

Inorganic Chemistry

including bioinorganic chemistry

Inorg. Chem., 1998, 37(17), 4162-4163, DOI:[10.1021/ic9805832](https://doi.org/10.1021/ic9805832)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

Table S1. Crystal data and structure refinement for Yb₄Se₄(SePh)₄py₈.

Identification code	YBPYSE2
Empirical formula	C ₆₄ H ₆₀ N ₈ Se ₈ Yb ₄ · 2.5(NC ₅ H ₅)
Formula weight	2462.79
Temperature	153(5) K
Radiation type, wavelength	MoK α , 0.71073 Å
Crystal system, space group	Triclinic, P-1
Number, θ range, for cell data	25, 17.0 < θ < 19.1 deg
Unit cell dimensions	a = 13.752(3) Å α = 89.45(1) deg b = 17.059(2) Å β = 75.97(1) deg c = 18.548(2) Å γ = 71.72(2) deg
Volume	3998.0(11) Å ³
Z, Calculated density	2, 2.046 Mg/m ³
Absorption coefficient	8.325 mm ⁻¹
F(000)	2314
Crystal colour, shape	red, lathe or rod
Crystal size	0.40 x 0.34 x 0.14 mm
θ range for data collection	2.19 to 22.50 deg.
Index ranges	0 ≤ h ≤ 14, -17 ≤ k ≤ 18, -19 ≤ l ≤ 19
Reflections collected / unique	10773 / 10234 [R(int) = 0.0208]
Completeness to 2 θ = 22.50	97.9%
Transmission factors, method	0.221 to 0.999, empirical ϕ -scan (MOLEN)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10234 / 1314 / 922
Goodness-of-fit on F ²	1.073
Final R indices [I > 2 σ (I)]	R1 = 0.0449, wR2 = 0.1026
R indices (all data)	R1 = 0.0644, wR2 = 0.1105
Largest diff. peak and hole	1.6 and -2.2 e.Å ⁻³ near Yb atoms 1.3 and -0.9 e.Å ⁻³ elsewhere

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Yb}_4\text{Se}_4(\text{SePh})_4\text{py}_8$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Yb(1)	2511(1)	-604(1)	-2966(1)	22(1)
Yb(2)	1218(1)	1329(1)	-3949(1)	22(1)
Yb(3)	-325(1)	887(1)	-2009(1)	21(1)
Yb(4)	2145(1)	1577(1)	-2118(1)	20(1)
Se(1)	592(1)	12(1)	-3384(1)	22(1)
Se(2)	3119(1)	752(1)	-3510(1)	21(1)
Se(3)	306(1)	2236(1)	-2586(1)	22(1)
Se(4)	1542(1)	233(1)	-1579(1)	21(1)
Se(5)	4572(1)	-1441(1)	-2816(1)	34(1)
Se(6)	-511(1)	1741(1)	-4592(1)	34(1)
Se(7)	-1198(1)	-272(1)	-1191(1)	29(1)
Se(8)	3157(1)	2806(1)	-2548(1)	31(1)
N(1)	2062(8)	-1889(6)	-2649(5)	28(2)
N(2)	3288(8)	-1354(6)	-4201(5)	28(2)
N(3)	1802(8)	2415(6)	-4600(5)	29(2)
N(4)	2234(8)	492(6)	-5116(5)	25(2)
N(5)	-1096(8)	1703(6)	-795(5)	30(2)
N(6)	-2084(8)	1662(6)	-2187(5)	28(2)
N(7)	3595(7)	994(6)	-1513(5)	24(2)
N(8)	1107(7)	2411(7)	-955(5)	27(2)
C(1)	4549(11)	-1845(9)	-1846(8)	38(3)
C(2)	5069(11)	-2661(9)	-1768(8)	45(3)
C(3)	5119(12)	-2934(10)	-1065(9)	50(3)
C(4)	4617(12)	-2426(10)	-442(9)	49(3)
C(5)	4060(12)	-1612(10)	-500(8)	48(3)
C(6)	4021(11)	-1318(9)	-1197(8)	38(3)
C(7)	-700(11)	2836(9)	-4925(8)	42(3)
C(8)	-651(13)	2946(10)	-5666(9)	55(3)
C(9)	-689(16)	3713(11)	-5929(10)	72(4)
C(10)	-840(16)	4383(12)	-5444(11)	80(4)
C(11)	-941(15)	4263(11)	-4692(11)	73(4)
C(12)	-863(12)	3494(9)	-4438(9)	52(3)
C(13)	-1761(9)	-886(7)	-1746(6)	23(2)
C(14)	-1637(9)	-883(7)	-2511(7)	27(2)
C(15)	-2064(10)	-1332(8)	-2878(7)	35(3)
C(16)	-2633(11)	-1799(8)	-2485(8)	39(3)
C(17)	-2763(10)	-1832(8)	-1725(7)	32(3)
C(18)	-2302(10)	-1385(7)	-1360(7)	28(3)
C(19)	2947(10)	3541(8)	-1705(7)	32(3)
C(20)	2551(12)	4386(9)	-1730(8)	45(3)
C(21)	2368(13)	4916(11)	-1094(9)	60(4)
C(22)	2543(13)	4595(10)	-436(9)	58(4)
C(23)	2990(12)	3761(10)	-431(8)	50(3)
C(24)	3183(11)	3229(9)	-1046(7)	37(3)
C(25)	2794(11)	-2617(8)	-2664(7)	37(3)
C(26)	2559(11)	-3349(8)	-2527(8)	41(3)
C(27)	1526(11)	-3317(9)	-2386(7)	40(3)
C(28)	761(11)	-2581(8)	-2348(7)	35(3)
C(29)	1040(10)	-1881(8)	-2491(6)	31(3)
C(30)	2829(10)	-1785(8)	-4502(7)	32(3)

C(31)	3322(11)	-2290(9)	-5155(7)	40(3)
C(32)	4316(11)	-2295(9)	-5537(7)	40(3)
C(33)	4792(11)	-1813(9)	-5247(7)	40(3)
C(34)	4261(10)	-1353(8)	-4589(7)	33(3)
C(35)	2200(12)	2878(8)	-4253(8)	42(3)
C(36)	2607(14)	3444(10)	-4606(10)	63(4)
C(37)	2635(14)	3553(10)	-5350(10)	64(4)
C(38)	2199(13)	3109(10)	-5703(9)	57(3)
C(39)	1804(11)	2527(9)	-5313(7)	39(3)
C(40)	1841(10)	17(8)	-5429(7)	32(3)
C(41)	2380(11)	-504(8)	-6062(7)	38(3)
C(42)	3388(11)	-504(8)	-6399(7)	38(3)
C(43)	3827(11)	9(8)	-6084(7)	35(3)
C(44)	3234(9)	494(8)	-5458(6)	30(3)
C(45)	-1620(10)	2486(8)	-741(7)	32(3)
C(46)	-2156(11)	2928(9)	-68(7)	41(3)
C(47)	-2141(11)	2551(9)	570(8)	44(3)
C(48)	-1584(11)	1731(9)	538(7)	35(3)
C(49)	-1061(10)	1313(8)	-154(6)	29(3)
C(50)	-2195(10)	2209(9)	-2704(7)	40(3)
C(51)	-3161(11)	2694(9)	-2797(7)	42(3)
C(52)	-4063(11)	2623(9)	-2327(8)	40(3)
C(53)	-3965(11)	2073(9)	-1808(8)	47(3)
C(54)	-2982(11)	1591(9)	-1743(8)	41(3)
C(55)	3601(10)	1139(8)	-798(6)	29(3)
C(56)	4478(10)	839(8)	-527(7)	32(3)
C(57)	5404(10)	347(8)	-989(7)	30(3)
C(58)	5426(10)	173(8)	-1717(7)	33(3)
C(59)	4506(10)	508(8)	-1955(7)	32(3)
C(60)	753(10)	3226(8)	-972(7)	33(3)
C(61)	261(11)	3742(9)	-340(8)	45(3)
C(62)	119(11)	3406(10)	339(8)	45(3)
C(63)	456(10)	2557(10)	372(7)	42(3)
C(64)	926(10)	2076(9)	-284(7)	33(3)
N(9)	108(11)	4561(10)	1986(9)	84(5)
C(65)	-184(11)	5279(9)	2441(10)	68(5)
C(66)	517(15)	5425(11)	2790(13)	107(6)
C(67)	1563(14)	4887(13)	2636(14)	116(6)
C(68)	1826(12)	4131(11)	2227(13)	101(6)
C(69)	1086(13)	3982(9)	1909(11)	81(5)
N(10)	3581(14)	5106(14)	6041(13)	120(6)
C(70)	3853(17)	5798(13)	5771(14)	116(7)
C(71)	4805(19)	5876(13)	5815(15)	120(7)
C(72)	5512(16)	5259(17)	6092(17)	134(7)
C(73)	5245(18)	4562(14)	6352(16)	128(7)
C(74)	4266(19)	4517(13)	6372(15)	121(7)
N(11)	4430(4)	5380(3)	811(19)	208(15)
C(75)	3330(4)	5600(4)	1010(3)	211(16)
C(76)	2790(2)	5550(4)	1740(3)	216(16)
C(77)	3370(4)	5190(4)	2250(2)	213(16)
C(78)	4450(4)	5070(4)	2070(3)	210(16)
C(79)	4970(3)	5190(4)	1370(3)	207(15)

Table S3. Bond lengths [Å] and angles [deg] for Yb₄Se₄(SePh)₄py₈.

Yb(1)-N(2)	2.458(9)	Yb(1)-N(1)	2.487(10)
Yb(1)-Se(4)	2.764(1)	Yb(1)-Se(2)	2.797(1)
Yb(1)-Se(1)	2.812(1)	Yb(1)-Se(5)	2.827(2)
Yb(2)-N(3)	2.440(10)	Yb(2)-N(4)	2.454(9)
Yb(2)-Se(1)	2.760(1)	Yb(2)-Se(3)	2.770(1)
Yb(2)-Se(2)	2.806(1)	Yb(2)-Se(6)	2.808(2)
Yb(3)-N(6)	2.466(10)	Yb(3)-N(5)	2.472(10)
Yb(3)-Se(4)	2.767(1)	Yb(3)-Se(1)	2.767(1)
Yb(3)-Se(3)	2.820(1)	Yb(3)-Se(7)	2.863(1)
Yb(4)-N(8)	2.451(9)	Yb(4)-N(7)	2.459(9)
Yb(4)-Se(2)	2.765(1)	Yb(4)-Se(3)	2.769(1)
Yb(4)-Se(4)	2.772(1)	Yb(4)-Se(8)	2.869(1)
Se(5)-C(1)	1.917(13)	Se(6)-C(7)	1.921(15)
Se(7)-C(13)	1.916(12)	Se(8)-C(19)	1.921(13)
N(1)-C(25)	1.325(16)	N(1)-C(29)	1.360(16)
N(2)-C(30)	1.311(15)	N(2)-C(34)	1.358(15)
N(3)-C(39)	1.334(16)	N(3)-C(35)	1.338(16)
N(4)-C(40)	1.313(15)	N(4)-C(44)	1.368(15)
N(5)-C(45)	1.295(16)	N(5)-C(49)	1.361(15)
N(6)-C(50)	1.333(16)	N(6)-C(54)	1.348(16)
N(7)-C(59)	1.339(15)	N(7)-C(55)	1.353(15)
N(8)-C(60)	1.324(16)	N(8)-C(64)	1.366(16)
C(1)-C(2)	1.376(19)	C(1)-C(6)	1.404(19)
C(2)-C(3)	1.39(2)	C(3)-C(4)	1.35(2)
C(4)-C(5)	1.38(2)	C(5)-C(6)	1.388(19)
C(7)-C(8)	1.37(2)	C(7)-C(12)	1.38(2)
C(8)-C(9)	1.38(2)	C(9)-C(10)	1.39(2)
C(10)-C(11)	1.39(2)	C(11)-C(12)	1.37(2)
C(13)-C(14)	1.387(16)	C(13)-C(18)	1.386(16)
C(14)-C(15)	1.372(17)	C(15)-C(16)	1.372(19)
C(16)-C(17)	1.380(18)	C(17)-C(18)	1.402(17)
C(19)-C(20)	1.377(19)	C(19)-C(24)	1.397(18)
C(20)-C(21)	1.42(2)	C(21)-C(22)	1.38(2)
C(22)-C(23)	1.36(2)	C(23)-C(24)	1.385(19)
C(25)-C(26)	1.392(19)	C(26)-C(27)	1.364(19)
C(27)-C(28)	1.351(19)	C(28)-C(29)	1.368(18)
C(30)-C(31)	1.388(17)	C(31)-C(32)	1.377(19)
C(32)-C(33)	1.381(19)	C(33)-C(34)	1.365(18)
C(35)-C(36)	1.35(2)	C(36)-C(37)	1.38(2)
C(37)-C(38)	1.36(2)	C(38)-C(39)	1.39(2)
C(40)-C(41)	1.379(18)	C(41)-C(42)	1.376(19)
C(42)-C(43)	1.407(18)	C(43)-C(44)	1.355(17)
C(45)-C(46)	1.376(18)	C(46)-C(47)	1.344(19)
C(47)-C(48)	1.36(2)	C(48)-C(49)	1.386(17)
C(50)-C(51)	1.378(18)	C(51)-C(52)	1.372(19)
C(52)-C(53)	1.338(19)	C(53)-C(54)	1.377(19)
C(55)-C(56)	1.367(17)	C(56)-C(57)	1.369(17)
C(57)-C(58)	1.377(17)	C(58)-C(59)	1.391(18)
C(60)-C(61)	1.366(18)	C(61)-C(62)	1.38(2)
C(62)-C(63)	1.38(2)	C(63)-C(64)	1.370(18)
N(9)-C(69)	1.372(13)	N(9)-C(65)	1.386(13)
C(65)-C(66)	1.367(14)	C(66)-C(67)	1.403(14)
C(67)-C(68)	1.402(14)	C(68)-C(69)	1.381(14)
N(10)-C(74)	1.396(14)	N(10)-C(70)	1.399(14)
C(70)-C(71)	1.378(14)	C(71)-C(72)	1.380(14)
C(72)-C(73)	1.400(14)	C(73)-C(74)	1.364(14)
N(11)-C(75)	1.387(15)	N(11)-C(79)	1.392(16)

C(75)-C(76)	1.393(16)	C(76)-C(77)	1.409(16)
C(77)-C(78)	1.392(16)	C(78)-C(79)	1.377(15)
N(2)-Yb(1)-N(1)	82.0(3)	N(2)-Yb(1)-Se(4)	177.2(2)
N(1)-Yb(1)-Se(4)	96.5(2)	N(2)-Yb(1)-Se(2)	90.7(2)
N(1)-Yb(1)-Se(2)	172.6(2)	Se(4)-Yb(1)-Se(2)	90.83(4)
N(2)-Yb(1)-Se(1)	87.7(2)	N(1)-Yb(1)-Se(1)	88.0(2)
Se(4)-Yb(1)-Se(1)	89.87(4)	Se(2)-Yb(1)-Se(1)	91.28(4)
N(2)-Yb(1)-Se(5)	80.6(2)	N(1)-Yb(1)-Se(5)	88.2(2)
Se(4)-Yb(1)-Se(5)	101.71(4)	Se(2)-Yb(1)-Se(5)	91.07(4)
Se(1)-Yb(1)-Se(5)	168.15(4)	N(3)-Yb(2)-N(4)	83.3(3)
N(3)-Yb(2)-Se(1)	172.9(2)	N(4)-Yb(2)-Se(1)	90.2(2)
N(3)-Yb(2)-Se(3)	95.5(2)	N(4)-Yb(2)-Se(3)	172.9(2)
Se(1)-Yb(2)-Se(3)	91.28(4)	N(3)-Yb(2)-Se(2)	90.1(2)
N(4)-Yb(2)-Se(2)	84.9(2)	Se(1)-Yb(2)-Se(2)	92.19(4)
Se(3)-Yb(2)-Se(2)	88.11(4)	N(3)-Yb(2)-Se(6)	89.5(2)
N(4)-Yb(2)-Se(6)	86.1(2)	Se(1)-Yb(2)-Se(6)	87.17(4)
Se(3)-Yb(2)-Se(6)	100.92(4)	Se(2)-Yb(2)-Se(6)	170.95(4)
N(6)-Yb(3)-N(5)	81.0(3)	N(6)-Yb(3)-Se(4)	169.0(2)
N(5)-Yb(3)-Se(4)	88.4(2)	N(6)-Yb(3)-Se(1)	99.8(2)
N(5)-Yb(3)-Se(1)	177.7(2)	Se(4)-Yb(3)-Se(1)	90.77(4)
N(6)-Yb(3)-Se(3)	86.3(2)	N(5)-Yb(3)-Se(3)	87.7(2)
Se(4)-Yb(3)-Se(3)	90.80(4)	Se(1)-Yb(3)-Se(3)	90.08(4)
N(6)-Yb(3)-Se(7)	89.8(2)	N(5)-Yb(3)-Se(7)	81.9(2)
Se(4)-Yb(3)-Se(7)	91.14(4)	Se(1)-Yb(3)-Se(7)	100.35(4)
Se(3)-Yb(3)-Se(7)	169.36(4)	N(8)-Yb(4)-N(7)	88.6(3)
N(8)-Yb(4)-Se(2)	172.9(2)	N(7)-Yb(4)-Se(2)	98.4(2)
N(8)-Yb(4)-Se(3)	84.1(2)	N(7)-Yb(4)-Se(3)	171.2(2)
Se(2)-Yb(4)-Se(3)	88.95(4)	N(8)-Yb(4)-Se(4)	90.7(2)
N(7)-Yb(4)-Se(4)	83.3(2)	Se(2)-Yb(4)-Se(4)	91.33(4)
Se(3)-Yb(4)-Se(4)	91.76(4)	N(8)-Yb(4)-Se(8)	90.0(2)
N(7)-Yb(4)-Se(8)	84.3(2)	Se(2)-Yb(4)-Se(8)	89.52(4)
Se(3)-Yb(4)-Se(8)	100.69(4)	Se(4)-Yb(4)-Se(8)	167.54(4)
Yb(2)-Se(1)-Yb(3)	89.97(4)	Yb(2)-Se(1)-Yb(1)	88.55(4)
Yb(3)-Se(1)-Yb(1)	89.15(4)	Yb(4)-Se(2)-Yb(1)	88.67(4)
Yb(4)-Se(2)-Yb(2)	91.01(4)	Yb(1)-Se(2)-Yb(2)	87.95(4)
Yb(4)-Se(3)-Yb(2)	91.68(4)	Yb(4)-Se(3)-Yb(3)	88.20(4)
Yb(2)-Se(3)-Yb(3)	88.67(4)	Yb(1)-Se(4)-Yb(3)	90.13(4)
Yb(1)-Se(4)-Yb(4)	89.18(4)	Yb(3)-Se(4)-Yb(4)	89.21(4)
C(1)-Se(5)-Yb(1)	111.7(4)	C(7)-Se(6)-Yb(2)	107.5(4)
C(13)-Se(7)-Yb(3)	115.1(3)	C(19)-Se(8)-Yb(4)	110.7(4)
C(25)-N(1)-C(29)	116.7(11)	C(25)-N(1)-Yb(1)	122.6(9)
C(29)-N(1)-Yb(1)	120.6(8)	C(30)-N(2)-C(34)	117.4(10)
C(30)-N(2)-Yb(1)	123.5(8)	C(34)-N(2)-Yb(1)	119.1(8)
C(39)-N(3)-C(35)	118.4(11)	C(39)-N(3)-Yb(2)	121.9(9)
C(35)-N(3)-Yb(2)	119.5(8)	C(40)-N(4)-C(44)	117.6(10)
C(40)-N(4)-Yb(2)	121.0(8)	C(44)-N(4)-Yb(2)	121.4(8)
C(45)-N(5)-C(49)	118.0(11)	C(45)-N(5)-Yb(3)	122.1(8)
C(49)-N(5)-Yb(3)	119.6(8)	C(50)-N(6)-C(54)	116.6(11)
C(50)-N(6)-Yb(3)	121.3(8)	C(54)-N(6)-Yb(3)	122.0(9)
C(59)-N(7)-C(55)	116.1(10)	C(59)-N(7)-Yb(4)	115.8(8)
C(55)-N(7)-Yb(4)	127.9(8)	C(60)-N(8)-C(64)	118.4(11)
C(60)-N(8)-Yb(4)	118.6(8)	C(64)-N(8)-Yb(4)	122.9(9)
C(2)-C(1)-C(6)	118.1(13)	C(2)-C(1)-Se(5)	120.6(11)
C(6)-C(1)-Se(5)	121.3(11)	C(1)-C(2)-C(3)	120.2(15)
C(4)-C(3)-C(2)	121.5(15)	C(3)-C(4)-C(5)	119.5(14)
C(4)-C(5)-C(6)	120.0(15)	C(5)-C(6)-C(1)	120.5(14)
C(8)-C(7)-C(12)	120.6(15)	C(8)-C(7)-Se(6)	118.5(12)
C(12)-C(7)-Se(6)	121.0(11)	C(7)-C(8)-C(9)	119.3(16)
C(8)-C(9)-C(10)	120.7(17)	C(11)-C(10)-C(9)	118.6(18)
C(12)-C(11)-C(10)	120.5(17)	C(11)-C(12)-C(7)	120.2(16)

C(14)-C(13)-C(18)	117.8(11)	C(14)-C(13)-Se(7)	124.5(9)
C(18)-C(13)-Se(7)	117.7(9)	C(13)-C(14)-C(15)	122.0(12)
C(16)-C(15)-C(14)	119.6(12)	C(15)-C(16)-C(17)	120.6(12)
C(16)-C(17)-C(18)	119.1(12)	C(13)-C(18)-C(17)	120.8(12)
C(20)-C(19)-C(24)	118.3(12)	C(20)-C(19)-Se(8)	121.1(10)
C(24)-C(19)-Se(8)	120.6(10)	C(19)-C(20)-C(21)	120.1(14)
C(22)-C(21)-C(20)	120.7(15)	C(23)-C(22)-C(21)	118.3(14)
C(22)-C(23)-C(24)	122.0(15)	C(23)-C(24)-C(19)	120.3(14)
N(1)-C(25)-C(26)	123.2(13)	C(27)-C(26)-C(25)	118.2(13)
C(28)-C(27)-C(26)	119.7(14)	C(27)-C(28)-C(29)	119.4(13)
N(1)-C(29)-C(28)	122.7(12)	N(2)-C(30)-C(31)	123.5(12)
C(32)-C(31)-C(30)	118.3(13)	C(31)-C(32)-C(33)	118.9(12)
C(34)-C(33)-C(32)	118.8(12)	N(2)-C(34)-C(33)	122.9(12)
N(3)-C(35)-C(36)	121.9(14)	C(35)-C(36)-C(37)	120.3(15)
C(38)-C(37)-C(36)	118.5(14)	C(37)-C(38)-C(39)	118.4(15)
N(3)-C(39)-C(38)	122.4(14)	N(4)-C(40)-C(41)	124.6(12)
C(42)-C(41)-C(40)	117.4(13)	C(41)-C(42)-C(43)	119.4(12)
C(44)-C(43)-C(42)	118.6(12)	C(43)-C(44)-N(4)	122.3(12)
N(5)-C(45)-C(46)	122.8(13)	C(47)-C(46)-C(45)	120.1(14)
C(46)-C(47)-C(48)	118.9(13)	C(47)-C(48)-C(49)	118.8(13)
N(5)-C(49)-C(48)	121.5(13)	N(6)-C(50)-C(51)	123.6(13)
C(52)-C(51)-C(50)	118.5(13)	C(53)-C(52)-C(51)	118.6(13)
C(52)-C(53)-C(54)	120.9(13)	N(6)-C(54)-C(53)	121.8(13)
N(7)-C(55)-C(56)	123.6(11)	C(55)-C(56)-C(57)	119.4(11)
C(56)-C(57)-C(58)	118.8(12)	C(57)-C(58)-C(59)	118.6(12)
N(7)-C(59)-C(58)	123.4(11)	N(8)-C(60)-C(61)	122.4(13)
C(60)-C(61)-C(62)	119.1(14)	C(61)-C(62)-C(63)	119.7(13)
C(64)-C(63)-C(62)	118.1(14)	N(8)-C(64)-C(63)	122.1(14)
C(69)-N(9)-C(65)	120.0(9)	C(66)-C(65)-N(9)	120.0(9)
C(65)-C(66)-C(67)	120.1(9)	C(66)-C(67)-C(68)	119.1(9)
C(69)-C(68)-C(67)	118.9(9)	N(9)-C(69)-C(68)	121.0(9)
C(74)-N(10)-C(70)	119.4(9)	C(71)-C(70)-N(10)	119.7(9)
C(70)-C(71)-C(72)	120.5(9)	C(71)-C(72)-C(73)	119.7(9)
C(74)-C(73)-C(72)	120.0(9)	C(73)-C(74)-N(10)	120.2(9)
C(75)-N(11)-C(79)	119.1(12)	N(11)-C(75)-C(76)	120.5(10)
C(75)-C(76)-C(77)	118.7(12)	C(78)-C(77)-C(76)	119.1(13)
C(79)-C(78)-C(77)	120.0(10)	C(78)-C(79)-N(11)	120.4(12)

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Yb}_4\text{Se}_4(\text{SePh})_4\text{py}_8$.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Yb(1)	20(1)	24(1)	21(1)	-2(1)	-3(1)	-7(1)
Yb(2)	20(1)	28(1)	18(1)	2(1)	-4(1)	-10(1)
Yb(3)	18(1)	26(1)	20(1)	0(1)	-2(1)	-8(1)
Yb(4)	19(1)	24(1)	18(1)	-2(1)	-4(1)	-7(1)
Se(1)	20(1)	27(1)	19(1)	0(1)	-3(1)	-11(1)
Se(2)	18(1)	27(1)	18(1)	-1(1)	-3(1)	-8(1)
Se(3)	19(1)	24(1)	22(1)	1(1)	-5(1)	-7(1)
Se(4)	21(1)	23(1)	20(1)	1(1)	-5(1)	-7(1)
Se(5)	23(1)	40(1)	37(1)	6(1)	-10(1)	-7(1)
Se(6)	29(1)	42(1)	36(1)	6(1)	-16(1)	-15(1)
Se(7)	35(1)	36(1)	23(1)	4(1)	-8(1)	-21(1)
Se(8)	30(1)	37(1)	30(1)	2(1)	-7(1)	-18(1)
N(1)	31(5)	27(5)	25(5)	0(4)	-6(4)	-10(4)
N(2)	31(5)	29(5)	22(5)	-4(4)	0(4)	-11(4)
N(3)	32(6)	23(5)	31(5)	1(4)	-2(4)	-12(4)
N(4)	27(5)	31(5)	18(5)	-3(4)	-8(4)	-6(4)
N(5)	37(6)	28(5)	25(4)	-2(4)	-4(4)	-14(4)
N(6)	25(5)	30(5)	34(5)	0(4)	-12(4)	-11(4)
N(7)	21(5)	29(5)	26(4)	3(4)	-7(4)	-14(4)
N(8)	14(5)	40(5)	28(4)	-8(4)	-5(4)	-9(4)
C(1)	32(7)	48(6)	44(6)	8(5)	-20(5)	-19(5)
C(2)	37(7)	44(6)	58(6)	7(5)	-22(6)	-12(6)
C(3)	47(7)	42(7)	70(7)	21(5)	-25(6)	-19(6)
C(4)	47(8)	60(7)	55(6)	19(5)	-28(6)	-26(6)
C(5)	46(7)	59(6)	49(6)	8(6)	-17(6)	-25(6)
C(6)	34(7)	37(6)	51(6)	8(5)	-19(5)	-17(5)
C(7)	33(7)	50(6)	51(6)	7(5)	-23(6)	-17(6)
C(8)	66(8)	59(7)	60(6)	18(6)	-40(7)	-30(7)
C(9)	97(9)	64(8)	66(7)	19(5)	-37(8)	-28(8)
C(10)	101(10)	58(7)	88(8)	16(6)	-39(8)	-24(8)
C(11)	88(9)	46(6)	81(7)	-3(6)	-33(8)	-7(8)
C(12)	50(8)	43(7)	63(7)	-3(5)	-19(6)	-10(7)
C(13)	22(6)	16(6)	31(5)	1(4)	-8(5)	-4(4)
C(14)	23(6)	24(6)	33(5)	-4(5)	-7(5)	-7(5)
C(15)	30(7)	44(7)	37(6)	-2(5)	-17(5)	-14(5)
C(16)	38(7)	35(7)	51(6)	-6(5)	-19(5)	-14(5)
C(17)	32(6)	22(6)	48(6)	6(5)	-15(5)	-11(5)
C(18)	31(6)	18(6)	35(5)	-1(4)	-4(5)	-10(5)
C(19)	28(6)	37(5)	41(6)	4(5)	-13(5)	-20(5)
C(20)	50(7)	38(6)	49(6)	5(5)	-19(6)	-12(6)
C(21)	64(8)	46(7)	64(7)	-8(5)	-19(7)	-8(7)
C(22)	62(8)	54(6)	58(7)	-24(6)	-24(7)	-12(7)
C(23)	51(8)	54(6)	47(6)	-12(5)	-22(6)	-10(6)
C(24)	36(7)	33(6)	44(6)	1(4)	-13(5)	-13(5)
C(25)	34(6)	24(5)	49(7)	-4(5)	-11(6)	-6(4)
C(26)	42(6)	24(5)	56(7)	-2(6)	-13(6)	-7(5)
C(27)	43(6)	33(5)	41(7)	-8(5)	-4(6)	-14(5)
C(28)	32(6)	38(6)	34(6)	-1(5)	-2(5)	-17(4)
C(29)	29(5)	34(5)	27(6)	-1(5)	-3(5)	-7(5)
C(30)	30(6)	41(7)	29(6)	-6(5)	-5(4)	-16(5)
C(31)	40(6)	44(7)	37(6)	-10(5)	-11(5)	-15(6)

C(32)	40(6)	46(7)	24(6)	-5(5)	-4(5)	-5(6)
C(33)	28(6)	54(7)	32(6)	1(5)	2(5)	-12(5)
C(34)	32(6)	38(7)	31(6)	-1(5)	-3(5)	-18(5)
C(35)	59(8)	28(6)	45(6)	6(5)	-21(6)	-18(6)
C(36)	85(9)	48(8)	72(7)	6(6)	-24(7)	-43(6)
C(37)	81(9)	48(8)	70(7)	23(6)	-4(7)	-42(7)
C(38)	72(9)	52(8)	45(7)	12(6)	-2(6)	-25(6)
C(39)	45(7)	38(7)	30(5)	5(5)	-3(5)	-13(5)
C(40)	32(6)	37(7)	30(6)	2(5)	-6(4)	-17(5)
C(41)	49(6)	33(7)	33(6)	-3(5)	-7(5)	-17(6)
C(42)	45(6)	37(7)	25(6)	-5(5)	0(5)	-8(5)
C(43)	30(6)	46(7)	25(6)	0(5)	-3(4)	-10(5)
C(44)	20(5)	41(7)	30(6)	-6(5)	-10(4)	-9(5)
C(45)	34(7)	29(5)	35(5)	3(5)	-9(5)	-14(5)
C(46)	38(7)	35(6)	44(6)	-7(4)	-2(5)	-10(5)
C(47)	43(7)	53(6)	32(5)	-13(5)	2(5)	-19(6)
C(48)	41(7)	49(6)	21(5)	-3(5)	-4(5)	-25(5)
C(49)	30(6)	36(6)	25(5)	5(4)	-5(5)	-18(5)
C(50)	26(5)	58(7)	27(6)	2(5)	-4(5)	-4(5)
C(51)	34(6)	51(7)	38(6)	10(5)	-15(5)	-7(5)
C(52)	24(5)	42(7)	49(7)	-2(5)	-11(5)	-3(5)
C(53)	24(5)	55(8)	62(7)	10(6)	-2(5)	-20(5)
C(54)	31(6)	40(7)	51(7)	6(5)	-8(5)	-13(5)
C(55)	30(5)	29(6)	23(5)	5(5)	-6(4)	-5(5)
C(56)	35(6)	36(7)	22(5)	0(5)	-13(4)	-4(5)
C(57)	31(6)	27(6)	31(5)	2(5)	-11(5)	-6(5)
C(58)	25(5)	35(7)	33(5)	-9(5)	-3(5)	-5(5)
C(59)	30(6)	31(6)	31(6)	-4(5)	-8(4)	-5(5)
C(60)	24(6)	40(6)	36(5)	-10(5)	-4(5)	-12(5)
C(61)	36(7)	40(6)	49(6)	-17(5)	1(6)	-7(6)
C(62)	27(7)	61(6)	38(5)	-23(5)	2(5)	-9(6)
C(63)	26(6)	66(6)	30(5)	-8(5)	-6(5)	-8(6)
C(64)	25(6)	50(6)	29(5)	-5(4)	-1(5)	-24(5)
N(9)	83(8)	85(9)	86(9)	-11(7)	-22(7)	-29(7)
C(65)	83(9)	54(8)	77(9)	13(7)	-30(7)	-29(7)
C(66)	109(10)	92(10)	123(11)	-22(8)	-61(9)	-12(8)
C(67)	112(9)	108(11)	132(12)	-35(9)	-68(9)	-11(8)
C(68)	99(9)	90(10)	117(11)	-18(8)	-47(9)	-19(8)
C(69)	75(9)	76(9)	97(10)	-12(8)	-17(8)	-33(7)
N(10)	130(11)	103(11)	127(11)	-6(9)	-18(9)	-48(8)
C(70)	129(11)	105(11)	108(12)	0(9)	-10(9)	-44(9)
C(71)	120(11)	117(11)	113(12)	10(9)	4(10)	-50(9)
C(72)	122(11)	137(12)	140(13)	23(10)	-9(9)	-54(9)
C(73)	128(11)	120(11)	135(12)	17(10)	-22(10)	-49(9)
C(74)	126(11)	102(11)	128(12)	0(9)	-12(10)	-42(9)
N(11)	208(18)	201(19)	231(18)	23(12)	-69(11)	-76(13)
C(75)	209(18)	205(19)	222(18)	26(12)	-60(11)	-67(13)
C(76)	216(17)	212(19)	216(19)	18(13)	-61(10)	-60(13)
C(77)	212(18)	213(19)	216(18)	13(12)	-61(11)	-64(13)
C(78)	211(18)	204(19)	220(18)	5(12)	-61(11)	-71(13)
C(79)	212(18)	200(19)	222(19)	9(13)	-65(10)	-76(13)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Yb}_4\text{Se}_4(\text{SePh})_4\text{py}_8$.

	x	y	z	U(eq)
H(2)	5394	-3040	-2196	54
H(3)	5516	-3492	-1023	60
H(4)	4649	-2628	34	59
H(5)	3702	-1251	-64	58
H(6)	3633	-757	-1235	46
H(8)	-591	2499	-5994	66
H(9)	-612	3784	-6446	87
H(10)	-873	4912	-5624	96
H(11)	-1065	4717	-4352	88
H(12)	-922	3416	-3923	63
H(14)	-1245	-561	-2788	32
H(15)	-1967	-1319	-3403	42
H(16)	-2938	-2103	-2738	46
H(17)	-3161	-2153	-1453	39
H(18)	-2360	-1425	-841	34
H(20)	2399	4614	-2175	55
H(21)	2123	5499	-1122	72
H(22)	2357	4946	4	69
H(23)	3174	3538	7	60
H(24)	3478	2649	-1020	44
H(25)	3514	-2640	-2774	44
H(26)	3103	-3858	-2532	50
H(27)	1344	-3811	-2313	48
H(28)	37	-2549	-2224	42
H(29)	498	-1370	-2480	38
H(30)	2122	-1750	-4259	39
H(31)	2981	-2625	-5334	48
H(32)	4669	-2623	-5992	47
H(33)	5476	-1802	-5501	48
H(34)	4587	-1017	-4395	39
H(35)	2195	2807	-3743	50
H(36)	2876	3768	-4342	75
H(37)	2952	3931	-5608	77
H(38)	2164	3194	-6205	69
H(39)	1526	2198	-5563	47
H(40)	1136	34	-5205	38
H(41)	2067	-850	-6257	45
H(42)	3785	-847	-6840	46
H(43)	4523	15	-6307	42
H(44)	3522	849	-5249	36
H(45)	-1634	2767	-1185	38
H(46)	-2538	3501	-55	49
H(47)	-2512	2852	1037	52
H(48)	-1556	1450	981	42
H(49)	-668	741	-181	35
H(50)	-1573	2268	-3025	48
H(51)	-3201	3069	-3179	50
H(52)	-4741	2956	-2369	48
H(53)	-4582	2014	-1480	56
H(54)	-2936	1198	-1376	49
H(55)	2960	1466	-466	34
H(56)	4445	971	-24	38

H(57)	6020	130	-810	36
H(58)	6056	-169	-2050	39
H(59)	4524	385	-2458	38
H(60)	845	3461	-1440	40
H(61)	20	4325	-370	54
H(62)	-210	3757	784	54
H(63)	364	2314	836	50
H(64)	1132	1491	-271	39
H(65)	-872	5669	2512	81
H(66)	297	5892	3136	128
H(67)	2085	5034	2807	139
H(68)	2503	3728	2169	121
H(69)	1256	3470	1632	97
H(70)	3384	6212	5558	139
H(71)	4976	6358	5654	144
H(72)	6177	5308	6106	161
H(73)	5745	4121	6515	153
H(74)	4049	4084	6613	145
H(75)	2948	5792	641	253
H(76)	2036	5765	1885	259
H(77)	3034	5021	2705	256
H(78)	4840	4896	2439	251
H(79)	5694	5148	1259	249

Table S6. Torsion angles [deg] for Yb₄Se₄(SePh)₄py₈.

N(3)-Yb(2)-Se(1)-Yb(3)	-163(2)	N(4)-Yb(2)-Se(1)-Yb(3)	172.9(2)
Se(3)-Yb(2)-Se(1)-Yb(3)	-0.21(4)	Se(2)-Yb(2)-Se(1)-Yb(3)	87.95(4)
Se(6)-Yb(2)-Se(1)-Yb(3)	-101.08(4)	N(3)-Yb(2)-Se(1)-Yb(1)	108(2)
N(4)-Yb(2)-Se(1)-Yb(1)	83.7(2)	Se(3)-Yb(2)-Se(1)-Yb(1)	-89.37(4)
Se(2)-Yb(2)-Se(1)-Yb(1)	-1.21(3)	Se(6)-Yb(2)-Se(1)-Yb(1)	169.76(4)
N(6)-Yb(3)-Se(1)-Yb(2)	86.5(2)	N(5)-Yb(3)-Se(1)-Yb(2)	-22(6)
Se(4)-Yb(3)-Se(1)-Yb(2)	-90.59(4)	Se(3)-Yb(3)-Se(1)-Yb(2)	0.21(4)
Se(7)-Yb(3)-Se(1)-Yb(2)	178.11(4)	N(6)-Yb(3)-Se(1)-Yb(1)	175.0(2)
N(5)-Yb(3)-Se(1)-Yb(1)	66(6)	Se(4)-Yb(3)-Se(1)-Yb(1)	-2.04(4)
Se(3)-Yb(3)-Se(1)-Yb(1)	88.76(4)	Se(7)-Yb(3)-Se(1)-Yb(1)	-93.33(4)
N(2)-Yb(1)-Se(1)-Yb(2)	-89.4(2)	N(1)-Yb(1)-Se(1)-Yb(2)	-171.5(2)
Se(4)-Yb(1)-Se(1)-Yb(2)	92.03(4)	Se(2)-Yb(1)-Se(1)-Yb(2)	1.21(3)
Se(5)-Yb(1)-Se(1)-Yb(2)	-100.1(2)	N(2)-Yb(1)-Se(1)-Yb(3)	-179.4(2)
N(1)-Yb(1)-Se(1)-Yb(3)	98.6(2)	Se(4)-Yb(1)-Se(1)-Yb(3)	2.04(4)
Se(2)-Yb(1)-Se(1)-Yb(3)	-88.78(4)	Se(5)-Yb(1)-Se(1)-Yb(3)	169.86(19)
N(8)-Yb(4)-Se(2)-Yb(1)	-106.2(19)	N(7)-Yb(4)-Se(2)-Yb(1)	83.4(2)
Se(3)-Yb(4)-Se(2)-Yb(1)	-91.72(4)	Se(4)-Yb(4)-Se(2)-Yb(1)	0.02(4)
Se(8)-Yb(4)-Se(2)-Yb(1)	167.59(4)	N(8)-Yb(4)-Se(2)-Yb(2)	-18.3(19)
N(7)-Yb(4)-Se(2)-Yb(2)	171.4(2)	Se(3)-Yb(4)-Se(2)-Yb(2)	-3.79(4)
Se(4)-Yb(4)-Se(2)-Yb(2)	87.95(4)	Se(8)-Yb(4)-Se(2)-Yb(2)	-104.49(4)
N(2)-Yb(1)-Se(2)-Yb(4)	177.6(2)	N(1)-Yb(1)-Se(2)-Yb(4)	174.1(18)
Se(4)-Yb(1)-Se(2)-Yb(4)	-0.02(4)	Se(1)-Yb(1)-Se(2)-Yb(4)	89.87(4)
Se(5)-Yb(1)-Se(2)-Yb(4)	-101.76(4)	N(2)-Yb(1)-Se(2)-Yb(2)	86.5(2)
N(1)-Yb(1)-Se(2)-Yb(2)	83.1(18)	Se(4)-Yb(1)-Se(2)-Yb(2)	-91.08(4)
Se(1)-Yb(1)-Se(2)-Yb(2)	-1.19(3)	Se(5)-Yb(1)-Se(2)-Yb(2)	167.19(4)
N(3)-Yb(2)-Se(2)-Yb(4)	99.3(2)	N(4)-Yb(2)-Se(2)-Yb(4)	-177.4(2)
Se(1)-Yb(2)-Se(2)-Yb(4)	-87.42(4)	Se(3)-Yb(2)-Se(2)-Yb(4)	3.79(4)
Se(6)-Yb(2)-Se(2)-Yb(4)	-173.2(3)	N(3)-Yb(2)-Se(2)-Yb(1)	-172.1(2)
N(4)-Yb(2)-Se(2)-Yb(1)	-88.8(2)	Se(1)-Yb(2)-Se(2)-Yb(1)	1.21(3)
Se(3)-Yb(2)-Se(2)-Yb(1)	92.42(4)	Se(6)-Yb(2)-Se(2)-Yb(1)	-84.6(3)
N(8)-Yb(4)-Se(3)-Yb(2)	-178.0(3)	N(7)-Yb(4)-Se(3)-Yb(2)	-143.1(15)
Se(2)-Yb(4)-Se(3)-Yb(2)	3.84(4)	Se(4)-Yb(4)-Se(3)-Yb(2)	-87.45(4)
Se(8)-Yb(4)-Se(3)-Yb(2)	93.16(4)	N(8)-Yb(4)-Se(3)-Yb(3)	-89.3(2)
N(7)-Yb(4)-Se(3)-Yb(3)	-54.5(15)	Se(2)-Yb(4)-Se(3)-Yb(3)	92.45(4)
Se(4)-Yb(4)-Se(3)-Yb(3)	1.16(3)	Se(8)-Yb(4)-Se(3)-Yb(3)	-178.23(3)
N(3)-Yb(2)-Se(3)-Yb(4)	-93.8(2)	N(4)-Yb(2)-Se(3)-Yb(4)	-13.6(19)
Se(1)-Yb(2)-Se(3)-Yb(4)	88.37(4)	Se(2)-Yb(2)-Se(3)-Yb(4)	-3.78(4)
Se(6)-Yb(2)-Se(3)-Yb(4)	175.73(4)	N(3)-Yb(2)-Se(3)-Yb(3)	178.1(2)
N(4)-Yb(2)-Se(3)-Yb(3)	-101.8(19)	Se(1)-Yb(2)-Se(3)-Yb(3)	0.21(4)
Se(2)-Yb(2)-Se(3)-Yb(3)	-91.94(4)	Se(6)-Yb(2)-Se(3)-Yb(3)	87.58(4)
N(6)-Yb(3)-Se(3)-Yb(4)	168.3(2)	N(5)-Yb(3)-Se(3)-Yb(4)	87.2(2)
Se(4)-Yb(3)-Se(3)-Yb(4)	-1.16(3)	Se(1)-Yb(3)-Se(3)-Yb(4)	-91.93(4)
Se(7)-Yb(3)-Se(3)-Yb(4)	99.3(2)	N(6)-Yb(3)-Se(3)-Yb(2)	-100.0(2)
N(5)-Yb(3)-Se(3)-Yb(2)	178.9(2)	Se(4)-Yb(3)-Se(3)-Yb(2)	90.57(4)
Se(1)-Yb(3)-Se(3)-Yb(2)	-0.21(4)	Se(7)-Yb(3)-Se(3)-Yb(2)	-169.0(2)
N(2)-Yb(1)-Se(4)-Yb(3)	-33(5)	N(1)-Yb(1)-Se(4)-Yb(3)	-90.0(2)
Se(2)-Yb(1)-Se(4)-Yb(3)	89.24(4)	Se(1)-Yb(1)-Se(4)-Yb(3)	-2.04(4)
Se(5)-Yb(1)-Se(4)-Yb(3)	-179.50(4)	N(2)-Yb(1)-Se(4)-Yb(4)	-122(5)
N(1)-Yb(1)-Se(4)-Yb(4)	-179.2(2)	Se(2)-Yb(1)-Se(4)-Yb(4)	0.02(4)
Se(1)-Yb(1)-Se(4)-Yb(4)	-91.25(4)	Se(5)-Yb(1)-Se(4)-Yb(4)	91.29(4)
N(6)-Yb(3)-Se(4)-Yb(1)	-162.5(12)	N(5)-Yb(3)-Se(4)-Yb(1)	-175.7(2)
Se(1)-Yb(3)-Se(4)-Yb(1)	2.07(4)	Se(3)-Yb(3)-Se(4)-Yb(1)	-88.02(4)
Se(7)-Yb(3)-Se(4)-Yb(1)	102.44(4)	N(6)-Yb(3)-Se(4)-Yb(4)	-73.3(12)
N(5)-Yb(3)-Se(4)-Yb(4)	-86.6(2)	Se(1)-Yb(3)-Se(4)-Yb(4)	91.25(4)
Se(3)-Yb(3)-Se(4)-Yb(4)	1.16(3)	Se(7)-Yb(3)-Se(4)-Yb(4)	-168.38(4)
N(8)-Yb(4)-Se(4)-Yb(1)	173.1(2)	N(7)-Yb(4)-Se(4)-Yb(1)	-98.4(2)
Se(2)-Yb(4)-Se(4)-Yb(1)	-0.02(4)	Se(3)-Yb(4)-Se(4)-Yb(1)	88.96(4)

Se(8)-Yb(4)-Se(4)-Yb(1)	-93.82(18)	N(8)-Yb(4)-Se(4)-Yb(3)	83.0(2)
N(7)-Yb(4)-Se(4)-Yb(3)	171.5(2)	Se(2)-Yb(4)-Se(4)-Yb(3)	-90.16(4)
Se(3)-Yb(4)-Se(4)-Yb(3)	-1.18(4)	Se(8)-Yb(4)-Se(4)-Yb(3)	176.04(17)
N(2)-Yb(1)-Se(5)-C(1)	-139.8(5)	N(1)-Yb(1)-Se(5)-C(1)	-57.6(5)
Se(4)-Yb(1)-Se(5)-C(1)	38.7(5)	Se(2)-Yb(1)-Se(5)-C(1)	129.7(5)
Se(1)-Yb(1)-Se(5)-C(1)	-128.9(5)	N(3)-Yb(2)-Se(6)-C(7)	-18.9(5)
N(4)-Yb(2)-Se(6)-C(7)	-102.3(5)	Se(1)-Yb(2)-Se(6)-C(7)	167.3(5)
Se(3)-Yb(2)-Se(6)-C(7)	76.5(5)	Se(2)-Yb(2)-Se(6)-C(7)	-106.5(5)
N(6)-Yb(3)-Se(7)-C(13)	62.9(4)	N(5)-Yb(3)-Se(7)-C(13)	143.8(5)
Se(4)-Yb(3)-Se(7)-C(13)	-128.0(4)	Se(1)-Yb(3)-Se(7)-C(13)	-37.1(4)
Se(3)-Yb(3)-Se(7)-C(13)	131.5(4)	N(8)-Yb(4)-Se(8)-C(19)	16.0(5)
N(7)-Yb(4)-Se(8)-C(19)	-72.6(5)	Se(2)-Yb(4)-Se(8)-C(19)	-171.1(4)
Se(3)-Yb(4)-Se(8)-C(19)	100.1(4)	Se(4)-Yb(4)-Se(8)-C(19)	-77.1(5)
N(2)-Yb(1)-N(1)-C(25)	65.5(9)	Se(4)-Yb(1)-N(1)-C(25)	-116.9(9)
Se(2)-Yb(1)-N(1)-C(25)	69(2)	Se(1)-Yb(1)-N(1)-C(25)	153.5(9)
Se(5)-Yb(1)-N(1)-C(25)	-15.3(9)	N(2)-Yb(1)-N(1)-C(29)	-110.7(9)
Se(4)-Yb(1)-N(1)-C(29)	66.9(8)	Se(2)-Yb(1)-N(1)-C(29)	-107.2(18)
Se(1)-Yb(1)-N(1)-C(29)	-22.7(8)	Se(5)-Yb(1)-N(1)-C(29)	168.5(8)
N(1)-Yb(1)-N(2)-C(30)	42.0(10)	Se(4)-Yb(1)-N(2)-C(30)	-16(6)
Se(2)-Yb(1)-N(2)-C(30)	-137.6(10)	Se(1)-Yb(1)-N(2)-C(30)	-46.3(10)
Se(5)-Yb(1)-N(2)-C(30)	131.5(10)	N(1)-Yb(1)-N(2)-C(34)	-135.6(9)
Se(4)-Yb(1)-N(2)-C(34)	167(4)	Se(2)-Yb(1)-N(2)-C(34)	44.8(9)
Se(1)-Yb(1)-N(2)-C(34)	136.1(9)	Se(5)-Yb(1)-N(2)-C(34)	-46.1(9)
N(4)-Yb(2)-N(3)-C(39)	42.3(10)	Se(1)-Yb(2)-N(3)-C(39)	18(3)
Se(3)-Yb(2)-N(3)-C(39)	-144.7(10)	Se(2)-Yb(2)-N(3)-C(39)	127.2(10)
Se(6)-Yb(2)-N(3)-C(39)	-43.8(10)	N(4)-Yb(2)-N(3)-C(35)	-133.1(10)
Se(1)-Yb(2)-N(3)-C(35)	-157.5(16)	Se(3)-Yb(2)-N(3)-C(35)	39.9(10)
Se(2)-Yb(2)-N(3)-C(35)	-48.2(10)	Se(6)-Yb(2)-N(3)-C(35)	140.8(10)
N(3)-Yb(2)-N(4)-C(40)	-134.1(10)	Se(1)-Yb(2)-N(4)-C(40)	43.0(9)
Se(3)-Yb(2)-N(4)-C(40)	145.1(16)	Se(2)-Yb(2)-N(4)-C(40)	135.2(9)
Se(6)-Yb(2)-N(4)-C(40)	-44.2(9)	N(3)-Yb(2)-N(4)-C(44)	46.8(9)
Se(1)-Yb(2)-N(4)-C(44)	-136.2(9)	Se(3)-Yb(2)-N(4)-C(44)	-34(3)
Se(2)-Yb(2)-N(4)-C(44)	-44.0(9)	Se(6)-Yb(2)-N(4)-C(44)	136.7(9)
N(6)-Yb(3)-N(5)-C(45)	-44.8(10)	Se(4)-Yb(3)-N(5)-C(45)	132.6(10)
Se(1)-Yb(3)-N(5)-C(45)	64(6)	Se(3)-Yb(3)-N(5)-C(45)	41.8(10)
Se(7)-Yb(3)-N(5)-C(45)	-136.0(10)	N(6)-Yb(3)-N(5)-C(49)	128.9(9)
Se(4)-Yb(3)-N(5)-C(49)	-53.6(9)	Se(1)-Yb(3)-N(5)-C(49)	-122(6)
Se(3)-Yb(3)-N(5)-C(49)	-144.5(9)	Se(7)-Yb(3)-N(5)-C(49)	37.8(8)
N(5)-Yb(3)-N(6)-C(50)	114.9(10)	Se(4)-Yb(3)-N(6)-C(50)	101.5(14)
Se(1)-Yb(3)-N(6)-C(50)	-62.9(10)	Se(3)-Yb(3)-N(6)-C(50)	26.6(9)
Se(7)-Yb(3)-N(6)-C(50)	-163.3(10)	N(5)-Yb(3)-N(6)-C(54)	-61.3(10)
Se(4)-Yb(3)-N(6)-C(54)	-74.7(17)	Se(1)-Yb(3)-N(6)-C(54)	120.9(9)
Se(3)-Yb(3)-N(6)-C(54)	-149.6(10)	Se(7)-Yb(3)-N(6)-C(54)	20.5(9)
N(8)-Yb(4)-N(7)-C(59)	-173.1(9)	Se(2)-Yb(4)-N(7)-C(59)	5.7(9)
Se(3)-Yb(4)-N(7)-C(59)	152.3(12)	Se(4)-Yb(4)-N(7)-C(59)	96.1(8)
Se(8)-Yb(4)-N(7)-C(59)	-82.9(8)	N(8)-Yb(4)-N(7)-C(55)	3.3(10)
Se(2)-Yb(4)-N(7)-C(55)	-177.9(9)	Se(3)-Yb(4)-N(7)-C(55)	-31(2)
Se(4)-Yb(4)-N(7)-C(55)	-87.6(10)	Se(8)-Yb(4)-N(7)-C(55)	93.4(10)
N(7)-Yb(4)-N(8)-C(60)	122.5(9)	Se(2)-Yb(4)-N(8)-C(60)	-48(2)
Se(3)-Yb(4)-N(8)-C(60)	-62.5(8)	Se(4)-Yb(4)-N(8)-C(60)	-154.2(8)
Se(8)-Yb(4)-N(8)-C(60)	38.2(8)	N(7)-Yb(4)-N(8)-C(64)	-53.9(9)
Se(2)-Yb(4)-N(8)-C(64)	135.6(17)	Se(3)-Yb(4)-N(8)-C(64)	121.1(9)
Se(4)-Yb(4)-N(8)-C(64)	29.4(8)	Se(8)-Yb(4)-N(8)-C(64)	-138.2(8)
Yb(1)-Se(5)-C(1)-C(2)	127.8(10)	Yb(1)-Se(5)-C(1)-C(6)	-53.3(11)
C(6)-C(1)-C(2)-C(3)	-4(2)	Se(5)-C(1)-C(2)-C(3)	174.9(11)
C(1)-C(2)-C(3)-C(4)	4(2)	C(2)-C(3)-C(4)-C(5)	-1(2)
C(3)-C(4)-C(5)-C(6)	0(2)	C(4)-C(5)-C(6)-C(1)	0(2)
C(2)-C(1)-C(6)-C(5)	2(2)	Se(5)-C(1)-C(6)-C(5)	-176.5(10)
Yb(2)-Se(6)-C(7)-C(8)	121.6(11)	Yb(2)-Se(6)-C(7)-C(12)	-57.3(13)
C(12)-C(7)-C(8)-C(9)	5(2)	Se(6)-C(7)-C(8)-C(9)	-174.2(13)
C(7)-C(8)-C(9)-C(10)	-4(3)	C(8)-C(9)-C(10)-C(11)	1(3)

C(9)-C(10)-C(11)-C(12)	2(3)	C(10)-C(11)-C(12)-C(7)	-1(3)
C(8)-C(7)-C(12)-C(11)	-2(2)	Se(6)-C(7)-C(12)-C(11)	176.6(13)
Yb(3)-Se(7)-C(13)-C(14)	9.3(11)	Yb(3)-Se(7)-C(13)-C(18)	-172.7(8)
C(18)-C(13)-C(14)-C(15)	2.4(18)	Se(7)-C(13)-C(14)-C(15)	-179.6(10)
C(13)-C(14)-C(15)-C(16)	0.0(19)	C(14)-C(15)-C(16)-C(17)	-1(2)
C(15)-C(16)-C(17)-C(18)	0(2)	C(14)-C(13)-C(18)-C(17)	-3.9(18)
Se(7)-C(13)-C(18)-C(17)	178.0(9)	C(16)-C(17)-C(18)-C(13)	2.9(19)
Yb(4)-Se(8)-C(19)-C(20)	-127.6(11)	Yb(4)-Se(8)-C(19)-C(24)	51.8(11)
C(24)-C(19)-C(20)-C(21)	-1(2)	Se(8)-C(19)-C(20)-C(21)	177.9(11)
C(19)-C(20)-C(21)-C(22)	-3(2)	C(20)-C(21)-C(22)-C(23)	6(3)
C(21)-C(22)-C(23)-C(24)	-6(3)	C(22)-C(23)-C(24)-C(19)	2(2)
C(20)-C(19)-C(24)-C(23)	2(2)	Se(8)-C(19)-C(24)-C(23)	-177.4(11)
C(29)-N(1)-C(25)-C(26)	-0.1(18)	Yb(1)-N(1)-C(25)-C(26)	-176.5(10)
N(1)-C(25)-C(26)-C(27)	1(2)	C(25)-C(26)-C(27)-C(28)	-3(2)
C(26)-C(27)-C(28)-C(29)	3(2)	C(25)-N(1)-C(29)-C(28)	0.4(17)
Yb(1)-N(1)-C(29)-C(28)	176.9(9)	C(27)-C(28)-C(29)-N(1)	-2.0(19)
C(34)-N(2)-C(30)-C(31)	6(2)	Yb(1)-N(2)-C(30)-C(31)	-171.8(10)
N(2)-C(30)-C(31)-C(32)	-5(2)	C(30)-C(31)-C(32)-C(33)	1(2)
C(31)-C(32)-C(33)-C(34)	0(2)	C(30)-N(2)-C(34)-C(33)	-3.8(19)
Yb(1)-N(2)-C(34)-C(33)	173.9(10)	C(32)-C(33)-C(34)-N(2)	1(2)
C(39)-N(3)-C(35)-C(36)	-1(2)	Yb(2)-N(3)-C(35)-C(36)	174.9(12)
N(3)-C(35)-C(36)-C(37)	-1(3)	C(35)-C(36)-C(37)-C(38)	3(3)
C(36)-C(37)-C(38)-C(39)	-4(3)	C(35)-N(3)-C(39)-C(38)	0(2)
Yb(2)-N(3)-C(39)-C(38)	-175.8(11)	C(37)-C(38)-C(39)-N(3)	3(2)
C(44)-N(4)-C(40)-C(41)	2.8(19)	Yb(2)-N(4)-C(40)-C(41)	-176.4(10)
N(4)-C(40)-C(41)-C(42)	-2(2)	C(40)-C(41)-C(42)-C(43)	1(2)
C(41)-C(42)-C(43)-C(44)	0(2)	C(42)-C(43)-C(44)-N(4)	1(2)
C(40)-N(4)-C(44)-C(43)	-2.2(19)	Yb(2)-N(4)-C(44)-C(43)	177.0(10)
C(49)-N(5)-C(45)-C(46)	-1.6(19)	Yb(3)-N(5)-C(45)-C(46)	172.3(10)
N(5)-C(45)-C(46)-C(47)	1(2)	C(45)-C(46)-C(47)-C(48)	0(2)
C(46)-C(47)-C(48)-C(49)	-1(2)	C(45)-N(5)-C(49)-C(48)	1.3(18)
Yb(3)-N(5)-C(49)-C(48)	-172.7(9)	C(47)-C(48)-C(49)-N(5)	-0.3(19)
C(54)-N(6)-C(50)-C(51)	0(2)	Yb(3)-N(6)-C(50)-C(51)	-176.0(11)
N(6)-C(50)-C(51)-C(52)	1(2)	C(50)-C(51)-C(52)-C(53)	-1(2)
C(51)-C(52)-C(53)-C(54)	0(2)	C(50)-N(6)-C(54)-C(53)	-1.5(19)
Yb(3)-N(6)-C(54)-C(53)	174.8(11)	C(52)-C(53)-C(54)-N(6)	1(2)
C(59)-N(7)-C(55)-C(56)	2.1(18)	Yb(4)-N(7)-C(55)-C(56)	-174.3(9)
N(7)-C(55)-C(56)-C(57)	-2(2)	C(55)-C(56)-C(57)-C(58)	0.5(19)
C(56)-C(57)-C(58)-C(59)	0.3(19)	C(55)-N(7)-C(59)-C(58)	-1.2(18)
Yb(4)-N(7)-C(59)-C(58)	175.5(10)	C(57)-C(58)-C(59)-N(7)	0(2)
C(64)-N(8)-C(60)-C(61)	3.2(18)	Yb(4)-N(8)-C(60)-C(61)	-173.3(10)
N(8)-C(60)-C(61)-C(62)	0(2)	C(60)-C(61)-C(62)-C(63)	-1(2)
C(61)-C(62)-C(63)-C(64)	0(2)	C(60)-N(8)-C(64)-C(63)	-4.4(17)
Yb(4)-N(8)-C(64)-C(63)	171.9(9)	C(62)-C(63)-C(64)-N(8)	2.8(19)
C(69)-N(9)-C(65)-C(66)	3(3)	N(9)-C(65)-C(66)-C(67)	6(4)
C(65)-C(66)-C(67)-C(68)	-11(4)	C(66)-C(67)-C(68)-C(69)	8(4)
C(65)-N(9)-C(69)-C(68)	-6(3)	C(67)-C(68)-C(69)-N(9)	0(4)
C(74)-N(10)-C(70)-C(71)	2(4)	N(10)-C(70)-C(71)-C(72)	3(4)
C(70)-C(71)-C(72)-C(73)	-2(5)	C(71)-C(72)-C(73)-C(74)	-4(5)
C(72)-C(73)-C(74)-N(10)	9(5)	C(70)-N(10)-C(74)-C(73)	-8(4)
C(79)-N(11)-C(75)-C(76)	-7(10)	N(11)-C(75)-C(76)-C(77)	-7(10)
C(75)-C(76)-C(77)-C(78)	15(10)	C(76)-C(77)-C(78)-C(79)	-10(10)
C(77)-C(78)-C(79)-N(11)	-5(10)	C(75)-N(11)-C(79)-C(78)	13(10)

Table S7. Crystal data and structure refinement for Yb₆S₆(SPh)₆py₁₂.

Identification code	YBSPHS2
Empirical formula	C ₈₆ H ₈₀ N ₁₀ S ₁₂ Yb ₆ · 2(NC ₅ H ₅)
Formula weight	2834.76
Temperature	153(5) K
Radiation type, wavelength	MoK α , 0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Number, θ range, for cell data	25, 12.1 < θ < 13.8 deg
Unit cell dimensions	a = 13.681(7) Å α = 90.00(2) deg b = 31.856(7) Å β = 93.75(4) deg c = 22.462(4) Å γ = 90.00(4) deg
Volume	9768(6) Å ³
Z, Calculated density	4, 1.928 Mg/m ³
Absorption coefficient	5.994 mm ⁻¹
F(000)	5448
Crystal colour, shape	orange-red, lathe
Crystal size	0.10 x 0.10 x 0.08 mm
θ range for data collection	2.12 to 20.03 deg.
Index ranges	0 ≤ h ≤ 13, 0 ≤ k ≤ 30, -21 ≤ l ≤ 21
Reflections collected / unique	9902 / 9090 [R(int) = 0.0805]
Completeness to 2 θ = 20.03	99.1%
Transmission factors, method	0.6184 to 0.6876, numerical grid (SHELX76)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9090 / 0 / 595
Goodness-of-fit on F ²	1.029
Final R indices [I > 2 σ (I)]	R1 = 0.0609, wR2 = 0.1190
R indices (all data)	R1 = 0.1677, wR2 = 0.1370
Largest diff. peak and hole	1.9 and -1.6 e.Å ⁻³ near the Yb atoms 1.1 and -1.0 e.Å ⁻³ elsewhere

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Yb}_6\text{S}_6(\text{SPh})_6\text{py}_{12}$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Yb(1)	2652(1)	1106(1)	9182(1)	33(1)
Yb(2)	891(1)	630(1)	7955(1)	34(1)
Yb(3)	-221(1)	1279(1)	9145(1)	34(1)
Yb(4)	1324(1)	1815(1)	7973(1)	31(1)
Yb(5)	-1489(1)	1978(1)	7867(1)	34(1)
Yb(6)	125(1)	2451(1)	9164(1)	35(1)
S(1)	1025(5)	654(2)	9145(3)	36(2)
S(2)	2419(5)	1133(2)	7993(3)	33(2)
S(3)	-239(5)	1308(2)	7952(3)	33(2)
S(4)	1365(4)	1791(2)	9172(3)	32(2)
S(5)	126(4)	2460(2)	7990(3)	32(2)
S(6)	-1392(4)	1934(2)	9055(3)	32(2)
S(7)	3966(5)	483(2)	9284(3)	40(2)
C(1)	4442(16)	218(7)	8682(10)	30(6)
C(2)	4869(18)	-169(8)	8787(12)	51(8)
C(3)	5203(19)	-402(9)	8339(12)	53(8)
C(4)	5120(2)	-272(9)	7747(13)	63(9)
C(5)	4709(17)	141(8)	7659(11)	42(7)
C(6)	4367(18)	366(8)	8112(11)	47(8)
S(8)	2884(5)	1112(3)	10375(3)	69(3)
C(7)	4001(19)	1284(9)	10678(12)	53(8)
C(8)	4000(2)	1536(8)	11235(11)	53(8)
C(9)	4870(2)	1661(9)	11485(13)	61(9)
C(10)	5770(2)	1566(8)	11236(12)	56(8)
C(11)	5758(19)	1364(8)	10710(11)	44(7)
C(12)	4883(18)	1212(8)	10434(11)	43(7)
S(9)	410(5)	618(2)	6771(3)	48(2)
C(13)	1360(2)	514(8)	6297(12)	52(8)
C(14)	1100(2)	485(8)	5683(11)	47(8)
C(15)	1820(2)	392(9)	5302(14)	70(10)
C(16)	2770(2)	369(8)	5516(12)	58(9)
C(17)	3030(2)	403(9)	6110(14)	76(10)
C(18)	2327(17)	486(7)	6508(10)	32(7)
S(10)	-2910(5)	2552(2)	7688(3)	42(2)
C(19)	-2649(19)	3103(8)	7640(11)	44(7)
C(20)	-1760(2)	3242(9)	7751(11)	55(8)
C(21)	-1580(2)	3677(10)	7743(12)	72(10)
C(22)	-2340(2)	3968(10)	7633(12)	66(9)
C(23)	-3240(2)	3823(9)	7566(11)	52(8)
C(24)	-3400(2)	3391(9)	7557(12)	60(9)
S(11)	-2792(5)	1369(2)	7656(3)	47(2)
C(25)	-3823(15)	1426(7)	7158(9)	19(6)
C(26)	-4673(17)	1274(7)	7272(10)	35(7)
C(27)	-5485(19)	1279(8)	6860(11)	47(8)
C(28)	-5410(2)	1453(9)	6321(14)	75(10)
C(29)	-4520(2)	1645(9)	6204(13)	65(9)
C(30)	-3770(2)	1603(9)	6604(13)	66(9)
S(12)	1635(5)	2952(2)	9446(3)	56(2)
C(31)	1460(2)	3456(9)	9194(13)	58(9)
C(32)	1150(2)	3557(10)	8620(14)	74(10)

C(33)	1010(3)	3972(12)	8414(17)	100(12)
C(34)	1110(3)	4285(14)	8770(2)	129(16)
C(35)	1320(3)	4229(14)	9350(2)	132(16)
C(36)	1530(2)	3822(11)	9603(15)	88(11)
N(1)	3980(14)	1624(6)	9131(8)	30(5)
C(37)	4782(18)	1508(8)	8927(11)	45(8)
C(38)	5636(18)	1748(8)	8941(10)	38(7)
C(39)	5640(2)	2113(10)	9241(12)	67(9)
C(40)	4790(2)	2249(10)	9511(13)	77(10)
C(41)	3977(19)	1963(8)	9429(10)	42(7)
N(2)	1654(14)	-55(6)	7890(9)	42(6)
C(42)	2269(18)	-187(8)	8318(11)	46(8)
C(43)	2726(19)	-592(8)	8315(12)	51(8)
C(44)	2540(2)	-822(10)	7819(13)	68(9)
C(45)	1920(2)	-692(9)	7359(13)	60(9)
C(46)	1470(2)	-316(10)	7406(14)	76(10)
N(3)	-585(14)	224(6)	8088(8)	36(5)
C(47)	-1440(2)	332(9)	7800(12)	58(8)
C(48)	-2360(2)	158(9)	7913(12)	59(9)
C(49)	-2320(2)	-136(10)	8335(13)	77(10)
C(50)	-1450(2)	-292(9)	8621(12)	63(9)
C(51)	-610(2)	-90(9)	8458(12)	59(9)
N(4)	-365(16)	1295(7)	10225(9)	47(6)
C(52)	346(19)	1255(8)	10541(11)	38(7)
C(53)	330(2)	1232(9)	11187(12)	65(9)
C(54)	-500(2)	1284(9)	11452(14)	72(10)
C(55)	-1330(2)	1366(10)	11061(14)	85(11)
C(56)	-1280(2)	1376(8)	10440(12)	52(8)
N(5)	-1520(13)	781(6)	9308(8)	30(5)
C(57)	-1403(18)	466(7)	9706(10)	38(7)
C(58)	-2161(18)	212(8)	9895(11)	44(7)
C(59)	-3110(2)	351(8)	9709(11)	50(8)
C(60)	-3210(2)	650(8)	9290(11)	49(8)
C(61)	-2450(2)	875(9)	9128(12)	56(8)
N(6)	2732(13)	2261(6)	7943(8)	32(5)
C(62)	3609(16)	2108(7)	7811(9)	30(6)
C(63)	4450(2)	2352(10)	7882(12)	63(9)
C(64)	4420(3)	2746(11)	8044(14)	91(11)
C(65)	3510(2)	2931(10)	8159(13)	75(10)
C(66)	2750(2)	2650(9)	8117(12)	59(9)
N(7)	1404(12)	1899(6)	6883(7)	21(5)
C(67)	1715(17)	1592(8)	6553(11)	41(7)
C(68)	1845(18)	1606(9)	5952(11)	50(8)
C(69)	1622(19)	1963(8)	5681(12)	52(8)
C(70)	1278(19)	2309(9)	5987(12)	55(8)
C(71)	1204(18)	2268(9)	6597(11)	50(8)
N(8)	-1214(12)	1977(6)	6799(7)	23(5)
C(72)	-1373(16)	2321(8)	6494(10)	35(7)
C(73)	-1434(17)	2340(8)	5879(11)	45(8)
C(74)	-1289(19)	1963(9)	5596(12)	55(8)
C(75)	-1047(17)	1598(8)	5868(11)	45(8)
C(76)	-1021(17)	1628(8)	6491(11)	44(7)
N(9)	53(18)	2348(7)	10248(10)	61(7)
C(77)	-800(2)	2406(9)	10507(14)	77(10)
C(78)	-700(2)	2403(9)	11136(14)	75(10)
C(79)	140(2)	2325(9)	11459(14)	68(9)
C(80)	950(2)	2286(9)	11182(13)	71(10)
C(81)	960(2)	2300(9)	10559(12)	63(9)
N(10)	-1035(16)	3008(7)	9338(9)	49(6)
C(82)	-1930(2)	3002(9)	9088(11)	54(8)
C(83)	-2620(2)	3319(8)	9150(11)	51(8)

C(84)	-2330(2)	3660(10)	9451(13)	73(10)
C(85)	-1419(19)	3683(8)	9712(11)	48(8)
C(86)	-720(2)	3354(8)	9644(11)	52(8)
N(11)	-2810(2)	572(10)	6248(13)	112(11)
C(87)	-2240(2)	208(10)	6229(13)	74(10)
C(88)	-2600(2)	-179(10)	6199(12)	68(9)
C(89)	-3560(3)	-191(12)	6102(14)	92(12)
C(90)	-4130(2)	114(11)	6053(13)	73(10)
C(91)	-3820(3)	499(11)	6116(14)	89(11)
N(12)	3890(3)	3944(12)	9408(15)	132(12)
C(92)	4160(3)	4369(15)	9310(19)	139(17)
C(93)	4900(3)	4464(12)	8969(16)	97(12)
C(94)	5410(3)	4159(16)	8796(19)	138(17)
C(95)	5230(3)	3781(16)	8855(19)	124(16)
C(96)	4620(3)	3665(14)	9148(17)	117(14)

Table S9. Bond lengths [Å] and angles [deg] for Yb6S6(SPh)6py12.

Yb(1)-N(1)	2.46(2)	Yb(1)-S(1)	2.648(7)
Yb(1)-S(2)	2.671(6)	Yb(1)-S(8)	2.679(7)
Yb(1)-S(7)	2.677(7)	Yb(1)-S(4)	2.803(7)
Yb(2)-N(2)	2.43(2)	Yb(2)-N(3)	2.43(2)
Yb(2)-S(2)	2.631(7)	Yb(2)-S(3)	2.656(7)
Yb(2)-S(1)	2.668(7)	Yb(2)-S(9)	2.699(7)
Yb(3)-N(5)	2.43(2)	Yb(3)-N(4)	2.45(2)
Yb(3)-S(1)	2.621(7)	Yb(3)-S(6)	2.632(7)
Yb(3)-S(3)	2.681(6)	Yb(3)-S(4)	2.713(7)
Yb(4)-N(6)	2.40(2)	Yb(4)-N(7)	2.47(2)
Yb(4)-S(5)	2.630(6)	Yb(4)-S(2)	2.640(7)
Yb(4)-S(3)	2.678(7)	Yb(4)-S(4)	2.692(6)
Yb(5)-N(8)	2.45(2)	Yb(5)-S(11)	2.654(7)
Yb(5)-S(6)	2.666(6)	Yb(5)-S(10)	2.680(7)
Yb(5)-S(5)	2.690(7)	Yb(5)-S(3)	2.733(7)
Yb(6)-N(10)	2.43(2)	Yb(6)-N(9)	2.47(2)
Yb(6)-S(5)	2.638(6)	Yb(6)-S(6)	2.648(7)
Yb(6)-S(12)	2.654(7)	Yb(6)-S(4)	2.700(7)
S(7)-C(1)	1.76(2)	C(1)-C(6)	1.36(3)
C(1)-C(2)	1.38(3)	C(2)-C(3)	1.36(3)
C(3)-C(4)	1.39(3)	C(4)-C(5)	1.44(3)
C(5)-C(6)	1.35(3)	S(8)-C(7)	1.72(3)
C(7)-C(12)	1.38(3)	C(7)-C(8)	1.49(3)
C(8)-C(9)	1.34(3)	C(9)-C(10)	1.42(3)
C(10)-C(11)	1.34(3)	C(11)-C(12)	1.40(3)
S(9)-C(13)	1.76(3)	C(13)-C(18)	1.38(3)
C(13)-C(14)	1.40(3)	C(14)-C(15)	1.37(3)
C(15)-C(16)	1.37(3)	C(16)-C(17)	1.36(3)
C(17)-C(18)	1.38(3)	S(10)-C(19)	1.80(3)
C(19)-C(20)	1.30(3)	C(19)-C(24)	1.38(3)
C(20)-C(21)	1.41(4)	C(21)-C(22)	1.40(4)
C(22)-C(23)	1.32(3)	C(23)-C(24)	1.39(3)
S(11)-C(25)	1.75(2)	C(25)-C(26)	1.30(3)
C(25)-C(30)	1.37(3)	C(26)-C(27)	1.40(3)
C(27)-C(28)	1.34(3)	C(28)-C(29)	1.40(4)
C(29)-C(30)	1.33(3)	S(12)-C(31)	1.72(3)
C(31)-C(32)	1.37(3)	C(31)-C(36)	1.48(4)
C(32)-C(33)	1.41(4)	C(33)-C(34)	1.29(4)
C(34)-C(35)	1.32(5)	C(35)-C(36)	1.44(5)
N(1)-C(37)	1.27(3)	N(1)-C(41)	1.27(3)
C(37)-C(38)	1.39(3)	C(38)-C(39)	1.34(3)
C(39)-C(40)	1.41(4)	C(40)-C(41)	1.44(4)
N(2)-C(42)	1.30(3)	N(2)-C(46)	1.38(3)
C(42)-C(43)	1.43(3)	C(43)-C(44)	1.34(3)
C(44)-C(45)	1.36(3)	C(45)-C(46)	1.35(4)
N(3)-C(51)	1.30(3)	N(3)-C(47)	1.34(3)
C(47)-C(48)	1.42(3)	C(48)-C(49)	1.33(3)
C(49)-C(50)	1.40(4)	C(50)-C(51)	1.40(3)
N(4)-C(52)	1.17(3)	N(4)-C(56)	1.39(3)
C(52)-C(53)	1.45(3)	C(53)-C(54)	1.33(3)
C(54)-C(55)	1.42(4)	C(55)-C(56)	1.40(3)
N(5)-C(61)	1.35(3)	N(5)-C(57)	1.35(3)
C(57)-C(58)	1.40(3)	C(58)-C(59)	1.41(3)
C(59)-C(60)	1.34(3)	C(60)-C(61)	1.33(3)
N(6)-C(66)	1.30(3)	N(6)-C(62)	1.35(3)
C(62)-C(63)	1.39(3)	C(63)-C(64)	1.31(4)
C(64)-C(65)	1.41(4)	C(65)-C(66)	1.37(4)
N(7)-C(67)	1.32(3)	N(7)-C(71)	1.36(3)

C(67)-C(68)	1.37(3)	C(68)-C(69)	1.32(3)
C(69)-C(70)	1.40(3)	C(70)-C(71)	1.39(3)
N(8)-C(72)	1.30(3)	N(8)-C(76)	1.35(3)
C(72)-C(73)	1.38(3)	C(73)-C(74)	1.38(3)
C(74)-C(75)	1.34(3)	C(75)-C(76)	1.40(3)
N(9)-C(77)	1.35(3)	N(9)-C(81)	1.39(3)
C(77)-C(78)	1.41(4)	C(78)-C(79)	1.34(4)
C(79)-C(80)	1.31(3)	C(80)-C(81)	1.40(3)
N(10)-C(82)	1.31(3)	N(10)-C(86)	1.36(3)
C(82)-C(83)	1.40(3)	C(83)-C(84)	1.33(3)
C(84)-C(85)	1.34(3)	C(85)-C(86)	1.43(3)
N(11)-C(87)	1.40(4)	N(11)-C(91)	1.41(4)
C(87)-C(88)	1.33(4)	C(88)-C(89)	1.31(4)
C(89)-C(90)	1.25(4)	C(90)-C(91)	1.30(4)
N(12)-C(92)	1.42(5)	N(12)-C(96)	1.48(4)
C(92)-C(93)	1.34(5)	C(93)-C(94)	1.27(5)
C(94)-C(95)	1.24(5)	C(95)-C(96)	1.16(5)

N(1)-Yb(1)-S(1)	169.9(5)	N(1)-Yb(1)-S(2)	88.4(4)
S(1)-Yb(1)-S(2)	86.6(2)	N(1)-Yb(1)-S(8)	90.1(5)
S(1)-Yb(1)-S(8)	94.6(2)	S(2)-Yb(1)-S(8)	177.8(3)
N(1)-Yb(1)-S(7)	90.4(5)	S(1)-Yb(1)-S(7)	99.1(2)
S(2)-Yb(1)-S(7)	98.3(2)	S(8)-Yb(1)-S(7)	83.4(2)
N(1)-Yb(1)-S(4)	86.8(5)	S(1)-Yb(1)-S(4)	84.1(2)
S(2)-Yb(1)-S(4)	86.2(2)	S(8)-Yb(1)-S(4)	92.1(2)
S(7)-Yb(1)-S(4)	174.6(2)	N(2)-Yb(2)-N(3)	83.8(6)
N(2)-Yb(2)-S(2)	101.8(5)	N(3)-Yb(2)-S(2)	169.8(5)
N(2)-Yb(2)-S(3)	169.6(5)	N(3)-Yb(2)-S(3)	86.9(5)
S(2)-Yb(2)-S(3)	88.1(2)	N(2)-Yb(2)-S(1)	94.8(5)
N(3)-Yb(2)-S(1)	84.0(5)	S(2)-Yb(2)-S(1)	87.0(2)
S(3)-Yb(2)-S(1)	88.9(2)	N(2)-Yb(2)-S(9)	90.3(5)
N(3)-Yb(2)-S(9)	87.9(5)	S(2)-Yb(2)-S(9)	100.5(2)
S(3)-Yb(2)-S(9)	84.5(2)	S(1)-Yb(2)-S(9)	169.9(2)
N(5)-Yb(3)-N(4)	76.0(6)	N(5)-Yb(3)-S(1)	89.2(5)
N(4)-Yb(3)-S(1)	96.4(5)	N(5)-Yb(3)-S(6)	94.7(5)
N(4)-Yb(3)-S(6)	88.4(5)	S(1)-Yb(3)-S(6)	174.5(2)
N(5)-Yb(3)-S(3)	102.4(4)	N(4)-Yb(3)-S(3)	174.0(5)
S(1)-Yb(3)-S(3)	89.4(2)	S(6)-Yb(3)-S(3)	86.0(2)
N(5)-Yb(3)-S(4)	169.2(4)	N(4)-Yb(3)-S(4)	94.7(5)
S(1)-Yb(3)-S(4)	86.4(2)	S(6)-Yb(3)-S(4)	90.4(2)
S(3)-Yb(3)-S(4)	87.5(2)	N(5)-Yb(3)-C(52)	88.3(6)
N(4)-Yb(3)-C(52)	18.9(6)	S(1)-Yb(3)-C(52)	82.3(5)
S(6)-Yb(3)-C(52)	101.7(5)	S(3)-Yb(3)-C(52)	166.4(5)
S(4)-Yb(3)-C(52)	81.3(5)	N(6)-Yb(4)-N(7)	79.7(6)
N(6)-Yb(4)-S(5)	92.3(5)	N(7)-Yb(4)-S(5)	89.9(4)
N(6)-Yb(4)-S(2)	91.8(5)	N(7)-Yb(4)-S(2)	92.5(4)
S(5)-Yb(4)-S(2)	175.5(2)	N(6)-Yb(4)-S(3)	177.3(4)
N(7)-Yb(4)-S(3)	97.8(4)	S(5)-Yb(4)-S(3)	88.5(2)
S(2)-Yb(4)-S(3)	87.4(2)	N(6)-Yb(4)-S(4)	94.6(4)
N(7)-Yb(4)-S(4)	174.1(4)	S(5)-Yb(4)-S(4)	88.9(2)
S(2)-Yb(4)-S(4)	89.1(2)	S(3)-Yb(4)-S(4)	88.0(2)
N(8)-Yb(5)-S(11)	88.2(4)	N(8)-Yb(5)-S(6)	168.0(4)
S(11)-Yb(5)-S(6)	97.5(2)	N(8)-Yb(5)-S(10)	90.5(4)
S(11)-Yb(5)-S(10)	90.0(2)	S(6)-Yb(5)-S(10)	100.0(2)
N(8)-Yb(5)-S(5)	85.5(4)	S(11)-Yb(5)-S(5)	166.5(2)
S(6)-Yb(5)-S(5)	86.6(2)	S(10)-Yb(5)-S(5)	102.0(2)
N(8)-Yb(5)-S(3)	86.1(4)	S(11)-Yb(5)-S(3)	81.5(2)
S(6)-Yb(5)-S(3)	84.3(2)	S(10)-Yb(5)-S(3)	170.9(2)
S(5)-Yb(5)-S(3)	86.2(2)	N(10)-Yb(6)-N(9)	82.5(7)
N(10)-Yb(6)-S(5)	101.3(5)	N(9)-Yb(6)-S(5)	172.6(6)
N(10)-Yb(6)-S(6)	87.3(5)	N(9)-Yb(6)-S(6)	85.8(6)

S(5)-Yb(6)-S(6)	88.1(2)	N(10)-Yb(6)-S(12)	91.6(6)
N(9)-Yb(6)-S(12)	85.7(6)	S(5)-Yb(6)-S(12)	100.4(2)
S(6)-Yb(6)-S(12)	171.5(2)	N(10)-Yb(6)-S(4)	169.8(5)
N(9)-Yb(6)-S(4)	87.4(6)	S(5)-Yb(6)-S(4)	88.5(2)
S(6)-Yb(6)-S(4)	90.3(2)	S(12)-Yb(6)-S(4)	89.3(2)
Yb(3)-S(1)-Yb(1)	97.6(2)	Yb(3)-S(1)-Yb(2)	91.1(2)
Yb(1)-S(1)-Yb(2)	92.8(2)	Yb(2)-S(2)-Yb(4)	93.0(2)
Yb(2)-S(2)-Yb(1)	93.2(2)	Yb(4)-S(2)-Yb(1)	94.2(2)
Yb(2)-S(3)-Yb(4)	91.5(2)	Yb(2)-S(3)-Yb(3)	90.1(2)
Yb(4)-S(3)-Yb(3)	92.8(2)	Yb(2)-S(3)-Yb(5)	175.2(3)
Yb(4)-S(3)-Yb(5)	91.4(2)	Yb(3)-S(3)-Yb(5)	93.5(2)
Yb(4)-S(4)-Yb(6)	89.9(2)	Yb(4)-S(4)-Yb(3)	91.8(2)
Yb(6)-S(4)-Yb(3)	88.1(2)	Yb(4)-S(4)-Yb(1)	90.1(2)
Yb(6)-S(4)-Yb(1)	179.9(2)	Yb(3)-S(4)-Yb(1)	91.9(2)
Yb(4)-S(5)-Yb(6)	92.7(2)	Yb(4)-S(5)-Yb(5)	93.5(2)
Yb(6)-S(5)-Yb(5)	92.4(2)	Yb(3)-S(6)-Yb(6)	90.9(2)
Yb(3)-S(6)-Yb(5)	96.2(2)	Yb(6)-S(6)-Yb(5)	92.7(2)
C(1)-S(7)-Yb(1)	124.9(8)	C(6)-C(1)-C(2)	118(2)
C(6)-C(1)-S(7)	123(2)	C(2)-C(1)-S(7)	118(2)
C(3)-C(2)-C(1)	122(3)	C(2)-C(3)-C(4)	123(3)
C(3)-C(4)-C(5)	114(3)	C(6)-C(5)-C(4)	122(3)
C(5)-C(6)-C(1)	121(3)	C(7)-S(8)-Yb(1)	116.2(9)
C(12)-C(7)-C(8)	118(2)	C(12)-C(7)-S(8)	125(2)
C(8)-C(7)-S(8)	117(2)	C(9)-C(8)-C(7)	118(3)
C(8)-C(9)-C(10)	123(3)	C(11)-C(10)-C(9)	119(3)
C(10)-C(11)-C(12)	121(3)	C(7)-C(12)-C(11)	121(2)
C(13)-S(9)-Yb(2)	117.2(9)	C(18)-C(13)-C(14)	120(2)
C(18)-C(13)-S(9)	122(2)	C(14)-C(13)-S(9)	117(2)
C(15)-C(14)-C(13)	119(3)	C(16)-C(15)-C(14)	120(3)
C(15)-C(16)-C(17)	121(3)	C(16)-C(17)-C(18)	120(3)
C(17)-C(18)-C(13)	119(3)	C(19)-S(10)-Yb(5)	122.1(9)
C(20)-C(19)-C(24)	118(3)	C(20)-C(19)-S(10)	120(2)
C(24)-C(19)-S(10)	121(2)	C(19)-C(20)-C(21)	120(3)
C(22)-C(21)-C(20)	122(3)	C(23)-C(22)-C(21)	118(3)
C(22)-C(23)-C(24)	119(3)	C(19)-C(24)-C(23)	123(3)
C(25)-S(11)-Yb(5)	122.8(8)	C(26)-C(25)-C(30)	115(2)
C(26)-C(25)-S(11)	122(2)	C(30)-C(25)-S(11)	122(2)
C(25)-C(26)-C(27)	123(2)	C(28)-C(27)-C(26)	120(3)
C(27)-C(28)-C(29)	118(3)	C(30)-C(29)-C(28)	118(3)
C(29)-C(30)-C(25)	125(3)	C(31)-S(12)-Yb(6)	113.2(10)
C(32)-C(31)-C(36)	114(3)	C(32)-C(31)-S(12)	124(2)
C(36)-C(31)-S(12)	122(2)	C(31)-C(32)-C(33)	124(3)
C(34)-C(33)-C(32)	121(4)	C(33)-C(34)-C(35)	121(5)
C(34)-C(35)-C(36)	123(5)	C(35)-C(36)-C(31)	117(3)
C(37)-N(1)-C(41)	118(2)	C(37)-N(1)-Yb(1)	119(2)
C(41)-N(1)-Yb(1)	121(2)	N(1)-C(37)-C(38)	125(3)
C(39)-C(38)-C(37)	118(3)	C(38)-C(39)-C(40)	120(3)
C(39)-C(40)-C(41)	114(3)	N(1)-C(41)-C(40)	125(3)
C(42)-N(2)-C(46)	118(2)	C(42)-N(2)-Yb(2)	120(2)
C(46)-N(2)-Yb(2)	122(2)	N(2)-C(42)-C(43)	123(3)
C(44)-C(43)-C(42)	116(3)	C(43)-C(44)-C(45)	122(3)
C(46)-C(45)-C(44)	119(3)	C(45)-C(46)-N(2)	122(3)
C(51)-N(3)-C(47)	117(2)	C(51)-N(3)-Yb(2)	123(2)
C(47)-N(3)-Yb(2)	120(2)	N(3)-C(47)-C(48)	125(3)
C(49)-C(48)-C(47)	114(3)	C(48)-C(49)-C(50)	125(3)
C(51)-C(50)-C(49)	114(3)	N(3)-C(51)-C(50)	125(3)
C(52)-N(4)-C(56)	123(2)	C(52)-N(4)-Yb(3)	119(2)
C(56)-N(4)-Yb(3)	119(2)	N(4)-C(52)-C(53)	123(3)
C(54)-C(53)-C(52)	121(3)	C(53)-C(54)-C(55)	115(3)
C(56)-C(55)-C(54)	122(3)	N(4)-C(56)-C(55)	117(3)
C(61)-N(5)-C(57)	116(2)	C(61)-N(5)-Yb(3)	120(2)

C(57)-N(5)-Yb(3)	122(2)	N(5)-C(57)-C(58)	125(2)
C(59)-C(58)-C(57)	114(2)	C(60)-C(59)-C(58)	119(3)
C(61)-C(60)-C(59)	122(3)	C(60)-C(61)-N(5)	123(3)
C(66)-N(6)-C(62)	114(2)	C(66)-N(6)-Yb(4)	124(2)
C(62)-N(6)-Yb(4)	122(2)	N(6)-C(62)-C(63)	121(2)
C(64)-C(63)-C(62)	122(3)	C(63)-C(64)-C(65)	120(4)
C(66)-C(65)-C(64)	113(3)	N(6)-C(66)-C(65)	130(3)
C(67)-N(7)-C(71)	116(2)	C(67)-N(7)-Yb(4)	121(2)
C(71)-N(7)-Yb(4)	123(2)	N(7)-C(67)-C(68)	127(2)
C(69)-C(68)-C(67)	116(3)	C(68)-C(69)-C(70)	122(3)
C(71)-C(70)-C(69)	117(3)	N(7)-C(71)-C(70)	122(3)
C(72)-N(8)-C(76)	117(2)	C(72)-N(8)-Yb(5)	119(2)
C(76)-N(8)-Yb(5)	123(2)	N(8)-C(72)-C(73)	124(2)
C(72)-C(73)-C(74)	115(3)	C(75)-C(74)-C(73)	126(3)
C(74)-C(75)-C(76)	113(3)	N(8)-C(76)-C(75)	125(2)
C(77)-N(9)-C(81)	125(3)	C(77)-N(9)-Yb(6)	120(2)
C(81)-N(9)-Yb(6)	115(2)	N(9)-C(77)-C(78)	114(3)
C(79)-C(78)-C(77)	125(3)	C(80)-C(79)-C(78)	119(3)
C(79)-C(80)-C(81)	123(3)	N(9)-C(81)-C(80)	116(3)
C(82)-N(10)-C(86)	119(2)	C(82)-N(10)-Yb(6)	121(2)
C(86)-N(10)-Yb(6)	119(2)	N(10)-C(82)-C(83)	124(3)
C(84)-C(83)-C(82)	117(3)	C(83)-C(84)-C(85)	120(3)
C(84)-C(85)-C(86)	121(3)	N(10)-C(86)-C(85)	117(2)
C(87)-N(11)-C(91)	114(3)	C(88)-C(87)-N(11)	124(3)
C(89)-C(88)-C(87)	113(3)	C(90)-C(89)-C(88)	128(4)
C(89)-C(90)-C(91)	121(4)	C(90)-C(91)-N(11)	119(4)
C(92)-N(12)-C(96)	109(4)	C(93)-C(92)-N(12)	121(4)
C(94)-C(93)-C(92)	117(5)	C(95)-C(94)-C(93)	127(5)
C(96)-C(95)-C(94)	121(6)	C(95)-C(96)-N(12)	124(5)

Table S10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Yb6S6(SPh)6py12.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Yb(1)	24(1)	43(1)	31(1)	5(1)	5(1)	3(1)
Yb(2)	31(1)	35(1)	37(1)	2(1)	4(1)	0(1)
Yb(3)	27(1)	41(1)	35(1)	9(1)	9(1)	1(1)
Yb(4)	26(1)	38(1)	31(1)	5(1)	6(1)	0(1)
Yb(5)	27(1)	40(1)	35(1)	4(1)	2(1)	-2(1)
Yb(6)	33(1)	42(1)	31(1)	-1(1)	5(1)	3(1)
S(1)	26(4)	44(5)	40(4)	9(4)	5(3)	1(4)
S(2)	32(4)	34(5)	33(4)	-4(3)	6(3)	2(3)
S(3)	28(4)	33(4)	37(4)	-3(3)	0(3)	1(3)
S(4)	25(4)	46(5)	24(4)	2(3)	2(3)	5(3)
S(5)	27(4)	33(5)	37(4)	1(3)	7(3)	2(3)
S(6)	16(4)	43(5)	38(4)	3(4)	10(3)	2(3)
S(7)	32(4)	42(5)	47(5)	9(4)	7(4)	1(4)
S(8)	38(5)	127(8)	41(5)	9(5)	0(4)	-5(5)
S(9)	48(5)	55(5)	38(4)	-2(4)	-8(4)	14(4)
S(10)	35(4)	44(5)	46(5)	8(4)	-2(3)	5(4)
S(11)	42(5)	50(5)	48(5)	12(4)	-3(4)	-13(4)
S(12)	49(5)	56(6)	59(5)	4(4)	-19(4)	-13(4)

Table S11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Yb6S6(SPh)6py12.

	x	y	z	U(eq)
H(2)	4931	-274	9184	61
H(3)	5504	-665	8433	64
H(4)	5322	-441	7428	76
H(5)	4675	259	7270	50
H(6)	4071	631	8031	56
H(8)	3409	1605	11408	63
H(9)	4878	1820	11843	73
H(10)	6371	1644	11440	67
H(11)	6355	1325	10524	52
H(12)	4898	1056	10074	51
H(14)	445	530	5533	56
H(15)	1647	342	4891	84
H(16)	3271	330	5246	70
H(17)	3692	369	6252	91
H(18)	2507	523	6920	38
H(20)	-1236	3051	7836	66
H(21)	-929	3777	7814	86
H(22)	-2211	4260	7608	79
H(23)	-3782	4011	7524	62
H(24)	-4051	3290	7491	72
H(26)	-4745	1152	7653	42
H(27)	-6089	1160	6962	56
H(28)	-5943	1446	6028	90
H(29)	-4460	1801	5849	77
H(30)	-3152	1703	6499	79
H(32)	1024	3334	8345	89
H(33)	840	4020	8003	120
H(34)	1024	4562	8622	155
H(35)	1346	4467	9604	159
H(36)	1702	3789	10017	105
H(37)	4801	1237	8751	54
H(38)	6193	1657	8745	46
H(39)	6217	2280	9271	81
H(40)	4763	2505	9726	92
H(41)	3392	2034	9612	50
H(42)	2421	-6	8647	55
H(43)	3135	-691	8643	61
H(44)	2858	-1087	7790	81
H(45)	1809	-860	7013	72
H(46)	1013	-229	7094	91
H(47)	-1421	540	7497	69
H(48)	-2955	243	7706	70
H(49)	-2923	-248	8451	92
H(50)	-1445	-515	8901	76
H(51)	2	-190	8630	71
H(52)	959	1237	10368	45
H(53)	922	1179	11422	77
H(54)	-535	1268	11873	87
H(55)	-1948	1416	11223	102
H(56)	-1834	1436	10179	63
H(57)	-758	411	9871	46
H(58)	-2044	-34	10130	53

H(59)	-3668	235	9877	60
H(60)	-3842	702	9103	59
H(61)	-2574	1110	8875	67
H(62)	3653	1829	7666	36
H(63)	5065	2229	7810	76
H(64)	5007	2907	8084	109
H(65)	3440	3219	8255	90
H(66)	2144	2757	8233	71
H(67)	1864	1333	6750	49
H(68)	2083	1371	5744	60
H(69)	1697	1986	5264	63
H(70)	1101	2562	5785	67
H(71)	1010	2504	6819	60
H(72)	-1451	2574	6708	42
H(73)	-1566	2594	5666	54
H(74)	-1366	1960	5172	66
H(75)	-909	1347	5660	53
H(76)	-854	1382	6714	53
H(77)	-1412	2446	10286	92
H(78)	-1269	2461	11345	90
H(79)	143	2298	11880	81
H(80)	1546	2246	11412	86
H(81)	1551	2279	10361	75
H(82)	-2115	2767	8848	65
H(83)	-3270	3292	8984	62
H(84)	-2763	3889	9482	88
H(85)	-1236	3921	9948	57
H(86)	-60	3379	9805	62
H(87)	-1546	240	6239	89
H(88)	-2203	-424	6243	82
H(89)	-3843	-462	6066	110
H(90)	-4812	64	5967	88
H(91)	-4264	727	6075	106
H(92)	3809	4588	9489	166
H(93)	5037	4746	8863	116
H(94)	5981	4228	8600	166
H(95)	5611	3581	8657	149
H(96)	4574	3372	9225	140

Table S12. Torsion angles [deg] for Yb6S6(SPh)6py12.

N(5)-Yb(3)-S(1)-Yb(1)	-169.6(4)	N(4)-Yb(3)-S(1)-Yb(1)	-93.8(5)
S(6)-Yb(3)-S(1)-Yb(1)	55(2)	S(3)-Yb(3)-S(1)-Yb(1)	88.1(2)
S(4)-Yb(3)-S(1)-Yb(1)	0.54(19)	N(5)-Yb(3)-S(1)-Yb(2)	97.4(4)
N(4)-Yb(3)-S(1)-Yb(2)	173.2(5)	S(6)-Yb(3)-S(1)-Yb(2)	-38(2)
S(3)-Yb(3)-S(1)-Yb(2)	-5.0(2)	S(4)-Yb(3)-S(1)-Yb(2)	-92.5(2)
N(1)-Yb(1)-S(1)-Yb(3)	-26(3)	S(2)-Yb(1)-S(1)-Yb(3)	-87.0(2)
S(8)-Yb(1)-S(1)-Yb(3)	91.1(3)	S(7)-Yb(1)-S(1)-Yb(3)	175.1(2)
S(4)-Yb(1)-S(1)-Yb(3)	-0.52(18)	N(1)-Yb(1)-S(1)-Yb(2)	65(3)
S(2)-Yb(1)-S(1)-Yb(2)	4.5(2)	S(8)-Yb(1)-S(1)-Yb(2)	-177.4(2)
S(7)-Yb(1)-S(1)-Yb(2)	-93.4(2)	S(4)-Yb(1)-S(1)-Yb(2)	91.0(2)
N(2)-Yb(2)-S(1)-Yb(3)	-165.2(5)	N(3)-Yb(2)-S(1)-Yb(3)	-81.9(5)
S(2)-Yb(2)-S(1)-Yb(3)	93.1(2)	S(3)-Yb(2)-S(1)-Yb(3)	5.0(2)
S(9)-Yb(2)-S(1)-Yb(3)	-44.9(14)	N(2)-Yb(2)-S(1)-Yb(1)	97.1(5)
N(3)-Yb(2)-S(1)-Yb(1)	-179.6(5)	S(2)-Yb(2)-S(1)-Yb(1)	-4.5(2)
S(3)-Yb(2)-S(1)-Yb(1)	-92.7(2)	S(9)-Yb(2)-S(1)-Yb(1)	-142.6(12)
N(2)-Yb(2)-S(2)-Yb(4)	175.8(5)	N(3)-Yb(2)-S(2)-Yb(4)	-61(3)
S(3)-Yb(2)-S(2)-Yb(4)	-0.84(19)	S(1)-Yb(2)-S(2)-Yb(4)	-89.9(2)
S(9)-Yb(2)-S(2)-Yb(4)	83.2(2)	N(2)-Yb(2)-S(2)-Yb(1)	-89.8(5)
N(3)-Yb(2)-S(2)-Yb(1)	33(3)	S(3)-Yb(2)-S(2)-Yb(1)	93.5(2)
S(1)-Yb(2)-S(2)-Yb(1)	4.5(2)	S(9)-Yb(2)-S(2)-Yb(1)	177.6(2)
N(6)-Yb(4)-S(2)-Yb(2)	-176.6(4)	N(7)-Yb(4)-S(2)-Yb(2)	-96.8(4)
S(5)-Yb(4)-S(2)-Yb(2)	26(3)	S(3)-Yb(4)-S(2)-Yb(2)	0.84(19)
S(4)-Yb(4)-S(2)-Yb(2)	88.8(2)	N(6)-Yb(4)-S(2)-Yb(1)	90.0(4)
N(7)-Yb(4)-S(2)-Yb(1)	169.8(4)	S(5)-Yb(4)-S(2)-Yb(1)	-68(3)
S(3)-Yb(4)-S(2)-Yb(1)	-92.6(2)	S(4)-Yb(4)-S(2)-Yb(1)	-4.5(2)
N(1)-Yb(1)-S(2)-Yb(2)	-175.7(5)	S(1)-Yb(1)-S(2)-Yb(2)	-4.5(2)
S(8)-Yb(1)-S(2)-Yb(2)	-127(6)	S(7)-Yb(1)-S(2)-Yb(2)	94.1(2)
S(4)-Yb(1)-S(2)-Yb(2)	-88.8(2)	N(1)-Yb(1)-S(2)-Yb(4)	-82.5(5)
S(1)-Yb(1)-S(2)-Yb(4)	88.7(2)	S(8)-Yb(1)-S(2)-Yb(4)	-34(6)
S(7)-Yb(1)-S(2)-Yb(4)	-172.7(2)	S(4)-Yb(1)-S(2)-Yb(4)	4.4(2)
N(2)-Yb(2)-S(3)-Yb(4)	-161(3)	N(3)-Yb(2)-S(3)-Yb(4)	172.0(5)
S(2)-Yb(2)-S(3)-Yb(4)	0.83(19)	S(1)-Yb(2)-S(3)-Yb(4)	87.9(2)
S(9)-Yb(2)-S(3)-Yb(4)	-99.9(2)	N(2)-Yb(2)-S(3)-Yb(3)	106(3)
N(3)-Yb(2)-S(3)-Yb(3)	79.2(5)	S(2)-Yb(2)-S(3)-Yb(3)	-92.0(2)
S(1)-Yb(2)-S(3)-Yb(3)	-4.9(2)	S(9)-Yb(2)-S(3)-Yb(3)	167.3(2)
N(2)-Yb(2)-S(3)-Yb(5)	-32(5)	N(3)-Yb(2)-S(3)-Yb(5)	-59(3)
S(2)-Yb(2)-S(3)-Yb(5)	129(3)	S(1)-Yb(2)-S(3)-Yb(5)	-144(3)
S(9)-Yb(2)-S(3)-Yb(5)	29(3)	N(6)-Yb(4)-S(3)-Yb(2)	72(10)
N(7)-Yb(4)-S(3)-Yb(2)	91.4(4)	S(5)-Yb(4)-S(3)-Yb(2)	-179.0(2)
S(2)-Yb(4)-S(3)-Yb(2)	-0.83(19)	S(4)-Yb(4)-S(3)-Yb(2)	-90.0(2)
N(6)-Yb(4)-S(3)-Yb(3)	163(10)	N(7)-Yb(4)-S(3)-Yb(3)	-178.5(4)
S(5)-Yb(4)-S(3)-Yb(3)	-88.8(2)	S(2)-Yb(4)-S(3)-Yb(3)	89.3(2)
S(4)-Yb(4)-S(3)-Yb(3)	0.1(2)	N(6)-Yb(4)-S(3)-Yb(5)	-104(10)
N(7)-Yb(4)-S(3)-Yb(5)	-84.9(4)	S(5)-Yb(4)-S(3)-Yb(5)	4.80(18)
S(2)-Yb(4)-S(3)-Yb(5)	-177.1(2)	S(4)-Yb(4)-S(3)-Yb(5)	93.7(2)
N(5)-Yb(3)-S(3)-Yb(2)	-84.1(5)	N(4)-Yb(3)-S(3)-Yb(2)	-157(5)
S(1)-Yb(3)-S(3)-Yb(2)	5.0(2)	S(6)-Yb(3)-S(3)-Yb(2)	-178.0(2)
S(4)-Yb(3)-S(3)-Yb(2)	91.4(2)	N(5)-Yb(3)-S(3)-Yb(4)	-175.7(5)
N(4)-Yb(3)-S(3)-Yb(4)	111(5)	S(1)-Yb(3)-S(3)-Yb(4)	-86.6(2)
S(6)-Yb(3)-S(3)-Yb(4)	90.4(2)	S(4)-Yb(3)-S(3)-Yb(4)	-0.1(2)
N(5)-Yb(3)-S(3)-Yb(5)	92.7(5)	N(4)-Yb(3)-S(3)-Yb(5)	19(5)
S(1)-Yb(3)-S(3)-Yb(5)	-178.2(2)	S(6)-Yb(3)-S(3)-Yb(5)	-1.22(19)
S(4)-Yb(3)-S(3)-Yb(5)	-91.8(2)	N(8)-Yb(5)-S(3)-Yb(2)	-47(3)
S(11)-Yb(5)-S(3)-Yb(2)	41(3)	S(6)-Yb(5)-S(3)-Yb(2)	140(3)
S(10)-Yb(5)-S(3)-Yb(2)	21(4)	S(5)-Yb(5)-S(3)-Yb(2)	-133(3)
N(8)-Yb(5)-S(3)-Yb(4)	81.1(4)	S(11)-Yb(5)-S(3)-Yb(4)	169.9(2)
S(6)-Yb(5)-S(3)-Yb(4)	-91.7(2)	S(10)-Yb(5)-S(3)-Yb(4)	149.6(12)

S(5)-Yb(5)-S(3)-Yb(4)	-4.70(18)	N(8)-Yb(5)-S(3)-Yb(3)	174.0(4)
S(11)-Yb(5)-S(3)-Yb(3)	-97.3(2)	S(6)-Yb(5)-S(3)-Yb(3)	1.20(19)
S(10)-Yb(5)-S(3)-Yb(3)	-117.6(12)	S(5)-Yb(5)-S(3)-Yb(3)	88.2(2)
N(6)-Yb(4)-S(4)-Yb(6)	92.6(5)	N(7)-Yb(4)-S(4)-Yb(6)	78(4)
S(5)-Yb(4)-S(4)-Yb(6)	0.3(2)	S(2)-Yb(4)-S(4)-Yb(6)	-175.7(2)
S(3)-Yb(4)-S(4)-Yb(6)	-88.3(2)	N(6)-Yb(4)-S(4)-Yb(3)	-179.3(5)
N(7)-Yb(4)-S(4)-Yb(3)	166(4)	S(5)-Yb(4)-S(4)-Yb(3)	88.4(2)
S(2)-Yb(4)-S(4)-Yb(3)	-87.6(2)	S(3)-Yb(4)-S(4)-Yb(3)	-0.1(2)
N(6)-Yb(4)-S(4)-Yb(1)	-87.4(5)	N(7)-Yb(4)-S(4)-Yb(1)	-102(4)
S(5)-Yb(4)-S(4)-Yb(1)	-179.67(19)	S(2)-Yb(4)-S(4)-Yb(1)	4.3(2)
S(3)-Yb(4)-S(4)-Yb(1)	91.8(2)	N(10)-Yb(6)-S(4)-Yb(4)	164(3)
N(9)-Yb(6)-S(4)-Yb(4)	173.5(6)	S(5)-Yb(6)-S(4)-Yb(4)	-0.3(2)
S(6)-Yb(6)-S(4)-Yb(4)	87.7(2)	S(12)-Yb(6)-S(4)-Yb(4)	-100.7(2)
N(10)-Yb(6)-S(4)-Yb(3)	72(3)	N(9)-Yb(6)-S(4)-Yb(3)	81.7(6)
S(5)-Yb(6)-S(4)-Yb(3)	-92.08(19)	S(6)-Yb(6)-S(4)-Yb(3)	-4.03(18)
S(12)-Yb(6)-S(4)-Yb(3)	167.5(2)	N(10)-Yb(6)-S(4)-Yb(1)	-36(100)*
N(9)-Yb(6)-S(4)-Yb(1)	-26(100)*	S(5)-Yb(6)-S(4)-Yb(1)	160(100)*
S(6)-Yb(6)-S(4)-Yb(1)	-112(100)*	S(12)-Yb(6)-S(4)-Yb(1)	60(100)*
N(5)-Yb(3)-S(4)-Yb(4)	156(2)	N(4)-Yb(3)-S(4)-Yb(4)	-174.2(5)
S(1)-Yb(3)-S(4)-Yb(4)	89.7(2)	S(6)-Yb(3)-S(4)-Yb(4)	-85.8(2)
S(3)-Yb(3)-S(4)-Yb(4)	0.1(2)	N(5)-Yb(3)-S(4)-Yb(6)	-114(2)
N(4)-Yb(3)-S(4)-Yb(6)	-84.3(5)	S(1)-Yb(3)-S(4)-Yb(6)	179.6(2)
S(6)-Yb(3)-S(4)-Yb(6)	4.06(18)	S(3)-Yb(3)-S(4)-Yb(6)	90.01(19)
N(5)-Yb(3)-S(4)-Yb(1)	66(2)	N(4)-Yb(3)-S(4)-Yb(1)	95.6(5)
S(1)-Yb(3)-S(4)-Yb(1)	-0.50(17)	S(6)-Yb(3)-S(4)-Yb(1)	-176.01(19)
S(3)-Yb(3)-S(4)-Yb(1)	-90.05(19)	N(1)-Yb(1)-S(4)-Yb(4)	84.4(5)
S(1)-Yb(1)-S(4)-Yb(4)	-91.3(2)	S(2)-Yb(1)-S(4)-Yb(4)	-4.28(19)
S(8)-Yb(1)-S(4)-Yb(4)	174.3(2)	S(7)-Yb(1)-S(4)-Yb(4)	142.6(19)
N(1)-Yb(1)-S(4)-Yb(6)	-76(100)*	S(1)-Yb(1)-S(4)-Yb(6)	108(100)*
S(2)-Yb(1)-S(4)-Yb(6)	-165(100)*	S(8)-Yb(1)-S(4)-Yb(6)	14(100)*
S(7)-Yb(1)-S(4)-Yb(6)	-18(100)*	N(1)-Yb(1)-S(4)-Yb(3)	176.1(4)
S(1)-Yb(1)-S(4)-Yb(3)	0.50(17)	S(2)-Yb(1)-S(4)-Yb(3)	87.49(19)
S(8)-Yb(1)-S(4)-Yb(3)	-93.9(2)	S(7)-Yb(1)-S(4)-Yb(3)	-126(2)
N(6)-Yb(4)-S(5)-Yb(6)	-94.9(4)	N(7)-Yb(4)-S(5)-Yb(6)	-174.5(4)
S(2)-Yb(4)-S(5)-Yb(6)	63(3)	S(3)-Yb(4)-S(5)-Yb(6)	87.7(2)
S(4)-Yb(4)-S(5)-Yb(6)	-0.3(2)	N(6)-Yb(4)-S(5)-Yb(5)	172.6(4)
N(7)-Yb(4)-S(5)-Yb(5)	92.9(4)	S(2)-Yb(4)-S(5)-Yb(5)	-30(3)
S(3)-Yb(4)-S(5)-Yb(5)	-4.88(18)	S(4)-Yb(4)-S(5)-Yb(5)	-92.9(2)
N(10)-Yb(6)-S(5)-Yb(4)	-176.8(5)	N(9)-Yb(6)-S(5)-Yb(4)	-57(5)
S(6)-Yb(6)-S(5)-Yb(4)	-90.0(2)	S(12)-Yb(6)-S(5)-Yb(4)	89.4(2)
S(4)-Yb(6)-S(5)-Yb(4)	0.3(2)	N(10)-Yb(6)-S(5)-Yb(5)	-83.3(5)
N(9)-Yb(6)-S(5)-Yb(5)	37(5)	S(6)-Yb(6)-S(5)-Yb(5)	3.5(2)
S(12)-Yb(6)-S(5)-Yb(5)	-177.1(2)	S(4)-Yb(6)-S(5)-Yb(5)	93.9(2)
N(8)-Yb(5)-S(5)-Yb(4)	-81.6(4)	S(11)-Yb(5)-S(5)-Yb(4)	-18.9(10)
S(6)-Yb(5)-S(5)-Yb(4)	89.3(2)	S(10)-Yb(5)-S(5)-Yb(4)	-171.18(19)
S(3)-Yb(5)-S(5)-Yb(4)	4.79(18)	N(8)-Yb(5)-S(5)-Yb(6)	-174.4(4)
S(11)-Yb(5)-S(5)-Yb(6)	-111.7(8)	S(6)-Yb(5)-S(5)-Yb(6)	-3.5(2)
S(10)-Yb(5)-S(5)-Yb(6)	96.0(2)	S(3)-Yb(5)-S(5)-Yb(6)	-88.0(2)
N(5)-Yb(3)-S(6)-Yb(6)	166.3(4)	N(4)-Yb(3)-S(6)-Yb(6)	90.5(5)
S(1)-Yb(3)-S(6)-Yb(6)	-58(2)	S(3)-Yb(3)-S(6)-Yb(6)	-91.6(2)
S(4)-Yb(3)-S(6)-Yb(6)	-4.13(18)	N(5)-Yb(3)-S(6)-Yb(5)	-100.8(4)
N(4)-Yb(3)-S(6)-Yb(5)	-176.6(5)	S(1)-Yb(3)-S(6)-Yb(5)	35(2)
S(3)-Yb(3)-S(6)-Yb(5)	1.3(2)	S(4)-Yb(3)-S(6)-Yb(5)	88.7(2)
N(10)-Yb(6)-S(6)-Yb(3)	-165.9(5)	N(9)-Yb(6)-S(6)-Yb(3)	-83.3(6)
S(5)-Yb(6)-S(6)-Yb(3)	92.7(2)	S(12)-Yb(6)-S(6)-Yb(3)	-83.3(15)
S(4)-Yb(6)-S(6)-Yb(3)	4.15(18)	N(10)-Yb(6)-S(6)-Yb(5)	97.8(5)
N(9)-Yb(6)-S(6)-Yb(5)	-179.5(6)	S(5)-Yb(6)-S(6)-Yb(5)	-3.6(2)
S(12)-Yb(6)-S(6)-Yb(5)	-179.6(14)	S(4)-Yb(6)-S(6)-Yb(5)	-92.1(2)
N(8)-Yb(5)-S(6)-Yb(3)	-38(2)	S(11)-Yb(5)-S(6)-Yb(3)	79.4(2)
S(10)-Yb(5)-S(6)-Yb(3)	170.7(2)	S(5)-Yb(5)-S(6)-Yb(3)	-87.7(2)
S(3)-Yb(5)-S(6)-Yb(3)	-1.2(2)	N(8)-Yb(5)-S(6)-Yb(6)	53(2)

S(11)-Yb(5)-S(6)-Yb(6)	170.6(2)	S(10)-Yb(5)-S(6)-Yb(6)	-98.1(2)
S(5)-Yb(5)-S(6)-Yb(6)	3.51(19)	S(3)-Yb(5)-S(6)-Yb(6)	90.0(2)
N(1)-Yb(1)-S(7)-C(1)	-88.0(11)	S(1)-Yb(1)-S(7)-C(1)	88.4(10)
S(2)-Yb(1)-S(7)-C(1)	0.5(10)	S(8)-Yb(1)-S(7)-C(1)	-178.0(10)
S(4)-Yb(1)-S(7)-C(1)	-146(2)	Yb(1)-S(7)-C(1)-C(6)	16(3)
Yb(1)-S(7)-C(1)-C(2)	-160.7(16)	C(6)-C(1)-C(2)-C(3)	-1(4)
S(7)-C(1)-C(2)-C(3)	176(2)	C(1)-C(2)-C(3)-C(4)	-1(4)
C(2)-C(3)-C(4)-C(5)	4(4)	C(3)-C(4)-C(5)-C(6)	-5(4)
C(4)-C(5)-C(6)-C(1)	3(4)	C(2)-C(1)-C(6)-C(5)	0(4)
S(7)-C(1)-C(6)-C(5)	-177.1(19)	N(1)-Yb(1)-S(8)-C(7)	-21.5(12)
S(1)-Yb(1)-S(8)-C(7)	167.5(11)	S(2)-Yb(1)-S(8)-C(7)	-70(6)
S(7)-Yb(1)-S(8)-C(7)	68.9(11)	S(4)-Yb(1)-S(8)-C(7)	-108.3(11)
Yb(1)-S(8)-C(7)-C(12)	-36(3)	Yb(1)-S(8)-C(7)-C(8)	143.1(18)
C(12)-C(7)-C(8)-C(9)	-3(4)	S(8)-C(7)-C(8)-C(9)	178(2)
C(7)-C(8)-C(9)-C(10)	1(4)	C(8)-C(9)-C(10)-C(11)	4(4)
C(9)-C(10)-C(11)-C(12)	-6(4)	C(8)-C(7)-C(12)-C(11)	1(4)
S(8)-C(7)-C(12)-C(11)	180(2)	C(10)-C(11)-C(12)-C(7)	4(4)
N(2)-Yb(2)-S(9)-C(13)	-52.3(11)	N(3)-Yb(2)-S(9)-C(13)	-136.2(11)
S(2)-Yb(2)-S(9)-C(13)	49.8(11)	S(3)-Yb(2)-S(9)-C(13)	136.8(11)
S(1)-Yb(2)-S(9)-C(13)	-173.0(14)	Yb(2)-S(9)-C(13)-C(18)	-7(3)
Yb(2)-S(9)-C(13)-C(14)	176.8(17)	C(18)-C(13)-C(14)-C(15)	6(4)
S(9)-C(13)-C(14)-C(15)	-178(2)	C(13)-C(14)-C(15)-C(16)	-7(4)
C(14)-C(15)-C(16)-C(17)	6(5)	C(15)-C(16)-C(17)-C(18)	-4(5)
C(16)-C(17)-C(18)-C(13)	3(4)	C(14)-C(13)-C(18)-C(17)	-4(4)
S(9)-C(13)-C(18)-C(17)	180(2)	N(8)-Yb(5)-S(10)-C(19)	-82.7(10)
S(11)-Yb(5)-S(10)-C(19)	-171.0(10)	S(6)-Yb(5)-S(10)-C(19)	91.4(10)
S(5)-Yb(5)-S(10)-C(19)	2.8(10)	S(3)-Yb(5)-S(10)-C(19)	-150.9(14)
Yb(5)-S(10)-C(19)-C(20)	-7(3)	Yb(5)-S(10)-C(19)-C(24)	-178.9(17)
C(24)-C(19)-C(20)-C(21)	-4(4)	S(10)-C(19)-C(20)-C(21)	-176(2)
C(19)-C(20)-C(21)-C(22)	2(4)	C(20)-C(21)-C(22)-C(23)	3(4)
C(21)-C(22)-C(23)-C(24)	-5(4)	C(20)-C(19)-C(24)-C(23)	2(4)
S(10)-C(19)-C(24)-C(23)	175(2)	C(22)-C(23)-C(24)-C(19)	3(4)
N(8)-Yb(5)-S(11)-C(25)	-58.5(10)	S(6)-Yb(5)-S(11)-C(25)	132.1(9)
S(10)-Yb(5)-S(11)-C(25)	32.0(9)	S(5)-Yb(5)-S(11)-C(25)	-120.9(11)
S(3)-Yb(5)-S(11)-C(25)	-144.8(9)	Yb(5)-S(11)-C(25)-C(26)	-140.4(17)
Yb(5)-S(11)-C(25)-C(30)	45(2)	C(30)-C(25)-C(26)-C(27)	1(4)
S(11)-C(25)-C(26)-C(27)	-173.8(19)	C(25)-C(26)-C(27)-C(28)	-1(4)
C(26)-C(27)-C(28)-C(29)	-4(4)	C(27)-C(28)-C(29)-C(30)	8(4)
C(28)-C(29)-C(30)-C(25)	-8(5)	C(26)-C(25)-C(30)-C(29)	4(4)
S(11)-C(25)-C(30)-C(29)	178(2)	N(10)-Yb(6)-S(12)-C(31)	-38.1(12)
N(9)-Yb(6)-S(12)-C(31)	-120.5(12)	S(5)-Yb(6)-S(12)-C(31)	63.6(11)
S(6)-Yb(6)-S(12)-C(31)	-120.4(17)	S(4)-Yb(6)-S(12)-C(31)	152.0(11)
Yb(6)-S(12)-C(31)-C(32)	-50(3)	Yb(6)-S(12)-C(31)-C(36)	124(2)
C(36)-C(31)-C(32)-C(33)	6(5)	S(12)-C(31)-C(32)-C(33)	-180(3)
C(31)-C(32)-C(33)-C(34)	-4(6)	C(32)-C(33)-C(34)-C(35)	-1(7)
C(33)-C(34)-C(35)-C(36)	4(7)	C(34)-C(35)-C(36)-C(31)	-2(6)
C(32)-C(31)-C(36)-C(35)	-3(4)	S(12)-C(31)-C(36)-C(35)	-177(3)
S(1)-Yb(1)-N(1)-C(37)	-132(2)	S(2)-Yb(1)-N(1)-C(37)	-70.7(18)
S(8)-Yb(1)-N(1)-C(37)	110.9(18)	S(7)-Yb(1)-N(1)-C(37)	27.5(18)
S(4)-Yb(1)-N(1)-C(37)	-157.0(18)	S(1)-Yb(1)-N(1)-C(41)	66(3)
S(2)-Yb(1)-N(1)-C(41)	126.6(18)	S(8)-Yb(1)-N(1)-C(41)	-51.8(18)
S(7)-Yb(1)-N(1)-C(41)	-135.1(18)	S(4)-Yb(1)-N(1)-C(41)	40.3(18)
C(41)-N(1)-C(37)-C(38)	-8(4)	Yb(1)-N(1)-C(37)-C(38)	-171.5(18)
N(1)-C(37)-C(38)-C(39)	7(4)	C(37)-C(38)-C(39)-C(40)	-2(4)
C(38)-C(39)-C(40)-C(41)	0(4)	C(37)-N(1)-C(41)-C(40)	6(4)
Yb(1)-N(1)-C(41)-C(40)	168.6(19)	C(39)-C(40)-C(41)-N(1)	-2(4)
N(3)-Yb(2)-N(2)-C(42)	-110.0(19)	S(2)-Yb(2)-N(2)-C(42)	61.4(18)
S(3)-Yb(2)-N(2)-C(42)	-137(2)	S(1)-Yb(2)-N(2)-C(42)	-26.6(18)
S(9)-Yb(2)-N(2)-C(42)	162.2(18)	N(3)-Yb(2)-N(2)-C(46)	71(2)
S(2)-Yb(2)-N(2)-C(46)	-117.7(19)	S(3)-Yb(2)-N(2)-C(46)	44(4)
S(1)-Yb(2)-N(2)-C(46)	154.3(19)	S(9)-Yb(2)-N(2)-C(46)	-17(2)

C(46)-N(2)-C(42)-C(43)	-2(4)	Yb(2)-N(2)-C(42)-C(43)	178.4(18)
N(2)-C(42)-C(43)-C(44)	5(4)	C(42)-C(43)-C(44)-C(45)	-3(4)
C(43)-C(44)-C(45)-C(46)	0(5)	C(44)-C(45)-C(46)-N(2)	3(4)
C(42)-N(2)-C(46)-C(45)	-2(4)	Yb(2)-N(2)-C(46)-C(45)	178(2)
N(2)-Yb(2)-N(3)-C(51)	47(2)	S(2)-Yb(2)-N(3)-C(51)	-77(4)
S(3)-Yb(2)-N(3)-C(51)	-137.4(19)	S(1)-Yb(2)-N(3)-C(51)	-48.2(19)
S(9)-Yb(2)-N(3)-C(51)	137.9(19)	N(2)-Yb(2)-N(3)-C(47)	-136.3(19)
S(2)-Yb(2)-N(3)-C(47)	99(3)	S(3)-Yb(2)-N(3)-C(47)	38.9(18)
S(1)-Yb(2)-N(3)-C(47)	128.2(18)	S(9)-Yb(2)-N(3)-C(47)	-45.7(18)
C(51)-N(3)-C(47)-C(48)	7(4)	Yb(2)-N(3)-C(47)-C(48)	-170(2)
N(3)-C(47)-C(48)-C(49)	-1(4)	C(47)-C(48)-C(49)-C(50)	-5(4)
C(48)-C(49)-C(50)-C(51)	4(5)	C(47)-N(3)-C(51)-C(50)	-7(4)
Yb(2)-N(3)-C(51)-C(50)	170(2)	C(49)-C(50)-C(51)-N(3)	2(4)
N(5)-Yb(3)-N(4)-C(52)	129(2)	S(1)-Yb(3)-N(4)-C(52)	42(2)
S(6)-Yb(3)-N(4)-C(52)	-135(2)	S(3)-Yb(3)-N(4)-C(52)	-156(4)
S(4)-Yb(3)-N(4)-C(52)	-45(2)	N(5)-Yb(3)-N(4)-C(56)	-54.3(18)
S(1)-Yb(3)-N(4)-C(56)	-142.0(18)	S(6)-Yb(3)-N(4)-C(56)	40.9(18)
S(3)-Yb(3)-N(4)-C(56)	20(6)	S(4)-Yb(3)-N(4)-C(56)	131.2(18)
C(56)-N(4)-C(52)-C(53)	8(4)	Yb(3)-N(4)-C(52)-C(53)	-175.8(19)
N(4)-C(52)-C(53)-C(54)	-5(4)	C(52)-C(53)-C(54)-C(55)	-1(4)
C(53)-C(54)-C(55)-C(56)	2(5)	C(52)-N(4)-C(56)-C(55)	-6(4)
Yb(3)-N(4)-C(56)-C(55)	177.6(19)	C(54)-C(55)-C(56)-N(4)	1(4)
N(4)-Yb(3)-N(5)-C(61)	109.3(18)	S(1)-Yb(3)-N(5)-C(61)	-153.9(17)
S(6)-Yb(3)-N(5)-C(61)	22.2(18)	S(3)-Yb(3)-N(5)-C(61)	-64.7(18)
S(4)-Yb(3)-N(5)-C(61)	140(2)	N(4)-Yb(3)-N(5)-C(57)	-52.6(17)
S(1)-Yb(3)-N(5)-C(57)	44.2(17)	S(6)-Yb(3)-N(5)-C(57)	-139.7(16)
S(3)-Yb(3)-N(5)-C(57)	133.4(16)	S(4)-Yb(3)-N(5)-C(57)	-22(4)
C(61)-N(5)-C(57)-C(58)	6(4)	Yb(3)-N(5)-C(57)-C(58)	168.7(18)
N(5)-C(57)-C(58)-C(59)	-10(4)	C(57)-C(58)-C(59)-C(60)	13(4)
C(58)-C(59)-C(60)-C(61)	-13(4)	C(59)-C(60)-C(61)-N(5)	10(4)
C(57)-N(5)-C(61)-C(60)	-6(4)	Yb(3)-N(5)-C(61)-C(60)	-169(2)
N(7)-Yb(4)-N(6)-C(66)	111(2)	S(5)-Yb(4)-N(6)-C(66)	22(2)
S(2)-Yb(4)-N(6)-C(66)	-156.8(19)	S(3)-Yb(4)-N(6)-C(66)	130(10)
S(4)-Yb(4)-N(6)-C(66)	-68(2)	N(7)-Yb(4)-N(6)-C(62)	-77.3(16)
S(5)-Yb(4)-N(6)-C(62)	-166.7(16)	S(2)-Yb(4)-N(6)-C(62)	14.9(16)
S(3)-Yb(4)-N(6)-C(62)	-58(11)	S(4)-Yb(4)-N(6)-C(62)	104.2(16)
C(66)-N(6)-C(62)-C(63)	2(3)	Yb(4)-N(6)-C(62)-C(63)	-170.2(18)
N(6)-C(62)-C(63)-C(64)	-4(4)	C(62)-C(63)-C(64)-C(65)	1(5)
C(63)-C(64)-C(65)-C(66)	4(5)	C(62)-N(6)-C(66)-C(65)	3(4)
Yb(4)-N(6)-C(66)-C(65)	176(2)	C(64)-C(65)-C(66)-N(6)	-6(5)
N(6)-Yb(4)-N(7)-C(67)	105.7(17)	S(5)-Yb(4)-N(7)-C(67)	-161.9(17)
S(2)-Yb(4)-N(7)-C(67)	14.3(17)	S(3)-Yb(4)-N(7)-C(67)	-73.4(17)
S(4)-Yb(4)-N(7)-C(67)	120(4)	N(6)-Yb(4)-N(7)-C(71)	-69.4(17)
S(5)-Yb(4)-N(7)-C(71)	23.0(17)	S(2)-Yb(4)-N(7)-C(71)	-160.8(17)
S(3)-Yb(4)-N(7)-C(71)	111.5(17)	S(4)-Yb(4)-N(7)-C(71)	-55(5)
C(71)-N(7)-C(67)-C(68)	-1(4)	Yb(4)-N(7)-C(67)-C(68)	-176.1(19)
N(7)-C(67)-C(68)-C(69)	-1(4)	C(67)-C(68)-C(69)-C(70)	0(4)
C(68)-C(69)-C(70)-C(71)	2(4)	C(67)-N(7)-C(71)-C(70)	3(3)
Yb(4)-N(7)-C(71)-C(70)	178.5(18)	C(69)-C(70)-C(71)-N(7)	-4(4)
S(11)-Yb(5)-N(8)-C(72)	120.7(16)	S(6)-Yb(5)-N(8)-C(72)	-121(2)
S(10)-Yb(5)-N(8)-C(72)	30.8(16)	S(5)-Yb(5)-N(8)-C(72)	-71.2(16)
S(3)-Yb(5)-N(8)-C(72)	-157.7(16)	S(11)-Yb(5)-N(8)-C(76)	-50.8(17)
S(6)-Yb(5)-N(8)-C(76)	68(3)	S(10)-Yb(5)-N(8)-C(76)	-140.8(17)
S(5)-Yb(5)-N(8)-C(76)	117.3(17)	S(3)-Yb(5)-N(8)-C(76)	30.8(17)
C(76)-N(8)-C(72)-C(73)	6(3)	Yb(5)-N(8)-C(72)-C(73)	-166.6(18)
N(8)-C(72)-C(73)-C(74)	-2(4)	C(72)-C(73)-C(74)-C(75)	-4(4)
C(73)-C(74)-C(75)-C(76)	4(4)	C(72)-N(8)-C(76)-C(75)	-5(4)
Yb(5)-N(8)-C(76)-C(75)	166.9(18)	C(74)-C(75)-C(76)-N(8)	0(4)
N(10)-Yb(6)-N(9)-C(77)	36(2)	S(5)-Yb(6)-N(9)-C(77)	-85(5)
S(6)-Yb(6)-N(9)-C(77)	-52(2)	S(12)-Yb(6)-N(9)-C(77)	128(2)
S(4)-Yb(6)-N(9)-C(77)	-142(2)	N(10)-Yb(6)-N(9)-C(81)	-134(2)

S(5)-Yb(6)-N(9)-C(81)	105(5)	S(6)-Yb(6)-N(9)-C(81)	138.4(19)
S(12)-Yb(6)-N(9)-C(81)	-41.6(19)	S(4)-Yb(6)-N(9)-C(81)	47.9(19)
C(81)-N(9)-C(77)-C(78)	-2(4)	Yb(6)-N(9)-C(77)-C(78)	-170.3(19)
N(9)-C(77)-C(78)-C(79)	-4(5)	C(77)-C(78)-C(79)-C(80)	7(5)
C(78)-C(79)-C(80)-C(81)	-4(5)	C(77)-N(9)-C(81)-C(80)	4(4)
Yb(6)-N(9)-C(81)-C(80)	174(2)	C(79)-C(80)-C(81)-N(9)	-2(5)
N(9)-Yb(6)-N(10)-C(82)	-118(2)	S(5)-Yb(6)-N(10)-C(82)	55.9(19)
S(6)-Yb(6)-N(10)-C(82)	-31.6(19)	S(12)-Yb(6)-N(10)-C(82)	156.8(19)
S(4)-Yb(6)-N(10)-C(82)	-108(3)	N(9)-Yb(6)-N(10)-C(86)	70.0(18)
S(5)-Yb(6)-N(10)-C(86)	-116.4(17)	S(6)-Yb(6)-N(10)-C(86)	156.1(18)
S(12)-Yb(6)-N(10)-C(86)	-15.5(18)	S(4)-Yb(6)-N(10)-C(86)	80(4)
C(86)-N(10)-C(82)-C(83)	-5(4)	Yb(6)-N(10)-C(82)-C(83)	-177.5(19)
N(10)-C(82)-C(83)-C(84)	5(4)	C(82)-C(83)-C(84)-C(85)	-4(4)
C(83)-C(84)-C(85)-C(86)	4(4)	C(82)-N(10)-C(86)-C(85)	5(3)
Yb(6)-N(10)-C(86)-C(85)	177.3(16)	C(84)-C(85)-C(86)-N(10)	-4(4)
C(91)-N(11)-C(87)-C(88)	-12(5)	N(11)-C(87)-C(88)-C(89)	9(5)
C(87)-C(88)-C(89)-C(90)	-2(6)	C(88)-C(89)-C(90)-C(91)	-2(6)
C(89)-C(90)-C(91)-N(11)	-1(5)	C(87)-N(11)-C(91)-C(90)	7(5)
C(96)-N(12)-C(92)-C(93)	7(6)	N(12)-C(92)-C(93)-C(94)	-7(7)
C(92)-C(93)-C(94)-C(95)	8(8)	C(93)-C(94)-C(95)-C(96)	-9(9)
C(94)-C(95)-C(96)-N(12)	9(8)	C(92)-N(12)-C(96)-C(95)	-8(6)

* These esd values are set to 100, since they are not well defined with the Yb(6)-S(4)-Yb(1) angle of 179.9(2) deg.



