2(3)
C(7)-C(8)-C(9)-F(7)	-177.9(3)	N(1)-C(13)-C(18)-N(2)	4.9(3)

C(17)-C(13)-C(18)-N(2)	-172.8(2)	C(26A)-O(1A)-C(23A)-C(24A)	-27.6(12)
N(1)-C(13)-C(18)-C(22)	-176.1(2)	O(1A)-C(23A)-C(24A)-C(25A)	5.8(15)
C(17)-C(13)-C(18)-C(22)	6.3(4)	C(23A)-C(24A)-C(25A)-C(26A)	16.8(14)
C(18)-N(2)-C(19)-C(20)	2.0(4)	C(23A)-O(1A)-C(26A)-C(25A)	38.4(11)
Th(1)-N(2)-C(19)-C(20)	-174.5(2)	C(24A)-C(25A)-C(26A)-O(1A)	-33.9(13)
N(2)-C(19)-C(20)-C(21)	0.8(4)	C(26B)-O(1B)-C(23B)-C(24B)	33.9(9)
C(19)-C(20)-C(21)-C(22)	-1.9(4)	O(1B)-C(23B)-C(24B)-C(25B)	-21.5(11)
C(20)-C(21)-C(22)-C(18)	0.2(5)	C(23B)-C(24B)-C(25B)-C(26B)	1.6(11)
N(2)-C(18)-C(22)-C(21)	2.7(4)	C(23B)-O(1B)-C(26B)-C(25B)	-32.7(8)
C(13)-C(18)-C(22)-C(21)	-176.3(3)	C(24B)-C(25B)-C(26B)-O(1B)	18.8(9)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

Table S22. Hydrogen bonds [Å and °] for **3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14)...S(1)#1	0.95	2.77	3.455(3)	129.3
C(14)-H(14)...F(1)#1	0.95	2.40	3.285(3)	154.2
C(15)-H(15)...F(6)#2	0.95	2.58	3.296(3)	132.6
C(19)-H(19)...S(2)#1	0.95	2.77	3.283(3)	114.5
C(23A)-H(23A)...F(5)#3	0.99	2.43	3.397(10)	166.9
C(25A)-H(25B)...F(3)#4	0.99	2.55	3.427(13)	147.0
C(25B)-H(25D)...F(4)#4	0.99	2.61	3.385(7)	135.2
C(26B)-H(26C)...F(8)	0.99	2.45	3.392(8)	158.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2 #2 -x+1,-y,-z+1 #3 -x+1/2,-y+1/2,-z+1 #4 -x+1/2,y+1/2,-z+1/2

Table S23. Crystal data and structure refinement for **4**.

Identification code	ThSeCF-bipyTHF_C2c	
Empirical formula	C52 H32 F20 N4 O2 Se4 Th	
Formula weight	1672.69	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 26.3395(13) Å	α= 90°.
	b = 12.7499(6) Å	β= 114.2965(9)°.
	c = 17.3963(8) Å	γ = 90°.
Volume	5324.7(4) $Å^3$	
Z	4	
Density (calculated)	2.087 Mg/m^3	
Absorption coefficient	5.652 mm^{-1}	
F(000)	3176	
Crystal size	0.300 x 0.250 x 0.150 mm^3	
Theta range for data collection	1.697 to 30.517°.	
Index ranges	-37<=h<=37, -18<=k<=18, -24<=l<=24	
Reflections collected	31323	
Independent reflections	8110 [R(int) = 0.0357]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.5608	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8110 / 805 / 420	
Goodness-of-fit on F^2	1.005	
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0605	
R indices (all data)	R1 = 0.0358, wR2 = 0.0635	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.423 and -1.473 $e.Å^{-3}$	

Table S24. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	5000	1842(1)	7500	19(1)
Se(1)	4106(1)	637(1)	7726(1)	25(1)
Se(2)	5441(1)	2827(1)	6321(1)	27(1)
F(1)	4605(1)	-1568(2)	7795(1)	36(1)
F(2)	4252(1)	-3168(1)	6705(1)	45(1)
F(3)	3312(1)	-2967(2)	5254(1)	46(1)
F(4)	2735(1)	-1139(2)	4906(1)	38(1)
F(5)	3068(1)	457(1)	6004(1)	32(1)
F(6)	4736(1)	1963(2)	4520(1)	42(1)
F(7)	3886(1)	2853(3)	3231(1)	76(1)
F(8)	3525(1)	4799(3)	3398(2)	93(1)
F(9)	4020(1)	5846(2)	4889(2)	77(1)
F(10)	4871(1)	4982(2)	6177(1)	50(1)
N(1)	4384(1)	1052(2)	6018(1)	24(1)
N(2)	4155(1)	2962(2)	6500(1)	26(1)
C(1)	3859(1)	-483(2)	6926(2)	25(1)
C(2)	4144(1)	-1433(2)	7078(2)	28(1)
C(3)	3968(1)	-2265(2)	6530(2)	32(1)
C(4)	3490(1)	-2166(2)	5792(2)	33(1)
C(5)	3195(1)	-1238(2)	5623(2)	30(1)
C(6)	3379(1)	-423(2)	6190(2)	26(1)
C(7)	4829(1)	3433(3)	5400(2)	33(1)
C(8)	4574(1)	2924(3)	4632(2)	38(1)
C(9)	4134(2)	3382(4)	3960(2)	55(1)
C(10)	3952(2)	4360(4)	4050(2)	64(1)
C(11)	4195(2)	4882(3)	4793(3)	57(1)
C(12)	4634(2)	4427(3)	5457(2)	42(1)
C(13)	3916(1)	1542(2)	5485(2)	26(1)
C(14)	4522(1)	138(2)	5761(2)	27(1)
C(15)	4215(1)	-309(3)	4981(2)	32(1)
C(16)	3740(1)	200(3)	4445(2)	37(1)

C(17)	3585(1)	1128(3)	4697(2)	35(1)
C(18)	3776(1)	2554(2)	5768(2)	27(1)
C(19)	4059(1)	3920(2)	6735(2)	30(1)
C(20)	3584(1)	4497(3)	6284(2)	37(1)
C(21)	3187(1)	4062(3)	5556(2)	40(1)
C(22)	3284(1)	3091(3)	5292(2)	36(1)
O(1A)	2580(2)	1974(5)	3175(3)	48(2)
C(23A)	2110(4)	2624(8)	2751(4)	62(2)
C(24A)	2078(4)	2835(7)	1896(4)	58(2)
C(25A)	2451(5)	2028(9)	1772(5)	68(3)
C(26A)	2646(3)	1359(6)	2544(4)	45(2)
O(1B)	2442(2)	2326(4)	3314(3)	42(1)
C(23B)	2236(3)	1469(6)	2748(4)	50(2)
C(24B)	2463(5)	1641(6)	2103(6)	58(2)
C(25B)	2456(5)	2824(6)	2020(5)	63(2)
C(26B)	2456(3)	3212(5)	2830(4)	47(2)

Table S25. Bond lengths [Å] and angles [°] for **4**.

Th(1)-N(2)	2.613(2)	C(10)-C(11)	1.357(6)
Th(1)-N(2)#1	2.613(2)	C(11)-C(12)	1.383(5)
Th(1)-N(1)	2.618(2)	C(13)-C(17)	1.390(4)
Th(1)-N(1)#1	2.618(2)	C(13)-C(18)	1.481(4)
Th(1)-Se(1)	2.9699(3)	C(14)-C(15)	1.386(4)
Th(1)-Se(1)#1	2.9699(3)	C(14)-H(14)	0.9500
Th(1)-Se(2)	3.0155(3)	C(15)-C(16)	1.377(4)
Th(1)-Se(2)#1	3.0155(3)	C(15)-H(15)	0.9500
Se(1)-C(1)	1.911(3)	C(16)-C(17)	1.380(4)
Se(2)-C(7)	1.907(3)	C(16)-H(16)	0.9500
F(1)-C(2)	1.346(3)	C(17)-H(17)	0.9500
F(2)-C(3)	1.338(3)	C(18)-C(22)	1.397(4)
F(3)-C(4)	1.334(3)	C(19)-C(20)	1.382(4)
F(4)-C(5)	1.340(3)	C(19)-H(19)	0.9500
F(5)-C(6)	1.348(3)	C(20)-C(21)	1.385(5)
F(6)-C(8)	1.339(4)	C(20)-H(20)	0.9500
F(7)-C(9)	1.345(5)	C(21)-C(22)	1.380(5)
F(8)-C(10)	1.347(4)	C(21)-H(21)	0.9500
F(9)-C(11)	1.347(4)	C(22)-H(22)	0.9500
F(10)-C(12)	1.347(4)	O(1A)-C(23A)	1.417(6)
N(1)-C(13)	1.352(3)	O(1A)-C(26A)	1.416(6)
N(1)-C(14)	1.351(4)	C(23A)-C(24A)	1.480(7)
N(2)-C(19)	1.345(4)	C(23A)-H(23A)	0.9900
N(2)-C(18)	1.357(4)	C(23A)-H(23B)	0.9900
C(1)-C(6)	1.383(4)	C(24A)-C(25A)	1.498(9)
C(1)-C(2)	1.391(4)	C(24A)-H(24A)	0.9900
C(2)-C(3)	1.373(4)	C(24A)-H(24B)	0.9900
C(3)-C(4)	1.386(4)	C(25A)-C(26A)	1.492(8)
C(4)-C(5)	1.379(4)	C(25A)-H(25A)	0.9900
C(5)-C(6)	1.378(4)	C(25A)-H(25B)	0.9900
C(7)-C(12)	1.386(4)	C(26A)-H(26A)	0.9900
C(7)-C(8)	1.385(5)	C(26A)-H(26B)	0.9900
C(8)-C(9)	1.390(4)	O(1B)-C(26B)	1.417(6)
C(9)-C(10)	1.368(6)	O(1B)-C(23B)	1.420(6)

C(23B)-C(24B)	1.489(8)	C(25B)-C(26B)	1.494(7)
C(23B)-H(23C)	0.9900	C(25B)-H(25C)	0.9900
C(23B)-H(23D)	0.9900	C(25B)-H(25D)	0.9900
C(24B)-C(25B)	1.515(9)	C(26B)-H(26C)	0.9900
C(24B)-H(24C)	0.9900	C(26B)-H(26D)	0.9900
C(24B)-H(24D)	0.9900		

N(2)-Th(1)-N(2)#1	113.77(11)	C(7)-Se(2)-Th(1)	108.15(9)
N(2)-Th(1)-N(1)	62.72(7)	C(13)-N(1)-C(14)	117.8(2)
N(2)#1-Th(1)-N(1)	151.52(7)	C(13)-N(1)-Th(1)	121.22(18)
N(2)-Th(1)-N(1)#1	151.52(7)	C(14)-N(1)-Th(1)	120.98(17)
N(2)#1-Th(1)-N(1)#1	62.72(7)	C(19)-N(2)-C(18)	118.3(2)
N(1)-Th(1)-N(1)#1	134.72(11)	C(19)-N(2)-Th(1)	120.65(18)
N(2)-Th(1)-Se(1)	82.32(5)	C(18)-N(2)-Th(1)	120.78(18)
N(2)#1-Th(1)-Se(1)	134.34(5)	C(6)-C(1)-C(2)	116.1(3)
N(1)-Th(1)-Se(1)	74.14(5)	C(6)-C(1)-Se(1)	122.7(2)
N(1)#1-Th(1)-Se(1)	82.82(5)	C(2)-C(1)-Se(1)	121.2(2)
N(2)-Th(1)-Se(1)#1	134.34(5)	F(1)-C(2)-C(3)	117.5(3)
N(2)#1-Th(1)-Se(1)#1	82.32(5)	F(1)-C(2)-C(1)	119.8(3)
N(1)-Th(1)-Se(1)#1	82.82(5)	C(3)-C(2)-C(1)	122.7(3)
N(1)#1-Th(1)-Se(1)#1	74.14(5)	F(2)-C(3)-C(2)	120.7(3)
Se(1)-Th(1)-Se(1)#1	117.697(12)	F(2)-C(3)-C(4)	120.0(3)
N(2)-Th(1)-Se(2)	77.33(5)	C(2)-C(3)-C(4)	119.4(3)
N(2)#1-Th(1)-Se(2)	76.37(5)	F(3)-C(4)-C(5)	120.1(3)
N(1)-Th(1)-Se(2)	75.35(5)	F(3)-C(4)-C(3)	120.3(3)
N(1)#1-Th(1)-Se(2)	124.99(5)	C(5)-C(4)-C(3)	119.6(3)
Se(1)-Th(1)-Se(2)	148.611(7)	F(4)-C(5)-C(6)	120.8(3)
Se(1)#1-Th(1)-Se(2)	64.987(8)	F(4)-C(5)-C(4)	119.7(3)
N(2)-Th(1)-Se(2)#1	76.37(5)	C(6)-C(5)-C(4)	119.5(3)
N(2)#1-Th(1)-Se(2)#1	77.34(5)	F(5)-C(6)-C(5)	117.1(2)
N(1)-Th(1)-Se(2)#1	124.99(5)	F(5)-C(6)-C(1)	120.2(2)
N(1)#1-Th(1)-Se(2)#1	75.35(5)	C(5)-C(6)-C(1)	122.7(3)
Se(1)-Th(1)-Se(2)#1	64.986(8)	C(12)-C(7)-C(8)	116.8(3)
Se(1)#1-Th(1)-Se(2)#1	148.612(7)	C(12)-C(7)-Se(2)	121.3(3)
Se(2)-Th(1)-Se(2)#1	130.783(12)	C(8)-C(7)-Se(2)	121.9(2)
C(1)-Se(1)-Th(1)	109.95(8)	F(6)-C(8)-C(7)	120.8(3)

F(6)-C(8)-C(9)	117.8(3)	C(19)-C(20)-H(20)	120.9
C(7)-C(8)-C(9)	121.4(3)	C(21)-C(20)-H(20)	120.9
F(7)-C(9)-C(10)	120.5(3)	C(22)-C(21)-C(20)	119.3(3)
F(7)-C(9)-C(8)	119.7(4)	C(22)-C(21)-H(21)	120.3
C(10)-C(9)-C(8)	119.7(4)	C(20)-C(21)-H(21)	120.3
F(8)-C(10)-C(11)	120.1(4)	C(21)-C(22)-C(18)	119.7(3)
F(8)-C(10)-C(9)	119.5(4)	C(21)-C(22)-H(22)	120.1
C(11)-C(10)-C(9)	120.4(3)	C(18)-C(22)-H(22)	120.1
F(9)-C(11)-C(10)	120.9(3)	C(23A)-O(1A)-C(26A)	106.2(5)
F(9)-C(11)-C(12)	119.4(4)	O(1A)-C(23A)-C(24A)	107.8(5)
C(10)-C(11)-C(12)	119.7(3)	O(1A)-C(23A)-H(23A)	110.1
F(10)-C(12)-C(11)	117.7(3)	C(24A)-C(23A)-H(23A)	110.1
F(10)-C(12)-C(7)	120.3(3)	O(1A)-C(23A)-H(23B)	110.1
C(11)-C(12)-C(7)	122.0(4)	C(24A)-C(23A)-H(23B)	110.1
N(1)-C(13)-C(17)	121.7(3)	H(23A)-C(23A)-H(23B)	108.5
N(1)-C(13)-C(18)	117.1(2)	C(23A)-C(24A)-C(25A)	104.5(5)
C(17)-C(13)-C(18)	121.2(3)	C(23A)-C(24A)-H(24A)	110.9
N(1)-C(14)-C(15)	123.4(3)	C(25A)-C(24A)-H(24A)	110.9
N(1)-C(14)-H(14)	118.3	C(23A)-C(24A)-H(24B)	110.9
C(15)-C(14)-H(14)	118.3	C(25A)-C(24A)-H(24B)	110.9
C(16)-C(15)-C(14)	118.2(3)	H(24A)-C(24A)-H(24B)	108.9
C(16)-C(15)-H(15)	120.9	C(26A)-C(25A)-C(24A)	105.4(5)
C(14)-C(15)-H(15)	120.9	C(26A)-C(25A)-H(25A)	110.7
C(15)-C(16)-C(17)	119.6(3)	C(24A)-C(25A)-H(25A)	110.7
C(15)-C(16)-H(16)	120.2	C(26A)-C(25A)-H(25B)	110.7
C(17)-C(16)-H(16)	120.2	C(24A)-C(25A)-H(25B)	110.7
C(16)-C(17)-C(13)	119.5(3)	H(25A)-C(25A)-H(25B)	108.8
C(16)-C(17)-H(17)	120.3	O(1A)-C(26A)-C(25A)	106.0(5)
C(13)-C(17)-H(17)	120.3	O(1A)-C(26A)-H(26A)	110.5
N(2)-C(18)-C(22)	120.9(3)	C(25A)-C(26A)-H(26A)	110.5
N(2)-C(18)-C(13)	117.2(2)	O(1A)-C(26A)-H(26B)	110.5
C(22)-C(18)-C(13)	121.8(3)	C(25A)-C(26A)-H(26B)	110.5
N(2)-C(19)-C(20)	123.5(3)	H(26A)-C(26A)-H(26B)	108.7
N(2)-C(19)-H(19)	118.3	C(26B)-O(1B)-C(23B)	107.4(5)
C(20)-C(19)-H(19)	118.3	O(1B)-C(23B)-C(24B)	104.5(5)
C(19)-C(20)-C(21)	118.2(3)	O(1B)-C(23B)-H(23C)	110.9

C(24B)-C(23B)-H(23C)	110.9	C(26B)-C(25B)-H(25C)	110.9
O(1B)-C(23B)-H(23D)	110.9	C(24B)-C(25B)-H(25C)	110.9
C(24B)-C(23B)-H(23D)	110.9	C(26B)-C(25B)-H(25D)	110.9
H(23C)-C(23B)-H(23D)	108.9	C(24B)-C(25B)-H(25D)	110.9
C(23B)-C(24B)-C(25B)	103.1(5)	H(25C)-C(25B)-H(25D)	108.9
C(23B)-C(24B)-H(24C)	111.1	O(1B)-C(26B)-C(25B)	107.8(5)
C(25B)-C(24B)-H(24C)	111.1	O(1B)-C(26B)-H(26C)	110.1
C(23B)-C(24B)-H(24D)	111.1	C(25B)-C(26B)-H(26C)	110.1
C(25B)-C(24B)-H(24D)	111.1	O(1B)-C(26B)-H(26D)	110.1
H(24C)-C(24B)-H(24D)	109.1	C(25B)-C(26B)-H(26D)	110.1
C(26B)-C(25B)-C(24B)	104.1(5)	H(26C)-C(26B)-H(26D)	108.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

Table S26. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	13(1)	34(1)	9(1)	0	3(1)	0
Se(1)	19(1)	40(1)	15(1)	-5(1)	7(1)	-5(1)
Se(2)	25(1)	39(1)	16(1)	7(1)	9(1)	4(1)
F(1)	28(1)	50(1)	24(1)	5(1)	5(1)	6(1)
F(2)	44(1)	38(1)	50(1)	4(1)	16(1)	11(1)
F(3)	41(1)	43(1)	48(1)	-20(1)	12(1)	-5(1)
F(4)	27(1)	50(1)	26(1)	-13(1)	-2(1)	0(1)
F(5)	23(1)	38(1)	26(1)	-7(1)	3(1)	6(1)
F(6)	32(1)	68(1)	22(1)	-4(1)	8(1)	15(1)
F(7)	40(1)	159(3)	19(1)	3(1)	4(1)	37(1)
F(8)	67(2)	173(3)	46(1)	57(2)	29(1)	85(2)
F(9)	100(2)	82(2)	82(2)	49(1)	71(2)	65(2)
F(10)	70(1)	44(1)	52(1)	10(1)	42(1)	16(1)
N(1)	16(1)	42(1)	13(1)	-2(1)	6(1)	1(1)
N(2)	20(1)	42(1)	15(1)	1(1)	7(1)	8(1)
C(1)	22(1)	37(2)	17(1)	-3(1)	9(1)	-2(1)
C(2)	23(1)	41(2)	20(1)	4(1)	7(1)	2(1)
C(3)	32(2)	33(2)	31(2)	1(1)	15(1)	6(1)
C(4)	33(2)	34(2)	31(2)	-10(1)	13(1)	-5(1)
C(5)	22(1)	42(2)	20(1)	-6(1)	3(1)	-2(1)
C(6)	21(1)	35(2)	23(1)	-4(1)	9(1)	0(1)
C(7)	32(2)	50(2)	24(1)	14(1)	16(1)	15(1)
C(8)	31(2)	66(2)	20(1)	10(1)	13(1)	21(1)
C(9)	40(2)	109(3)	19(2)	18(2)	16(1)	37(2)
C(10)	53(2)	114(3)	34(2)	42(2)	28(2)	54(2)
C(11)	66(2)	73(3)	53(2)	38(2)	46(2)	45(2)
C(12)	50(2)	54(2)	35(2)	18(2)	31(2)	20(2)
C(13)	16(1)	49(2)	13(1)	-2(1)	6(1)	2(1)
C(14)	20(1)	44(2)	18(1)	-6(1)	8(1)	2(1)
C(15)	21(1)	53(2)	21(1)	-15(1)	7(1)	0(1)
C(16)	23(1)	68(2)	16(1)	-12(1)	5(1)	2(1)

C(17)	20(1)	66(2)	15(1)	-7(1)	3(1)	8(1)
C(18)	18(1)	46(2)	16(1)	2(1)	7(1)	6(1)
C(19)	26(1)	44(2)	20(1)	-1(1)	10(1)	6(1)
C(20)	32(2)	50(2)	28(2)	3(1)	12(1)	15(1)
C(21)	26(2)	59(2)	31(2)	5(1)	6(1)	18(1)
C(22)	22(1)	59(2)	21(1)	3(1)	4(1)	8(1)
O(1A)	37(3)	76(4)	25(3)	9(2)	7(2)	29(3)
C(23A)	56(4)	96(5)	35(4)	16(4)	21(3)	39(4)
C(24A)	57(4)	80(5)	38(4)	25(3)	22(3)	29(4)
C(25A)	68(5)	98(6)	36(4)	12(4)	21(4)	40(5)
C(26A)	38(4)	51(4)	32(4)	-9(3)	0(3)	16(3)
O(1B)	37(3)	58(3)	22(2)	2(2)	4(2)	8(2)
C(23B)	43(4)	66(4)	40(4)	-10(3)	17(3)	-12(3)
C(24B)	65(5)	70(5)	47(5)	-8(4)	31(4)	-3(4)
C(25B)	80(5)	72(5)	39(4)	17(4)	25(4)	14(5)
C(26B)	46(4)	55(4)	37(3)	4(3)	13(3)	20(3)

Table S27. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **4**.

	x	y	z	U(eq)
H(14)	4848	-216	6135	33
H(15)	4328	-950	4821	38
H(16)	3520	-85	3904	44
H(17)	3255	1480	4336	42
H(19)	4331	4216	7237	36
H(20)	3533	5174	6469	44
H(21)	2851	4428	5241	48
H(22)	3017	2789	4789	43
H(23A)	2150	3290	3063	74
H(23B)	1767	2268	2714	74
H(24A)	2211	3552	1860	69
H(24B)	1691	2758	1467	69
H(25A)	2244	1603	1262	81
H(25B)	2771	2367	1712	81
H(26A)	2420	712	2437	54
H(26B)	3041	1162	2720	54
H(23C)	1823	1468	2485	60
H(23D)	2368	794	3045	60
H(24C)	2224	1306	1561	70
H(24D)	2846	1361	2297	70
H(25C)	2790	3074	1949	76
H(25D)	2119	3061	1533	76
H(26C)	2795	3632	3141	56
H(26D)	2126	3660	2717	56

Table S28. Torsion angles [°] for **4**.

C(6)-C(1)-C(2)-F(1)	-177.8(2)	F(7)-C(9)-C(10)-C(11)	178.4(4)
Se(1)-C(1)-C(2)-F(1)	-0.8(4)	C(8)-C(9)-C(10)-C(11)	-0.5(6)
C(6)-C(1)-C(2)-C(3)	0.9(4)	F(8)-C(10)-C(11)-F(9)	-0.8(6)
Se(1)-C(1)-C(2)-C(3)	177.9(2)	C(9)-C(10)-C(11)-F(9)	180.0(4)
F(1)-C(2)-C(3)-F(2)	-0.7(4)	F(8)-C(10)-C(11)-C(12)	-179.8(4)
C(1)-C(2)-C(3)-F(2)	-179.5(3)	C(9)-C(10)-C(11)-C(12)	1.0(6)
F(1)-C(2)-C(3)-C(4)	179.0(3)	F(9)-C(11)-C(12)-F(10)	-0.4(5)
C(1)-C(2)-C(3)-C(4)	0.2(5)	C(10)-C(11)-C(12)-F(10)	178.6(3)
F(2)-C(3)-C(4)-F(3)	0.1(5)	F(9)-C(11)-C(12)-C(7)	179.3(3)
C(2)-C(3)-C(4)-F(3)	-179.6(3)	C(10)-C(11)-C(12)-C(7)	-1.7(6)
F(2)-C(3)-C(4)-C(5)	178.9(3)	C(8)-C(7)-C(12)-F(10)	-178.4(3)
C(2)-C(3)-C(4)-C(5)	-0.8(5)	Se(2)-C(7)-C(12)-F(10)	-1.0(4)
F(3)-C(4)-C(5)-F(4)	-1.7(4)	C(8)-C(7)-C(12)-C(11)	1.9(5)
C(3)-C(4)-C(5)-F(4)	179.5(3)	Se(2)-C(7)-C(12)-C(11)	179.4(3)
F(3)-C(4)-C(5)-C(6)	179.0(3)	C(14)-N(1)-C(13)-C(17)	0.0(4)
C(3)-C(4)-C(5)-C(6)	0.2(5)	Th(1)-N(1)-C(13)-C(17)	-179.9(2)
F(4)-C(5)-C(6)-F(5)	2.2(4)	C(14)-N(1)-C(13)-C(18)	-178.7(2)
C(4)-C(5)-C(6)-F(5)	-178.5(3)	Th(1)-N(1)-C(13)-C(18)	1.4(3)
F(4)-C(5)-C(6)-C(1)	-178.3(3)	C(13)-N(1)-C(14)-C(15)	0.8(4)
C(4)-C(5)-C(6)-C(1)	1.1(4)	Th(1)-N(1)-C(14)-C(15)	-179.3(2)
C(2)-C(1)-C(6)-F(5)	178.0(2)	N(1)-C(14)-C(15)-C(16)	-0.7(5)
Se(1)-C(1)-C(6)-F(5)	1.0(4)	C(14)-C(15)-C(16)-C(17)	-0.2(5)
C(2)-C(1)-C(6)-C(5)	-1.6(4)	C(15)-C(16)-C(17)-C(13)	1.0(5)
Se(1)-C(1)-C(6)-C(5)	-178.5(2)	N(1)-C(13)-C(17)-C(16)	-0.9(5)
C(12)-C(7)-C(8)-F(6)	179.9(3)	C(18)-C(13)-C(17)-C(16)	177.8(3)
Se(2)-C(7)-C(8)-F(6)	2.5(4)	C(19)-N(2)-C(18)-C(22)	-3.2(4)
C(12)-C(7)-C(8)-C(9)	-1.4(5)	Th(1)-N(2)-C(18)-C(22)	170.8(2)
Se(2)-C(7)-C(8)-C(9)	-178.9(3)	C(19)-N(2)-C(18)-C(13)	174.6(3)
F(6)-C(8)-C(9)-F(7)	0.5(5)	Th(1)-N(2)-C(18)-C(13)	-11.3(3)
C(7)-C(8)-C(9)-F(7)	-178.2(3)	N(1)-C(13)-C(18)-N(2)	6.5(4)
F(6)-C(8)-C(9)-C(10)	179.4(3)	C(17)-C(13)-C(18)-N(2)	-172.3(3)
C(7)-C(8)-C(9)-C(10)	0.8(6)	N(1)-C(13)-C(18)-C(22)	-175.7(3)
F(7)-C(9)-C(10)-F(8)	-0.8(6)	C(17)-C(13)-C(18)-C(22)	5.6(4)
C(8)-C(9)-C(10)-F(8)	-179.8(4)	C(18)-N(2)-C(19)-C(20)	2.2(4)

Th(1)-N(2)-C(19)-C(20)	-171.9(2)	C(23A)-C(24A)-C(25A)-C(26A)	3.6(12)
N(2)-C(19)-C(20)-C(21)	0.4(5)	C(23A)-O(1A)-C(26A)-C(25A)	32.1(10)
C(19)-C(20)-C(21)-C(22)	-2.0(5)	C(24A)-C(25A)-C(26A)-O(1A)	-21.7(11)
C(20)-C(21)-C(22)-C(18)	0.9(5)	C(26B)-O(1B)-C(23B)-C(24B)	35.2(9)
N(2)-C(18)-C(22)-C(21)	1.7(5)	O(1B)-C(23B)-C(24B)-C(25B)	-35.2(10)
C(13)-C(18)-C(22)-C(21)	-176.0(3)	C(23B)-C(24B)-C(25B)-C(26B)	22.3(10)
C(26A)-O(1A)-C(23A)-C(24A)	-30.2(11)	C(23B)-O(1B)-C(26B)-C(25B)	-20.6(9)
O(1A)-C(23A)-C(24A)-C(25A)	15.8(12)	C(24B)-C(25B)-C(26B)-O(1B)	-2.0(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+3/2

Table S29. Hydrogen bonds [Å and °] for **4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14)...Se(1)#1	0.95	2.87	3.544(3)	129.3
C(14)-H(14)...F(1)#1	0.95	2.51	3.402(3)	156.1
C(15)-H(15)...F(6)#2	0.95	2.60	3.297(3)	130.8
C(19)-H(19)...Se(2)#1	0.95	2.92	3.383(3)	111.1
C(23A)-H(23A)...F(5)#3	0.99	2.51	3.425(8)	154.3
C(25A)-H(25A)...F(3)#4	0.99	2.49	3.260(9)	134.0
C(26A)-H(26A)...F(8)#5	0.99	2.58	3.463(8)	147.8
C(26B)-H(26C)...F(8)	0.99	2.32	3.273(9)	160.1
C(26B)-H(26D)...Se(1)#3	0.99	3.14	4.091(8)	161.3

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2 #2 -x+1,-y,-z+1 #3 -x+1/2,-y+1/2,-z+1

#4 -x+1/2,y+1/2,-z+1/2 #5 -x+1/2,y-1/2,-z+1/2

Table S30. Crystal data and structure refinement for **5**.

Identification code	ter py_P21n	
Empirical formula	C54 H46 N6 S4 Th	
Formula weight	1139.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 15.1881(10) Å	α= 90°.
	b = 21.6317(14) Å	β= 111.1460(10)°.
	c = 15.6510(10) Å	γ = 90°.
Volume	4795.8(5) $Å^3$	
Z	4	
Density (calculated)	1.578 Mg/m^3	
Absorption coefficient	3.328 mm^{-1}	
F(000)	2264	
Crystal size	.55 x .14 x .12 mm^3	
Theta range for data collection	1.683 to 29.574°.	
Index ranges	-21<=h<=15, -29<=k<=25, -11<=l<=21	
Reflections collected	27936	
Independent reflections	13310 [R(int) = 0.0398]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7464 and 0.4586	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13310 / 0 / 586	
Goodness-of-fit on F^2	0.987	
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0733	
R indices (all data)	R1 = 0.0541, wR2 = 0.0786	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.018 and -2.023 $e.Å^{-3}$	

Table S31. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Th(1)	6743(1)	4351(1)	2347(1)	11(1)
S(1)	8723(1)	4435(1)	2809(1)	18(1)
S(2)	6510(1)	5614(1)	1847(1)	16(1)
S(3)	5238(1)	4703(1)	2924(1)	19(1)
S(4)	5015(1)	3771(1)	1292(1)	17(1)
N(1)	6910(2)	3448(1)	3500(2)	18(1)
N(2)	7333(2)	3287(1)	1967(2)	14(1)
N(3)	6780(2)	4204(1)	713(2)	14(1)
N(4)	7739(2)	4790(2)	4063(2)	17(1)
C(1)	9107(3)	4218(2)	1908(2)	18(1)
C(2)	9542(3)	3650(2)	1922(3)	23(1)
C(3)	9854(3)	3492(2)	1217(3)	32(1)
C(4)	9747(3)	3895(2)	505(3)	35(1)
C(5)	9319(3)	4461(2)	488(3)	29(1)
C(6)	9006(3)	4628(2)	1187(2)	21(1)
C(7)	7487(3)	5902(2)	1602(2)	17(1)
C(8)	7404(3)	6038(2)	694(2)	21(1)
C(9)	8165(3)	6289(2)	520(3)	25(1)
C(10)	8997(3)	6423(2)	1228(3)	26(1)
C(11)	9081(3)	6299(2)	2127(3)	24(1)
C(12)	8338(3)	6038(2)	2308(2)	20(1)
C(13)	5288(3)	5429(2)	3477(2)	20(1)
C(14)	4992(3)	5968(2)	2973(2)	21(1)
C(15)	4919(3)	6515(2)	3391(3)	28(1)
C(16)	5163(3)	6543(2)	4338(3)	32(1)
C(17)	5486(3)	6013(2)	4845(3)	33(1)
C(18)	5549(3)	5461(2)	4426(2)	24(1)
C(19)	5150(3)	3137(2)	636(2)	17(1)
C(20)	5300(3)	2539(2)	999(2)	20(1)
C(21)	5369(3)	2035(2)	476(2)	24(1)
C(22)	5303(3)	2121(2)	-426(2)	23(1)

C(23)	5163(3)	2711(2)	-794(2)	21(1)
C(24)	5088(2)	3217(2)	-274(2)	17(1)
C(25)	6697(3)	3529(2)	4256(2)	23(1)
C(26)	7059(3)	3164(2)	5029(2)	27(1)
C(27)	7696(3)	2709(2)	5039(2)	25(1)
C(28)	7900(3)	2600(2)	4259(2)	23(1)
C(29)	7481(3)	2967(2)	3492(2)	16(1)
C(30)	7604(2)	2839(2)	2606(2)	15(1)
C(31)	7950(3)	2271(2)	2448(2)	21(1)
C(32)	8010(3)	2159(2)	1605(2)	20(1)
C(33)	7743(3)	2617(2)	946(2)	21(1)
C(34)	7427(2)	3184(2)	1153(2)	16(1)
C(35)	7155(2)	3694(2)	476(2)	14(1)
C(36)	7270(3)	3651(2)	-363(2)	18(1)
C(37)	6969(3)	4134(2)	-984(2)	23(1)
C(38)	6539(3)	4637(2)	-764(2)	22(1)
C(39)	6453(3)	4654(2)	82(2)	18(1)
C(40)	7606(3)	5380(2)	4241(2)	17(1)
C(41)	8146(3)	5677(2)	5047(2)	26(1)
C(42)	8856(3)	5350(2)	5700(2)	30(1)
C(43)	9001(3)	4744(2)	5519(2)	29(1)
C(44)	8429(3)	4479(2)	4706(2)	24(1)
N(5)	7566(3)	3931(2)	6930(3)	45(1)
C(45)	7095(3)	4447(2)	6714(3)	36(1)
C(46)	7442(4)	5012(3)	7081(3)	44(1)
C(47)	8350(3)	5039(2)	7710(3)	39(1)
C(48)	8869(3)	4502(2)	7941(3)	32(1)
C(49)	8454(3)	3955(2)	7541(3)	38(1)
N(6)	7944(4)	2408(2)	8690(3)	48(1)
C(50)	8797(4)	2403(2)	8629(3)	49(2)
C(51)	9025(4)	2064(3)	7995(3)	47(1)
C(52)	8328(4)	1718(2)	7380(3)	44(1)
C(53)	7454(4)	1721(3)	7422(3)	48(1)
C(54)	7296(4)	2066(3)	8085(3)	50(1)

Table S32. Bond lengths [Å] and angles [°] for **5**.

Th(1)-N(3)	2.598(3)	C(8)-H(8)	0.9500
Th(1)-N(1)	2.609(3)	C(9)-C(10)	1.378(6)
Th(1)-N(2)	2.614(3)	C(9)-H(9)	0.9500
Th(1)-N(4)	2.734(3)	C(10)-C(11)	1.392(5)
Th(1)-S(2)	2.8282(9)	C(10)-H(10)	0.9500
Th(1)-S(1)	2.8348(10)	C(11)-C(12)	1.379(5)
Th(1)-S(4)	2.8384(9)	C(11)-H(11)	0.9500
Th(1)-S(3)	2.8479(9)	C(12)-H(12)	0.9500
S(1)-C(1)	1.772(4)	C(13)-C(14)	1.388(5)
S(2)-C(7)	1.775(4)	C(13)-C(18)	1.394(5)
S(3)-C(13)	1.780(4)	C(14)-C(15)	1.376(5)
S(4)-C(19)	1.770(4)	C(14)-H(14)	0.9500
N(1)-C(25)	1.346(4)	C(15)-C(16)	1.393(5)
N(1)-C(29)	1.357(5)	C(15)-H(15)	0.9500
N(2)-C(30)	1.346(4)	C(16)-C(17)	1.378(6)
N(2)-C(34)	1.350(4)	C(16)-H(16)	0.9500
N(3)-C(39)	1.347(4)	C(17)-C(18)	1.383(6)
N(3)-C(35)	1.353(4)	C(17)-H(17)	0.9500
N(4)-C(40)	1.336(5)	C(18)-H(18)	0.9500
N(4)-C(44)	1.344(5)	C(19)-C(20)	1.399(5)
C(1)-C(2)	1.391(5)	C(19)-C(24)	1.403(4)
C(1)-C(6)	1.399(5)	C(20)-C(21)	1.388(5)
C(2)-C(3)	1.392(5)	C(20)-H(20)	0.9500
C(2)-H(2)	0.9500	C(21)-C(22)	1.391(5)
C(3)-C(4)	1.378(6)	C(21)-H(21)	0.9500
C(3)-H(3)	0.9500	C(22)-C(23)	1.385(5)
C(4)-C(5)	1.382(6)	C(22)-H(22)	0.9500
C(4)-H(4)	0.9500	C(23)-C(24)	1.393(5)
C(5)-C(6)	1.387(5)	C(23)-H(23)	0.9500
C(5)-H(5)	0.9500	C(24)-H(24)	0.9500
C(6)-H(6)	0.9500	C(25)-C(26)	1.381(5)
C(7)-C(12)	1.396(5)	C(25)-H(25)	0.9500
C(7)-C(8)	1.411(5)	C(26)-C(27)	1.378(6)
C(8)-C(9)	1.390(5)	C(26)-H(26)	0.9500

C(27)-C(28)	1.383(5)	C(42)-H(42)	0.9500
C(27)-H(27)	0.9500	C(43)-C(44)	1.380(5)
C(28)-C(29)	1.388(5)	C(43)-H(43)	0.9500
C(28)-H(28)	0.9500	C(44)-H(44)	0.9500
C(29)-C(30)	1.490(4)	N(5)-C(45)	1.303(6)
C(30)-C(31)	1.393(5)	N(5)-C(49)	1.344(6)
C(31)-C(32)	1.377(5)	C(45)-C(46)	1.370(7)
C(31)-H(31)	0.9500	C(45)-H(45)	0.9500
C(32)-C(33)	1.381(5)	C(46)-C(47)	1.377(6)
C(32)-H(32)	0.9500	C(46)-H(46)	0.9500
C(33)-C(34)	1.398(5)	C(47)-C(48)	1.377(6)
C(33)-H(33)	0.9500	C(47)-H(47)	0.9500
C(34)-C(35)	1.482(5)	C(48)-C(49)	1.379(6)
C(35)-C(36)	1.389(4)	C(48)-H(48)	0.9500
C(36)-C(37)	1.387(5)	C(49)-H(49)	0.9500
C(36)-H(36)	0.9500	N(6)-C(54)	1.319(7)
C(37)-C(38)	1.376(5)	N(6)-C(50)	1.332(7)
C(37)-H(37)	0.9500	C(50)-C(51)	1.377(7)
C(38)-C(39)	1.377(5)	C(50)-H(50)	0.9500
C(38)-H(38)	0.9500	C(51)-C(52)	1.368(7)
C(39)-H(39)	0.9500	C(51)-H(51)	0.9500
C(40)-C(41)	1.389(5)	C(52)-C(53)	1.352(7)
C(40)-H(40)	0.9500	C(52)-H(52)	0.9500
C(41)-C(42)	1.384(6)	C(53)-C(54)	1.367(7)
C(41)-H(41)	0.9500	C(53)-H(53)	0.9500
C(42)-C(43)	1.375(6)	C(54)-H(54)	0.9500

N(3)-Th(1)-N(1)	123.94(9)	N(4)-Th(1)-S(2)	84.59(7)
N(3)-Th(1)-N(2)	62.45(9)	N(3)-Th(1)-S(1)	81.99(7)
N(1)-Th(1)-N(2)	62.79(9)	N(1)-Th(1)-S(1)	92.40(7)
N(3)-Th(1)-N(4)	143.97(9)	N(2)-Th(1)-S(1)	72.23(7)
N(1)-Th(1)-N(4)	72.51(9)	N(4)-Th(1)-S(1)	64.35(7)
N(2)-Th(1)-N(4)	114.58(9)	S(2)-Th(1)-S(1)	91.38(3)
N(3)-Th(1)-S(2)	83.70(6)	N(3)-Th(1)-S(4)	73.59(7)
N(1)-Th(1)-S(2)	152.36(6)	N(1)-Th(1)-S(4)	84.88(7)
N(2)-Th(1)-S(2)	143.68(6)	N(2)-Th(1)-S(4)	78.46(6)

N(4)-Th(1)-S(4)	142.45(6)	C(3)-C(4)-H(4)	120.2
S(2)-Th(1)-S(4)	105.57(3)	C(5)-C(4)-H(4)	120.2
S(1)-Th(1)-S(4)	148.19(3)	C(4)-C(5)-C(6)	120.5(4)
N(3)-Th(1)-S(3)	130.54(7)	C(4)-C(5)-H(5)	119.8
N(1)-Th(1)-S(3)	82.53(7)	C(6)-C(5)-H(5)	119.8
N(2)-Th(1)-S(3)	133.46(7)	C(5)-C(6)-C(1)	120.2(4)
N(4)-Th(1)-S(3)	79.54(7)	C(5)-C(6)-H(6)	119.9
S(2)-Th(1)-S(3)	78.17(3)	C(1)-C(6)-H(6)	119.9
S(1)-Th(1)-S(3)	143.27(3)	C(12)-C(7)-C(8)	118.4(3)
S(4)-Th(1)-S(3)	67.87(3)	C(12)-C(7)-S(2)	120.7(3)
C(1)-S(1)-Th(1)	113.77(12)	C(8)-C(7)-S(2)	120.8(3)
C(7)-S(2)-Th(1)	111.59(12)	C(9)-C(8)-C(7)	120.0(3)
C(13)-S(3)-Th(1)	119.40(13)	C(9)-C(8)-H(8)	120.0
C(19)-S(4)-Th(1)	113.80(12)	C(7)-C(8)-H(8)	120.0
C(25)-N(1)-C(29)	117.7(3)	C(10)-C(9)-C(8)	120.7(3)
C(25)-N(1)-Th(1)	121.1(2)	C(10)-C(9)-H(9)	119.6
C(29)-N(1)-Th(1)	118.0(2)	C(8)-C(9)-H(9)	119.6
C(30)-N(2)-C(34)	118.3(3)	C(9)-C(10)-C(11)	119.7(4)
C(30)-N(2)-Th(1)	120.2(2)	C(9)-C(10)-H(10)	120.1
C(34)-N(2)-Th(1)	121.4(2)	C(11)-C(10)-H(10)	120.1
C(39)-N(3)-C(35)	117.9(3)	C(12)-C(11)-C(10)	120.2(4)
C(39)-N(3)-Th(1)	120.0(2)	C(12)-C(11)-H(11)	119.9
C(35)-N(3)-Th(1)	122.0(2)	C(10)-C(11)-H(11)	119.9
C(40)-N(4)-C(44)	117.3(3)	C(11)-C(12)-C(7)	121.1(3)
C(40)-N(4)-Th(1)	117.7(2)	C(11)-C(12)-H(12)	119.5
C(44)-N(4)-Th(1)	124.5(2)	C(7)-C(12)-H(12)	119.5
C(2)-C(1)-C(6)	119.0(3)	C(14)-C(13)-C(18)	118.2(4)
C(2)-C(1)-S(1)	120.8(3)	C(14)-C(13)-S(3)	121.1(3)
C(6)-C(1)-S(1)	120.2(3)	C(18)-C(13)-S(3)	120.5(3)
C(1)-C(2)-C(3)	120.0(4)	C(15)-C(14)-C(13)	121.2(3)
C(1)-C(2)-H(2)	120.0	C(15)-C(14)-H(14)	119.4
C(3)-C(2)-H(2)	120.0	C(13)-C(14)-H(14)	119.4
C(4)-C(3)-C(2)	120.7(4)	C(14)-C(15)-C(16)	120.5(4)
C(4)-C(3)-H(3)	119.7	C(14)-C(15)-H(15)	119.8
C(2)-C(3)-H(3)	119.7	C(16)-C(15)-H(15)	119.8
C(3)-C(4)-C(5)	119.6(4)	C(17)-C(16)-C(15)	118.7(4)

C(17)-C(16)-H(16)	120.7	C(27)-C(28)-H(28)	120.4
C(15)-C(16)-H(16)	120.7	C(29)-C(28)-H(28)	120.4
C(16)-C(17)-C(18)	121.0(4)	N(1)-C(29)-C(28)	121.7(3)
C(16)-C(17)-H(17)	119.5	N(1)-C(29)-C(30)	116.5(3)
C(18)-C(17)-H(17)	119.5	C(28)-C(29)-C(30)	121.8(3)
C(17)-C(18)-C(13)	120.5(4)	N(2)-C(30)-C(31)	122.5(3)
C(17)-C(18)-H(18)	119.8	N(2)-C(30)-C(29)	116.8(3)
C(13)-C(18)-H(18)	119.8	C(31)-C(30)-C(29)	120.7(3)
C(20)-C(19)-C(24)	117.8(3)	C(32)-C(31)-C(30)	119.1(3)
C(20)-C(19)-S(4)	121.2(3)	C(32)-C(31)-H(31)	120.5
C(24)-C(19)-S(4)	121.0(3)	C(30)-C(31)-H(31)	120.5
C(21)-C(20)-C(19)	121.5(3)	C(31)-C(32)-C(33)	119.0(3)
C(21)-C(20)-H(20)	119.2	C(31)-C(32)-H(32)	120.5
C(19)-C(20)-H(20)	119.2	C(33)-C(32)-H(32)	120.5
C(20)-C(21)-C(22)	120.0(3)	C(32)-C(33)-C(34)	119.3(3)
C(20)-C(21)-H(21)	120.0	C(32)-C(33)-H(33)	120.3
C(22)-C(21)-H(21)	120.0	C(34)-C(33)-H(33)	120.3
C(23)-C(22)-C(21)	119.3(3)	N(2)-C(34)-C(33)	121.7(3)
C(23)-C(22)-H(22)	120.4	N(2)-C(34)-C(35)	117.0(3)
C(21)-C(22)-H(22)	120.4	C(33)-C(34)-C(35)	121.2(3)
C(22)-C(23)-C(24)	120.9(3)	N(3)-C(35)-C(36)	121.6(3)
C(22)-C(23)-H(23)	119.6	N(3)-C(35)-C(34)	116.6(3)
C(24)-C(23)-H(23)	119.6	C(36)-C(35)-C(34)	121.9(3)
C(23)-C(24)-C(19)	120.5(3)	C(37)-C(36)-C(35)	119.3(3)
C(23)-C(24)-H(24)	119.8	C(37)-C(36)-H(36)	120.4
C(19)-C(24)-H(24)	119.8	C(35)-C(36)-H(36)	120.4
N(1)-C(25)-C(26)	123.4(4)	C(38)-C(37)-C(36)	119.1(3)
N(1)-C(25)-H(25)	118.3	C(38)-C(37)-H(37)	120.5
C(26)-C(25)-H(25)	118.3	C(36)-C(37)-H(37)	120.5
C(27)-C(26)-C(25)	118.3(4)	C(37)-C(38)-C(39)	118.7(3)
C(27)-C(26)-H(26)	120.9	C(37)-C(38)-H(38)	120.6
C(25)-C(26)-H(26)	120.9	C(39)-C(38)-H(38)	120.6
C(26)-C(27)-C(28)	119.5(3)	N(3)-C(39)-C(38)	123.2(3)
C(26)-C(27)-H(27)	120.3	N(3)-C(39)-H(39)	118.4
C(28)-C(27)-H(27)	120.3	C(38)-C(39)-H(39)	118.4
C(27)-C(28)-C(29)	119.2(4)	N(4)-C(40)-C(41)	123.2(4)

N(4)-C(40)-H(40)	118.4	C(46)-C(47)-H(47)	120.6
C(41)-C(40)-H(40)	118.4	C(47)-C(48)-C(49)	118.7(4)
C(42)-C(41)-C(40)	118.8(4)	C(47)-C(48)-H(48)	120.7
C(42)-C(41)-H(41)	120.6	C(49)-C(48)-H(48)	120.7
C(40)-C(41)-H(41)	120.6	N(5)-C(49)-C(48)	122.2(5)
C(43)-C(42)-C(41)	118.4(4)	N(5)-C(49)-H(49)	118.9
C(43)-C(42)-H(42)	120.8	C(48)-C(49)-H(49)	118.9
C(41)-C(42)-H(42)	120.8	C(54)-N(6)-C(50)	115.9(4)
C(42)-C(43)-C(44)	119.5(4)	N(6)-C(50)-C(51)	124.0(5)
C(42)-C(43)-H(43)	120.2	N(6)-C(50)-H(50)	118.0
C(44)-C(43)-H(43)	120.2	C(51)-C(50)-H(50)	118.0
N(4)-C(44)-C(43)	122.9(4)	C(52)-C(51)-C(50)	117.8(5)
N(4)-C(44)-H(44)	118.6	C(52)-C(51)-H(51)	121.1
C(43)-C(44)-H(44)	118.6	C(50)-C(51)-H(51)	121.1
C(45)-N(5)-C(49)	117.9(4)	C(53)-C(52)-C(51)	119.2(4)
N(5)-C(45)-C(46)	124.2(5)	C(53)-C(52)-H(52)	120.4
N(5)-C(45)-H(45)	117.9	C(51)-C(52)-H(52)	120.4
C(46)-C(45)-H(45)	117.9	C(52)-C(53)-C(54)	118.9(5)
C(45)-C(46)-C(47)	118.2(5)	C(52)-C(53)-H(53)	120.5
C(45)-C(46)-H(46)	120.9	C(54)-C(53)-H(53)	120.5
C(47)-C(46)-H(46)	120.9	N(6)-C(54)-C(53)	124.1(5)
C(48)-C(47)-C(46)	118.9(5)	N(6)-C(54)-H(54)	117.9
C(48)-C(47)-H(47)	120.6	C(53)-C(54)-H(54)	117.9

Table S33. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Th(1)	12(1)	11(1)	10(1)	0(1)	2(1)	1(1)
S(1)	14(1)	21(1)	17(1)	-2(1)	4(1)	0(1)
S(2)	17(1)	14(1)	18(1)	2(1)	6(1)	2(1)
S(3)	19(1)	20(1)	19(1)	-1(1)	8(1)	1(1)
S(4)	15(1)	18(1)	17(1)	-3(1)	4(1)	-2(1)
N(1)	24(2)	13(2)	15(1)	2(1)	6(1)	-1(1)
N(2)	12(2)	14(2)	15(1)	-1(1)	3(1)	-1(1)
N(3)	14(2)	14(2)	12(1)	0(1)	2(1)	-1(1)
N(4)	17(2)	23(2)	12(1)	-1(1)	4(1)	-3(1)
C(1)	10(2)	21(2)	18(2)	-3(1)	1(1)	-3(1)
C(2)	18(2)	21(2)	29(2)	-4(2)	7(2)	2(2)
C(3)	20(2)	31(2)	45(2)	-13(2)	13(2)	-1(2)
C(4)	28(2)	51(3)	33(2)	-16(2)	19(2)	-7(2)
C(5)	22(2)	41(3)	24(2)	-2(2)	7(2)	-14(2)
C(6)	15(2)	23(2)	24(2)	-1(2)	4(1)	-3(2)
C(7)	20(2)	11(2)	22(2)	2(1)	10(1)	6(2)
C(8)	23(2)	19(2)	21(2)	2(1)	7(2)	2(2)
C(9)	28(2)	24(2)	26(2)	7(2)	14(2)	2(2)
C(10)	25(2)	20(2)	41(2)	2(2)	22(2)	0(2)
C(11)	17(2)	27(2)	30(2)	-9(2)	9(2)	-3(2)
C(12)	20(2)	19(2)	21(2)	-3(1)	7(2)	1(2)
C(13)	17(2)	25(2)	20(2)	-5(1)	11(1)	-3(2)
C(14)	20(2)	20(2)	24(2)	-4(2)	11(2)	-3(2)
C(15)	30(2)	24(2)	34(2)	-2(2)	15(2)	-5(2)
C(16)	30(3)	35(3)	36(2)	-15(2)	17(2)	-3(2)
C(17)	31(3)	45(3)	23(2)	-10(2)	10(2)	0(2)
C(18)	24(2)	33(2)	15(2)	-1(2)	7(2)	-2(2)
C(19)	13(2)	18(2)	17(2)	0(1)	1(1)	-1(2)
C(20)	17(2)	21(2)	18(2)	2(1)	1(1)	-2(2)
C(21)	24(2)	15(2)	27(2)	3(2)	2(2)	0(2)
C(22)	22(2)	21(2)	23(2)	-9(2)	3(2)	-1(2)

C(23)	18(2)	26(2)	16(2)	-1(1)	4(1)	0(2)
C(24)	16(2)	16(2)	16(2)	2(1)	4(1)	0(2)
C(25)	32(2)	22(2)	17(2)	3(1)	11(2)	3(2)
C(26)	40(3)	24(2)	19(2)	5(2)	13(2)	-2(2)
C(27)	27(2)	27(2)	18(2)	8(2)	5(2)	2(2)
C(28)	23(2)	22(2)	21(2)	9(2)	6(2)	6(2)
C(29)	16(2)	12(2)	19(2)	2(1)	5(1)	-1(1)
C(30)	12(2)	16(2)	16(1)	3(1)	4(1)	-2(1)
C(31)	14(2)	16(2)	28(2)	1(2)	4(1)	-4(2)
C(32)	20(2)	8(2)	29(2)	-3(1)	7(2)	1(1)
C(33)	21(2)	19(2)	23(2)	-6(1)	7(2)	-2(2)
C(34)	13(2)	18(2)	17(2)	-2(1)	5(1)	0(2)
C(35)	7(2)	19(2)	15(1)	-3(1)	2(1)	-4(1)
C(36)	16(2)	22(2)	16(2)	-3(1)	5(1)	-5(2)
C(37)	25(2)	32(2)	11(2)	2(1)	7(1)	-3(2)
C(38)	22(2)	25(2)	17(2)	3(1)	6(1)	0(2)
C(39)	18(2)	17(2)	16(2)	2(1)	3(1)	2(2)
C(40)	15(2)	18(2)	18(2)	-2(1)	5(1)	-2(2)
C(41)	25(2)	27(2)	25(2)	-8(2)	6(2)	-5(2)
C(42)	21(2)	43(3)	19(2)	-9(2)	0(2)	-3(2)
C(43)	20(2)	42(3)	18(2)	0(2)	-1(2)	3(2)
C(44)	28(2)	26(2)	17(2)	1(1)	6(2)	3(2)
N(5)	42(3)	61(3)	41(2)	-19(2)	26(2)	-14(2)
C(45)	23(2)	67(4)	19(2)	0(2)	7(2)	-9(2)
C(46)	33(3)	53(3)	42(3)	15(2)	11(2)	9(2)
C(47)	35(3)	38(3)	37(2)	0(2)	5(2)	-3(2)
C(48)	23(2)	40(3)	28(2)	-3(2)	4(2)	-3(2)
C(49)	31(3)	33(3)	57(3)	-8(2)	26(2)	0(2)
N(6)	80(4)	34(2)	39(2)	-2(2)	31(2)	12(2)
C(50)	64(4)	41(3)	30(2)	3(2)	3(2)	-26(3)
C(51)	37(3)	69(4)	40(3)	20(3)	19(2)	4(3)
C(52)	53(3)	48(3)	35(2)	0(2)	21(2)	22(3)
C(53)	39(3)	54(4)	47(3)	-14(2)	13(2)	-6(3)
C(54)	37(3)	69(4)	50(3)	2(3)	23(2)	11(3)

Table S34. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for **5**.

	x	y	z	U(eq)
H(2)	9626	3370	2413	28
H(3)	10145	3102	1227	38
H(4)	9966	3785	29	43
H(5)	9239	4739	-5	35
H(6)	8723	5021	1175	25
H(8)	6828	5957	202	25
H(9)	8110	6370	-93	30
H(10)	9511	6600	1104	31
H(11)	9652	6394	2617	29
H(12)	8406	5950	2924	24
H(14)	4838	5959	2329	25
H(15)	4700	6876	3031	34
H(16)	5108	6919	4628	39
H(17)	5667	6028	5493	40
H(18)	5773	5101	4787	29
H(20)	5356	2475	1617	24
H(21)	5460	1632	734	28
H(22)	5353	1778	-786	28
H(23)	5118	2772	-1410	25
H(24)	4995	3618	-537	20
H(25)	6277	3854	4258	28
H(26)	6873	3226	5541	32
H(27)	7993	2471	5576	30
H(28)	8322	2278	4249	27
H(31)	8141	1966	2916	25
H(32)	8233	1772	1479	24
H(33)	7773	2547	358	25
H(36)	7551	3294	-510	22
H(37)	7060	4117	-1553	27
H(38)	6306	4966	-1187	26
H(39)	6147	4999	227	21

H(40)	7120	5607	3795	21
H(41)	8029	6097	5148	32
H(42)	9234	5539	6260	36
H(43)	9490	4510	5950	34
H(44)	8529	4057	4596	29
H(45)	6472	4432	6273	44
H(46)	7066	5374	6906	52
H(47)	8615	5422	7979	47
H(48)	9499	4507	8368	38
H(49)	8808	3583	7703	45
H(50)	9276	2650	9049	58
H(51)	9647	2069	7984	57
H(52)	8457	1478	6930	52
H(53)	6958	1488	6997	57
H(54)	6681	2059	8111	60

Table S35. Torsion angles [°] for **5**.

Th(1)-S(1)-C(1)-C(2)	-104.4(3)	C(19)-C(20)-C(21)-C(22)	1.0(6)
Th(1)-S(1)-C(1)-C(6)	78.0(3)	C(20)-C(21)-C(22)-C(23)	-0.4(6)
C(6)-C(1)-C(2)-C(3)	-1.2(6)	C(21)-C(22)-C(23)-C(24)	0.0(6)
S(1)-C(1)-C(2)-C(3)	-178.8(3)	C(22)-C(23)-C(24)-C(19)	-0.2(6)
C(1)-C(2)-C(3)-C(4)	0.7(6)	C(20)-C(19)-C(24)-C(23)	0.8(5)
C(2)-C(3)-C(4)-C(5)	-0.4(7)	S(4)-C(19)-C(24)-C(23)	-177.8(3)
C(3)-C(4)-C(5)-C(6)	0.6(6)	C(29)-N(1)-C(25)-C(26)	2.6(6)
C(4)-C(5)-C(6)-C(1)	-1.1(6)	Th(1)-N(1)-C(25)-C(26)	-157.0(3)
C(2)-C(1)-C(6)-C(5)	1.4(6)	N(1)-C(25)-C(26)-C(27)	2.4(6)
S(1)-C(1)-C(6)-C(5)	179.0(3)	C(25)-C(26)-C(27)-C(28)	-4.7(6)
Th(1)-S(2)-C(7)-C(12)	-76.2(3)	C(26)-C(27)-C(28)-C(29)	2.1(6)
Th(1)-S(2)-C(7)-C(8)	108.1(3)	C(25)-N(1)-C(29)-C(28)	-5.4(5)
C(12)-C(7)-C(8)-C(9)	1.3(5)	Th(1)-N(1)-C(29)-C(28)	154.8(3)
S(2)-C(7)-C(8)-C(9)	177.1(3)	C(25)-N(1)-C(29)-C(30)	172.3(3)
C(7)-C(8)-C(9)-C(10)	-1.7(6)	Th(1)-N(1)-C(29)-C(30)	-27.5(4)
C(8)-C(9)-C(10)-C(11)	0.7(6)	C(27)-C(28)-C(29)-N(1)	3.1(6)
C(9)-C(10)-C(11)-C(12)	0.6(6)	C(27)-C(28)-C(29)-C(30)	-174.4(4)
C(10)-C(11)-C(12)-C(7)	-0.9(6)	C(34)-N(2)-C(30)-C(31)	-1.8(5)
C(8)-C(7)-C(12)-C(11)	-0.1(6)	Th(1)-N(2)-C(30)-C(31)	-178.1(3)
S(2)-C(7)-C(12)-C(11)	-175.8(3)	C(34)-N(2)-C(30)-C(29)	-179.4(3)
Th(1)-S(3)-C(13)-C(14)	84.1(3)	Th(1)-N(2)-C(30)-C(29)	4.3(4)
Th(1)-S(3)-C(13)-C(18)	-101.5(3)	N(1)-C(29)-C(30)-N(2)	15.4(5)
C(18)-C(13)-C(14)-C(15)	-2.8(6)	C(28)-C(29)-C(30)-N(2)	-166.9(3)
S(3)-C(13)-C(14)-C(15)	171.8(3)	N(1)-C(29)-C(30)-C(31)	-162.3(3)
C(13)-C(14)-C(15)-C(16)	1.6(6)	C(28)-C(29)-C(30)-C(31)	15.4(5)
C(14)-C(15)-C(16)-C(17)	0.5(6)	N(2)-C(30)-C(31)-C(32)	-0.7(6)
C(15)-C(16)-C(17)-C(18)	-1.3(7)	C(29)-C(30)-C(31)-C(32)	176.9(3)
C(16)-C(17)-C(18)-C(13)	0.1(6)	C(30)-C(31)-C(32)-C(33)	1.2(6)
C(14)-C(13)-C(18)-C(17)	1.9(6)	C(31)-C(32)-C(33)-C(34)	0.6(6)
S(3)-C(13)-C(18)-C(17)	-172.6(3)	C(30)-N(2)-C(34)-C(33)	3.7(5)
Th(1)-S(4)-C(19)-C(20)	88.7(3)	Th(1)-N(2)-C(34)-C(33)	179.9(3)
Th(1)-S(4)-C(19)-C(24)	-92.8(3)	C(30)-N(2)-C(34)-C(35)	-177.9(3)
C(24)-C(19)-C(20)-C(21)	-1.2(6)	Th(1)-N(2)-C(34)-C(35)	-1.6(4)
S(4)-C(19)-C(20)-C(21)	177.3(3)	C(32)-C(33)-C(34)-N(2)	-3.2(6)

C(32)-C(33)-C(34)-C(35)	178.5(3)	N(4)-C(40)-C(41)-C(42)	0.0(6)
C(39)-N(3)-C(35)-C(36)	5.0(5)	C(40)-C(41)-C(42)-C(43)	0.5(6)
Th(1)-N(3)-C(35)-C(36)	-172.6(2)	C(41)-C(42)-C(43)-C(44)	-1.1(6)
C(39)-N(3)-C(35)-C(34)	-174.4(3)	C(40)-N(4)-C(44)-C(43)	-0.9(6)
Th(1)-N(3)-C(35)-C(34)	8.0(4)	Th(1)-N(4)-C(44)-C(43)	171.1(3)
N(2)-C(34)-C(35)-N(3)	-4.1(5)	C(42)-C(43)-C(44)-N(4)	1.4(6)
C(33)-C(34)-C(35)-N(3)	174.3(3)	C(49)-N(5)-C(45)-C(46)	-1.2(7)
N(2)-C(34)-C(35)-C(36)	176.5(3)	N(5)-C(45)-C(46)-C(47)	1.0(7)
C(33)-C(34)-C(35)-C(36)	-5.1(5)	C(45)-C(46)-C(47)-C(48)	0.0(7)
N(3)-C(35)-C(36)-C(37)	-1.8(5)	C(46)-C(47)-C(48)-C(49)	-0.7(7)
C(34)-C(35)-C(36)-C(37)	177.6(3)	C(45)-N(5)-C(49)-C(48)	0.4(6)
C(35)-C(36)-C(37)-C(38)	-1.9(6)	C(47)-C(48)-C(49)-N(5)	0.5(7)
C(36)-C(37)-C(38)-C(39)	2.4(6)	C(54)-N(6)-C(50)-C(51)	-1.0(7)
C(35)-N(3)-C(39)-C(38)	-4.6(5)	N(6)-C(50)-C(51)-C(52)	1.1(8)
Th(1)-N(3)-C(39)-C(38)	173.0(3)	C(50)-C(51)-C(52)-C(53)	-0.2(7)
C(37)-C(38)-C(39)-N(3)	0.9(6)	C(51)-C(52)-C(53)-C(54)	-0.7(8)
C(44)-N(4)-C(40)-C(41)	0.2(5)	C(50)-N(6)-C(54)-C(53)	-0.1(8)
Th(1)-N(4)-C(40)-C(41)	-172.4(3)	C(52)-C(53)-C(54)-N(6)	0.9(9)

Table S36. Hydrogen bonds [Å and °] for **5**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...S(4)#1	0.95	2.99	3.885(4)	158.0
C(14)-H(14)...S(2)	0.95	2.99	3.455(4)	111.5
C(24)-H(24)...S(2)#1	0.95	2.97	3.748(4)	140.3
C(25)-H(25)...S(3)	0.95	2.80	3.518(4)	132.9
C(26)-H(26)...N(5)	0.95	2.55	3.247(5)	130.3
C(31)-H(31)...S(2)#2	0.95	2.97	3.755(4)	140.5
C(36)-H(36)...N(6)#3	0.95	2.48	3.402(5)	164.3
C(38)-H(38)...S(3)#1	0.95	2.97	3.765(4)	142.4
C(39)-H(39)...S(2)	0.95	2.74	3.432(4)	130.6
C(40)-H(40)...S(2)	0.95	2.85	3.545(3)	131.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+3/2,y-1/2,-z+1/2 #3 x,y,z-1

8. Crystal structure unit cell packing diagrams for 1-5.

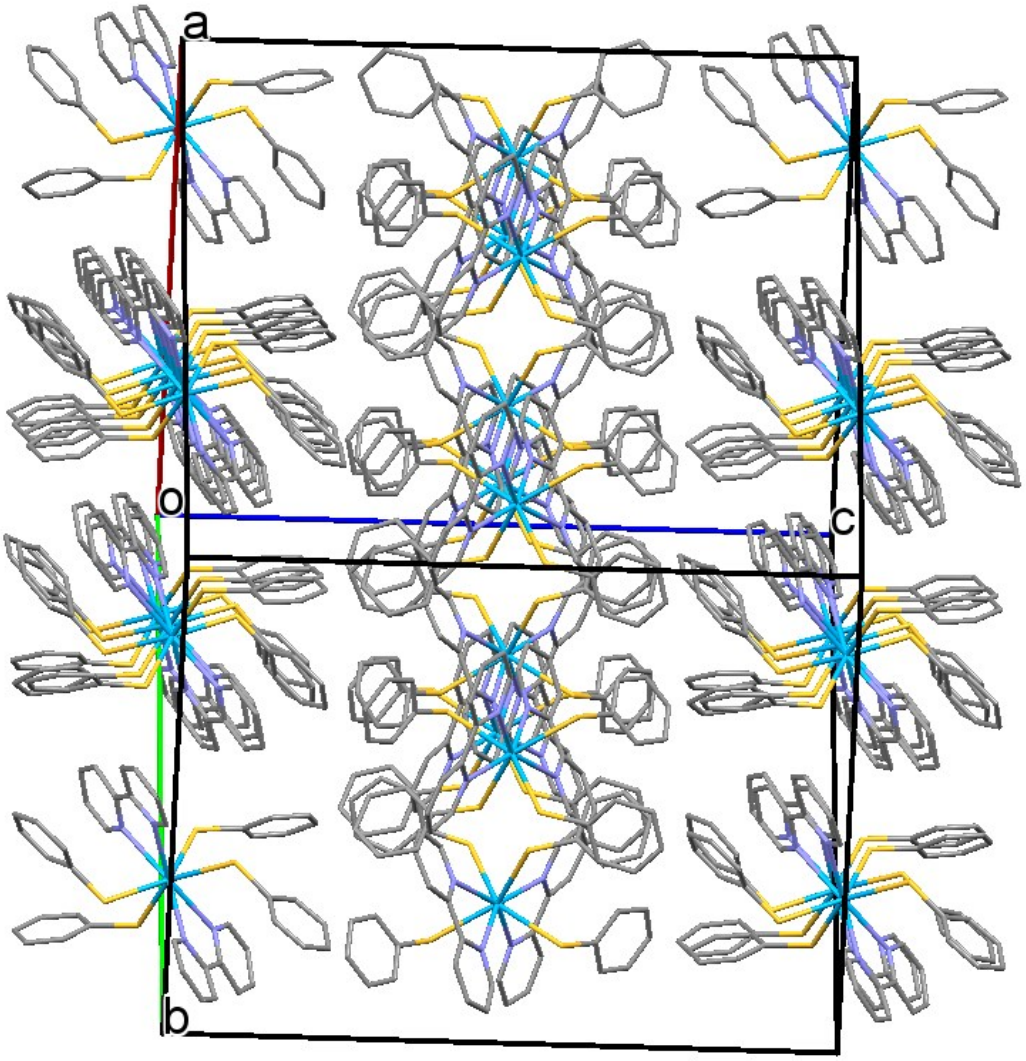

Figure S22. Unit cell packing viewed along the crystallographic **(a+b)**-axis for **$(bipy)_2Th(SPh)_4$ (1).**

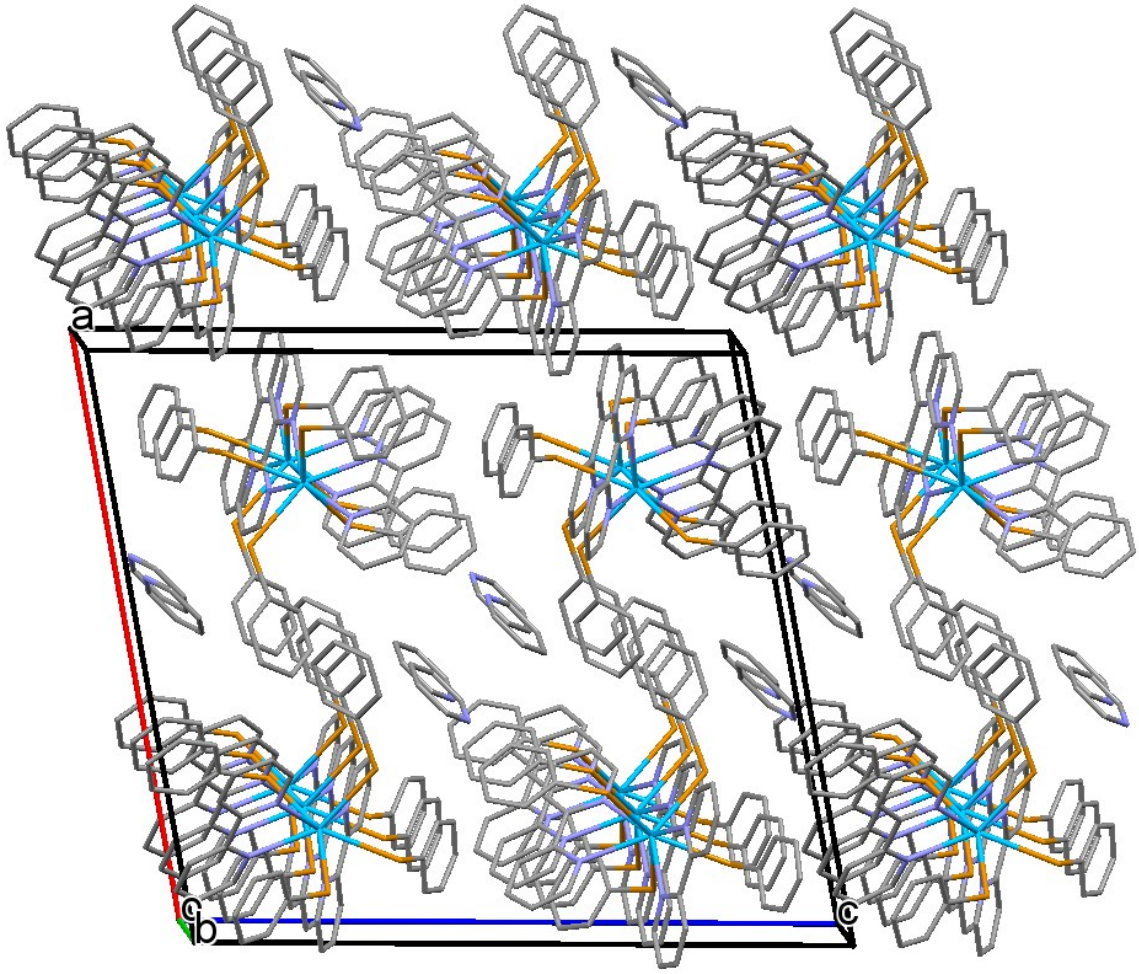

Figure S23. Unit cell packing viewed along the crystallographic **b**-axis for **$(bipy)_2Th(SePh)_4 \cdot py$ (2).**

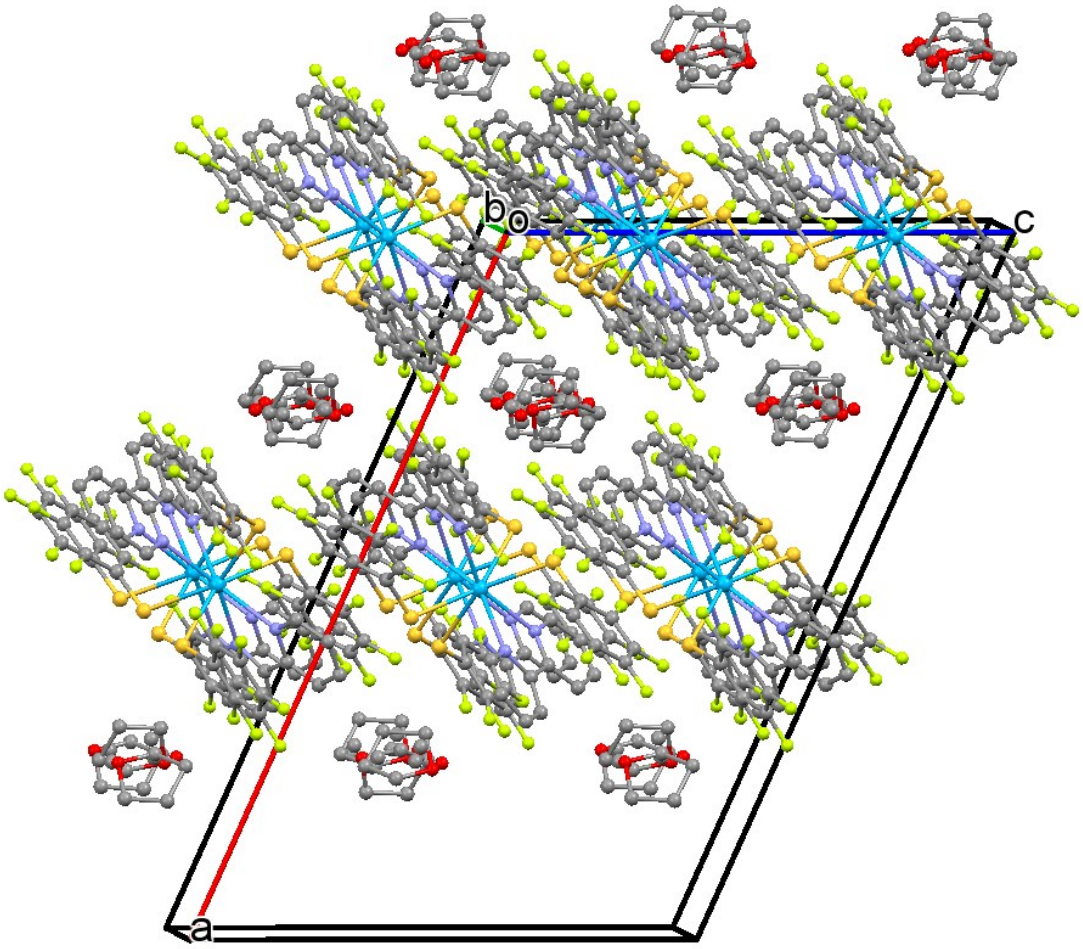

Figure S24. Unit cell packing viewed along the crystallographic **b**-axis for **$(bipy)_2Th(SC_6F_5)_4 \cdot 2THF$ (3).** Note that the crystal packing of the isomorphous **$(bipy)_2Th(SeC_6F_5)_4 \cdot 2THF$ (4)** is equivalent to that of **(3).**

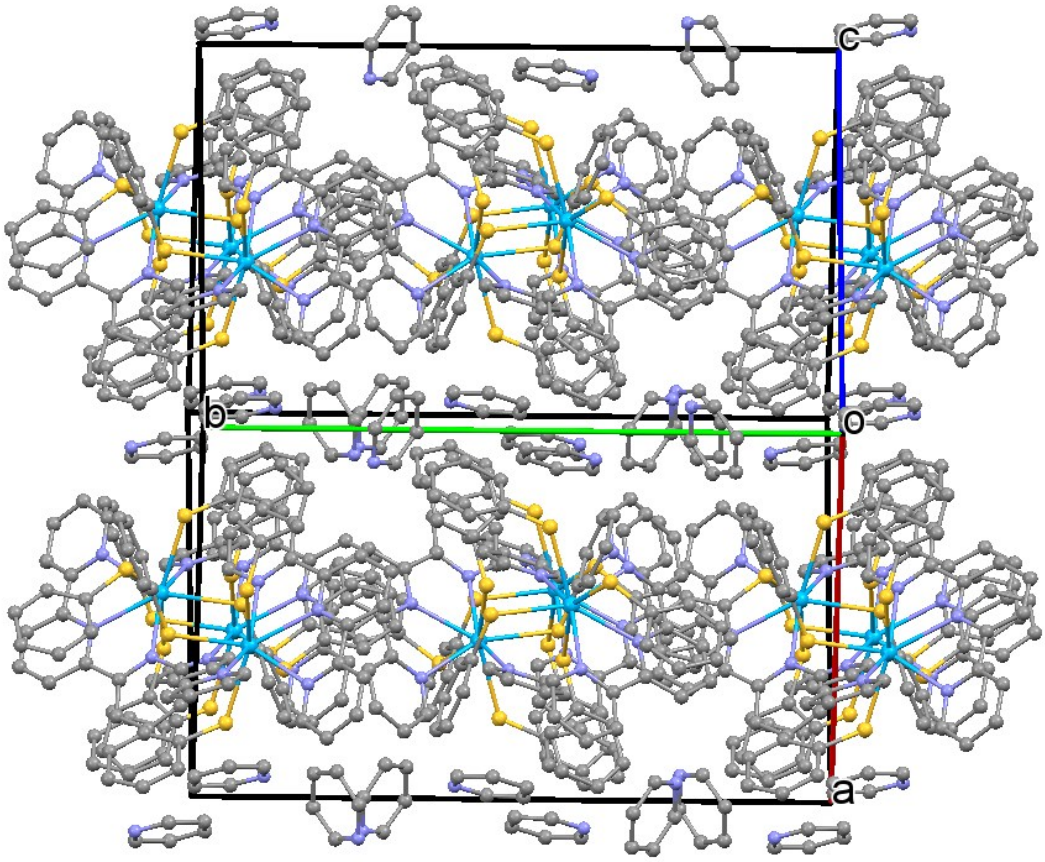

Figure S25. Unit cell packing viewed along the crystallographic **(a+c)**-axis for **(py)(terpy)Th(SPh)$_4$· 2py (5).**

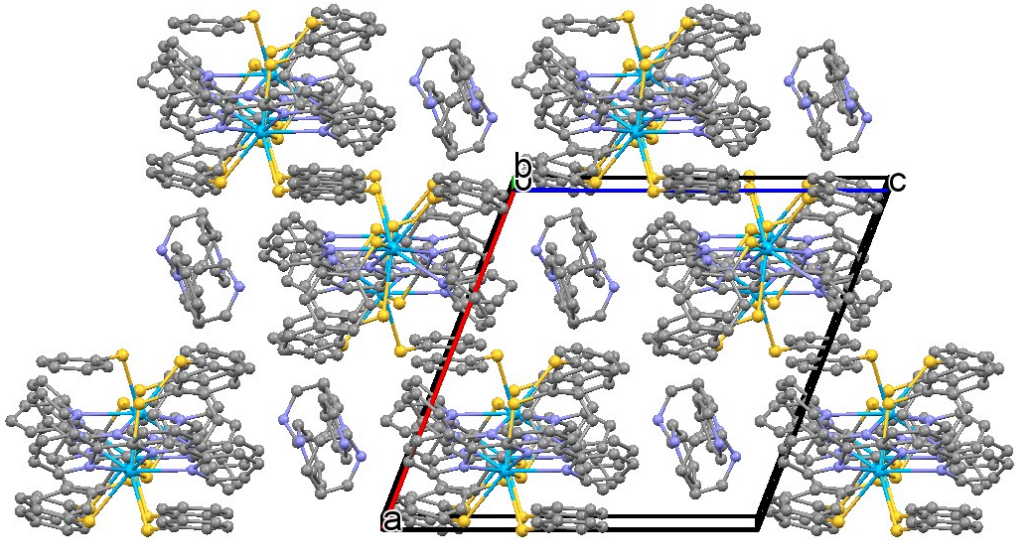

Figure S26. Unit cell packing viewed along the crystallographic **b**-axis for **(py)(terpy)Th(SPh)$_4$· 2py (5).**

9. Intra- and inter-molecular π…π interaction motifs for 1-5.

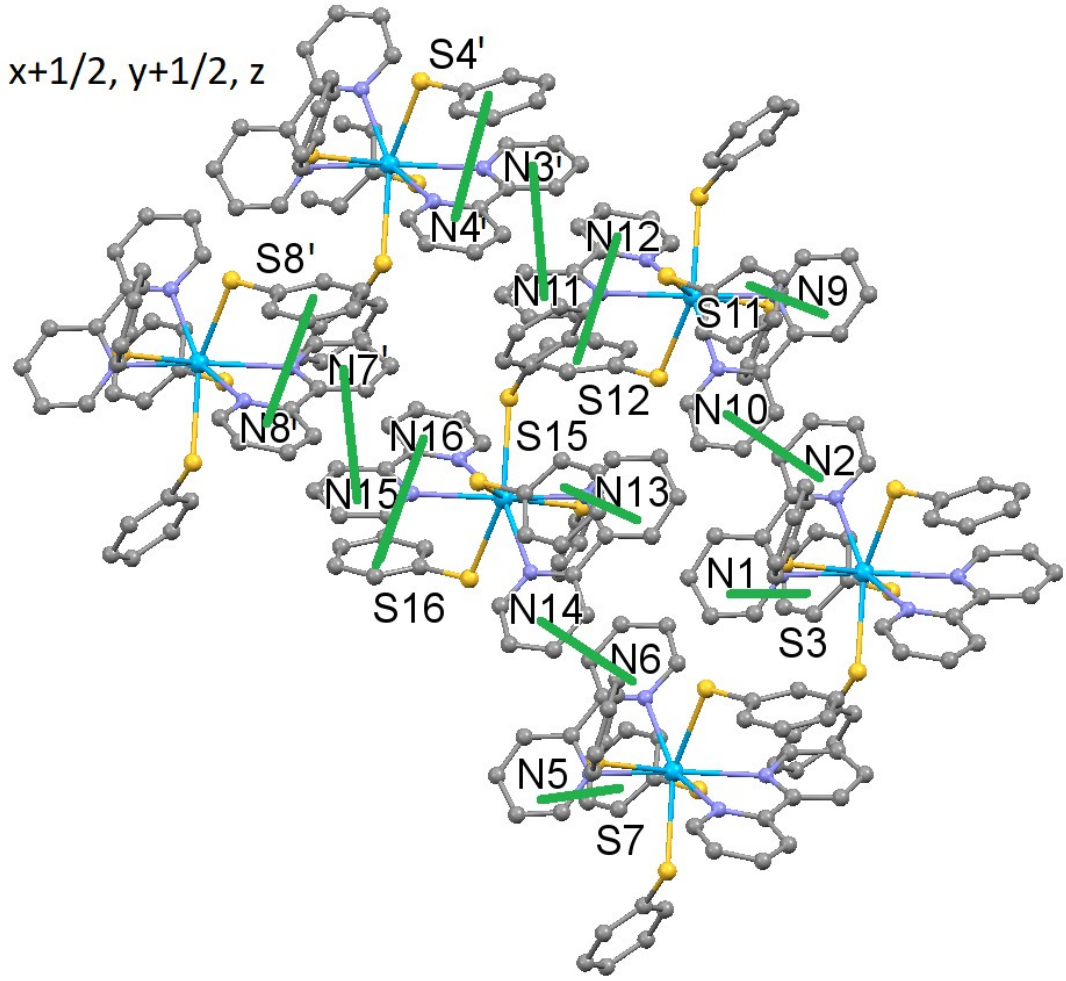

Figure S27. The intra- and inter-molecular π…π interactions in **$(bipy)_2Th(SPh)_4$ (1).** Green lines are drawn to show the pairs of rings having the π…π interactions listed in Table 1. Primed labels are for atoms related by the C-centering symmetry operation x+1/2, y+1/2, z.

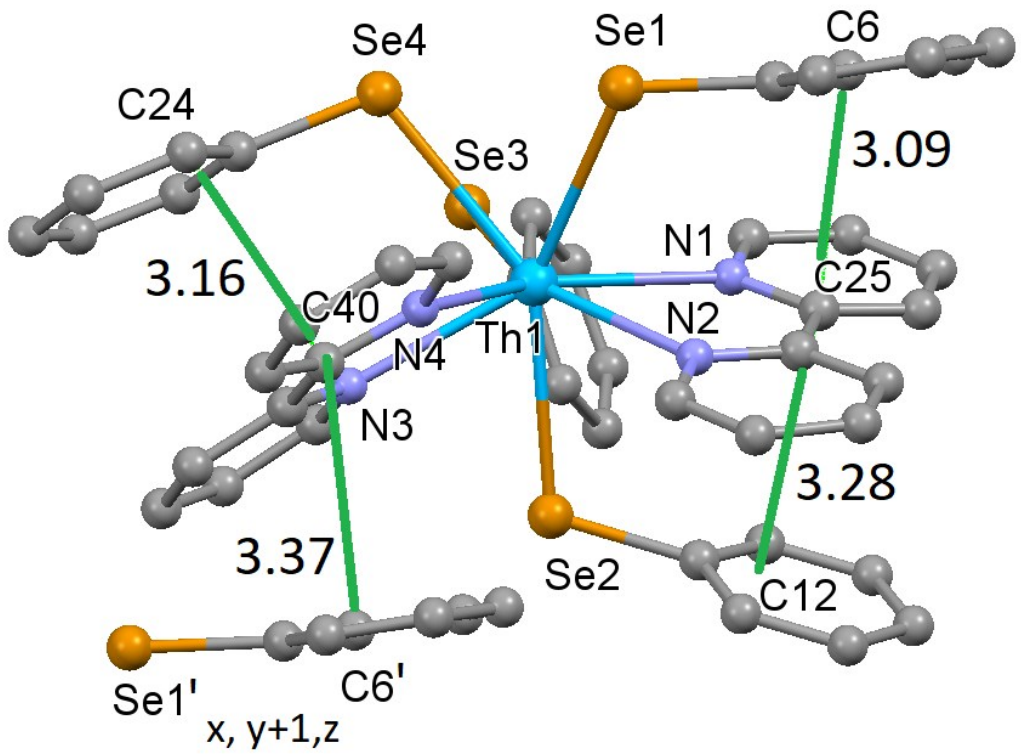

Figure S28. The intra- and inter-molecular π…π interactions in **$(bipy)_2Th(SePh)_4 \cdot py$ (2).** Green lines are drawn to show the pairs of rings having the π…π interactions listed in Table 1. Primed labels are for atoms related by the translation (y) symmetry operation x, y+1, z.

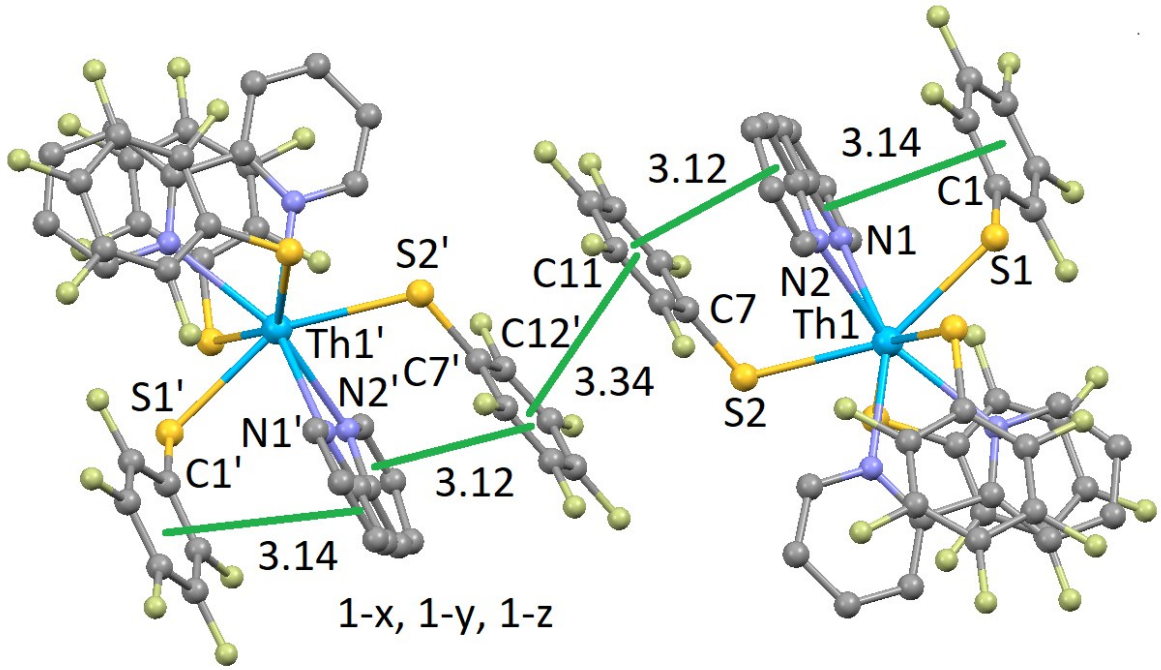

Figure S29. The intra- and inter-molecular π…π interactions in **$(bipy)_2Th(SC_6F_5)_4 \cdot 2THF$ (3).** Green lines are drawn to show the pairs of rings having the π…π interactions listed in Table 1. Primed labels are for atoms related by inversion/translation symmetry operation 1–x, 1-y, 1-z.

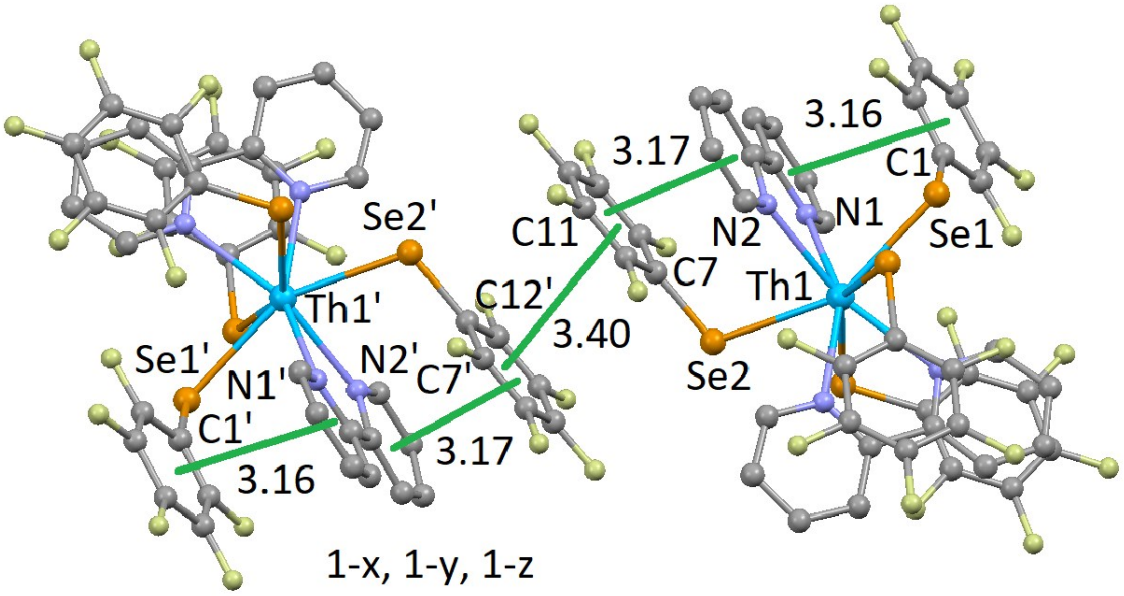

Figure S30. The intra- and inter-molecular π…π interactions in **$(bipy)_2Th(SeC_6F_5)_4 \cdot 2THF$ (4).** Green lines are drawn to show the pairs of rings having the π…π interactions listed in Table 1. Primed labels are for atoms related by inversion/translation symmetry operation 1–x, 1-y, 1-z.

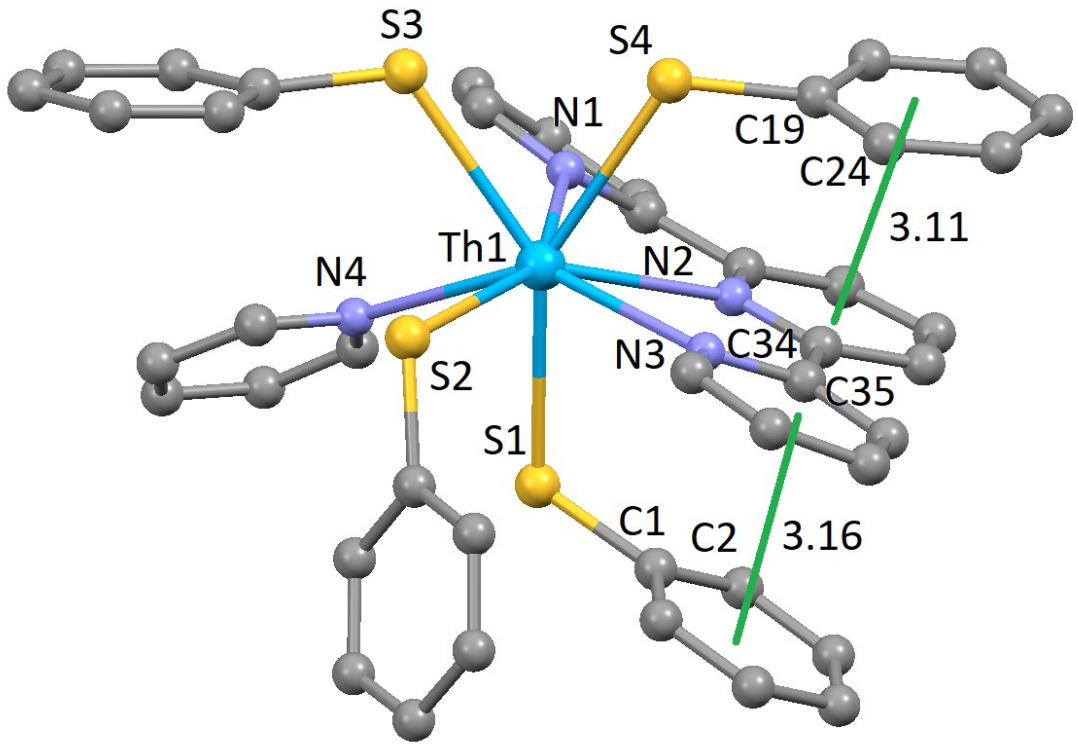

Figure S31. The intra-molecular π…π interactions in **(py)(terpy)Th(SPh)$_4$· 2py (5).** Green lines are drawn to show the pairs of rings having the π…π interactions listed in Table 1. Unlike **1 – 4**, there are no significant intermolecular π…π interactions in **5**.