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Table S1. Crystal data and structure refinement for [P(Et)4][Ce(Spy)4].

Empirical formula	C56 H72 Ce2 N8 P2 S8
formula weight	1455.88
Temperature	153(2) K
Radiation (type, wavelength)	MoKα, 0.71073 Å
Diffractometer, monochromator	CAD4, graphite
Stnd reflcns: no., interval, decay	3, 3600 s, < 1 %
Crystal system, space group	Monoclinic, P2/n
No. refls, Θ range for cell det'n	25, 12.6 to 16.9 °
Unit cell dimensions	a = 15.118(6) Å b = 16.117(4) Å c = 26.443(7) Å β = 90.14(3) °
Volume	6443(4) Å^3
Z	4
Density (calculated)	1.501 Mg/m^3
Absorption coefficient	1.746 mm^{-1}
F(000)	2952
Crystal color, description	orange, lathe
Crystal size	0.20 x 0.20 x 0.10 mm
Θ range for data collection	2 to 21 °
Index ranges	0<=h<=15, 0<=k<=16, -26<=l<=26
Reflections collected	7561
Independent reflections	6904 [R(int) = 0.034]
Transmission factors	0.704 to 0.753
Observed reflections	4251
Data / restraints / parameters	5826 / 384 / 687
Goodness-of-fit on all F^2 data	1.032
Final R(F), wR(F^2) [4251 I>2σ data]	0.045, 0.077
Final R(F), wR(F^2) [5826 I>0 data]	0.078, 0.086
Weights	$1/[\sigma^2(F_o^2)+(0.0279P)^2]$, where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.6 and -0.5 e·Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for [P(Et)4][Ce(Spy)4]. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ce(1)	2606(1)	2837(1)	-8(1)	23(1)
S(1)	3612(2)	3278(2)	-906(1)	35(1)
S(2)	1979(2)	4566(1)	37(1)	29(1)
S(3)	3858(2)	3345(2)	771(1)	42(1)
S(4)	1529(2)	1357(2)	-193(1)	45(1)
N(1)	3875(5)	1913(4)	-377(3)	27(2)
C(1)	4130(6)	2334(6)	-786(3)	28(2)
C(2)	4795(6)	2009(6)	-1111(4)	30(2)
C(3)	5164(6)	1257(6)	-986(4)	39(3)
C(4)	4884(6)	834(6)	-569(4)	39(3)
C(5)	4227(6)	1171(6)	-278(4)	39(3)
N(2)	1315(5)	3313(5)	548(3)	29(2)
C(6)	1249(6)	4141(6)	472(3)	26(2)
C(7)	631(6)	4613(6)	739(4)	35(3)
C(8)	84(6)	4240(6)	1085(4)	40(3)
C(9)	135(6)	3391(6)	1156(4)	39(3)
C(10)	750(6)	2953(6)	875(4)	34(3)
N(3)	3059(5)	1908(5)	748(3)	34(2)
C(11)	3709(6)	2340(6)	983(3)	32(3)
C(12)	4200(6)	1987(6)	1372(4)	42(3)
C(13)	4026(7)	1173(7)	1518(4)	43(3)
C(14)	3358(6)	744(6)	1289(4)	40(3)
C(15)	2903(6)	1133(6)	901(4)	37(3)
N(4)	1239(4)	2804(5)	-610(3)	30(2)
C(16)	960(6)	2030(6)	-605(3)	28(2)
C(17)	267(6)	1768(6)	-906(4)	37(3)

C(18)	-125(6)	2329(7)	-1221(4)	43(3)
C(19)	140(6)	3138(6)	-1240(3)	36(3)
C(20)	844(6)	3367(6)	-922(4)	36(3)
Ce(2)	2500	7772(1)	2500	21(1)
S(5)	721(1)	7073(2)	2580(1)	32(1)
S(6)	2358(2)	8491(2)	3516(1)	34(1)
N(5)	2133(4)	6516(4)	3073(2)	20(2)
C(21)	1233(5)	6459(5)	3039(3)	20(2)
C(22)	773(6)	5957(6)	3375(3)	30(3)
C(23)	1216(6)	5495(6)	3732(3)	32(3)
C(24)	2141(6)	5551(5)	3748(4)	31(3)
C(25)	2560(6)	6064(6)	3422(4)	35(3)
N(6)	3487(5)	8984(5)	2828(3)	30(2)
C(26)	3235(6)	9101(6)	3311(4)	26(2)
C(27)	3689(6)	9657(6)	3619(4)	30(2)
C(28)	4420(6)	10087(6)	3438(4)	32(3)
C(29)	4674(7)	9948(6)	2951(4)	44(3)
C(30)	4194(6)	9407(6)	2653(4)	43(3)
Ce(3)	7500	2336(1)	2500	22(1)
S(7)	6355(2)	1590(2)	3284(1)	32(1)
S(8)	9248(2)	3037(2)	2668(1)	37(1)
N(7)	7921(5)	1056(5)	3047(3)	29(2)
C(31)	7197(6)	857(6)	3309(3)	29(2)
C(32)	7164(7)	122(6)	3588(4)	44(3)
C(33)	7869(8)	-402(7)	3584(4)	49(3)
C(34)	8603(8)	-226(7)	3299(4)	59(3)
C(35)	8606(7)	514(8)	3041(4)	56(3)
N(8)	7806(5)	3554(4)	3125(3)	25(2)
C(36)	8695(6)	3617(5)	3120(3)	27(2)
C(37)	9130(6)	4136(6)	3473(4)	34(3)
C(38)	8657(7)	4591(6)	3806(4)	38(3)
C(39)	7734(7)	4550(6)	3796(3)	36(3)
C(40)	7350(6)	4020(6)	3452(3)	26(2)
P(1)	7579(2)	2377(2)	4857(1)	36(1)
C(41)	8364(7)	2750(6)	5300(4)	46(3)
C(42)	8935(6)	3473(7)	5121(4)	47(3)
C(43)	8119(6)	2173(7)	4269(4)	45(3)
C(44)	8829(7)	1492(8)	4315(5)	84(4)
C(45)	6729(6)	3137(6)	4706(4)	48(3)
C(46)	6085(7)	3278(7)	5125(4)	62(4)
C(47)	7066(7)	1443(6)	5098(4)	49(3)
C(48)	6292(8)	1127(7)	4775(4)	69(4)
P(2)	2500	3089(2)	7500	27(1)
C(49)	2857(6)	2441(6)	6995(3)	33(3)
C(50)	3547(6)	1796(6)	7160(4)	48(3)
C(51)	1615(6)	3729(5)	7268(4)	35(3)
C(52)	1319(6)	4389(6)	7647(4)	36(3)
P(3)	2500	3262(2)	2500	25(1)
C(53)	2885(6)	2624(6)	3013(3)	33(3)
C(54)	3602(6)	2011(6)	2873(4)	49(3)
C(55)	1616(6)	3883(6)	2728(3)	31(3)
C(56)	1263(6)	4515(6)	2354(4)	52(3)

Table S3. Bond lengths [Å] and angles [°] for [P(Et)4][Ce(Spy)4].

Ce(1)-N(2)	2.564(7)	Ce(1)-N(3)	2.588(7)
Ce(1)-N(4)	2.606(7)	Ce(1)-N(1)	2.619(7)
Ce(1)-S(1)	2.912(3)	Ce(1)-S(3)	2.912(3)
Ce(1)-S(4)	2.928(3)	Ce(1)-S(2)	2.947(2)
S(1)-C(1)	1.740(9)	S(2)-C(6)	1.737(9)
S(3)-C(11)	1.729(10)	S(4)-C(16)	1.761(10)
N(1)-C(1)	1.335(11)	N(1)-C(5)	1.336(11)
C(1)-C(2)	1.424(12)	C(2)-C(3)	1.374(12)
C(3)-C(4)	1.364(13)	C(4)-C(5)	1.370(13)
N(2)-C(10)	1.347(11)	N(2)-C(6)	1.354(11)
C(6)-C(7)	1.396(12)	C(7)-C(8)	1.374(12)

C(8)-C(9)	1.382(13)	C(9)-C(10)	1.386(12)
N(3)-C(15)	1.334(11)	N(3)-C(11)	1.354(11)
C(11)-C(12)	1.389(13)	C(12)-C(13)	1.393(13)
C(13)-C(14)	1.364(13)	C(14)-C(15)	1.383(13)
N(4)-C(16)	1.318(11)	N(4)-C(20)	1.363(11)
C(16)-C(17)	1.379(11)	C(17)-C(18)	1.366(13)
C(18)-C(19)	1.364(13)	C(19)-C(20)	1.403(12)
Ce(2)-N(5)'	2.588(7)	Ce(2)-N(5)	2.588(7)
Ce(2)-N(6)	2.606(7)	Ce(2)-N(6)'	2.606(7)
Ce(2)-S(5)	2.924(3)	Ce(2)-S(5)'	2.924(2)
Ce(2)-S(6)	2.935(3)	Ce(2)-S(6)'	2.935(3)
S(5)-C(21)	1.748(9)	S(6)-C(26)	1.739(9)
N(5)-C(25)	1.341(11)	N(5)-C(21)	1.366(10)
C(21)-C(22)	1.388(12)	C(22)-C(23)	1.375(12)
C(23)-C(24)	1.401(12)	C(24)-C(25)	1.353(13)
N(6)-C(26)	1.345(11)	N(6)-C(30)	1.351(11)
C(26)-C(27)	1.392(12)	C(27)-C(28)	1.390(12)
C(28)-C(29)	1.361(12)	C(29)-C(30)	1.381(13)
Ce(3)-N(7)"	2.597(8)	Ce(3)-N(7)	2.597(8)
Ce(3)-N(8)	2.606(7)	Ce(3)-N(8)"	2.606(7)
Ce(3)-S(8)	2.907(3)	Ce(3)-S(8)"	2.907(3)
Ce(3)-S(7)	2.961(3)	Ce(3)-S(7)"	2.961(3)
S(7)-C(31)	1.737(9)	S(8)-C(36)	1.734(9)
N(7)-C(31)	1.336(11)	N(7)-C(35)	1.355(12)
C(31)-C(32)	1.396(13)	C(32)-C(33)	1.360(14)
C(33)-C(34)	1.37(2)	C(34)-C(35)	1.374(14)
N(8)-C(40)	1.338(10)	N(8)-C(36)	1.348(10)
C(36)-C(37)	1.415(12)	C(37)-C(38)	1.352(13)
C(38)-C(39)	1.396(12)	C(39)-C(40)	1.376(12)
P(1)-C(41)	1.771(10)	P(1)-C(43)	1.787(10)
P(1)-C(47)	1.810(10)	P(1)-C(45)	1.818(10)
C(41)-C(42)	1.526(13)	C(43)-C(44)	1.539(14)
C(45)-C(46)	1.494(12)	C(47)-C(48)	1.535(13)
P(2)-C(49)	1.780(9)	P(2)-C(49)'"	1.780(9)
P(2)-C(51)'"	1.796(9)	P(2)-C(51)	1.796(9)
C(49)-C(50)	1.535(12)	C(51)-C(52)	1.527(12)
P(3)-C(55)'	1.776(9)	P(3)-C(55)	1.776(9)
P(3)-C(53)'	1.798(9)	P(3)-C(53)	1.798(9)
C(53)-C(54)	1.513(12)	C(55)-C(56)	1.515(12)

N(2)-Ce(1)-N(3)	86.0(2)	N(2)-Ce(1)-N(4)	75.7(2)
N(3)-Ce(1)-N(4)	131.9(2)	N(2)-Ce(1)-N(1)	160.6(2)
N(3)-Ce(1)-N(1)	76.5(2)	N(4)-Ce(1)-N(1)	110.0(2)
N(2)-Ce(1)-S(1)	142.6(2)	N(3)-Ce(1)-S(1)	129.3(2)
N(4)-Ce(1)-S(1)	85.5(2)	N(1)-Ce(1)-S(1)	56.7(2)
N(2)-Ce(1)-S(3)	90.3(2)	N(3)-Ce(1)-S(3)	56.4(2)
N(4)-Ce(1)-S(3)	162.0(2)	N(1)-Ce(1)-S(3)	87.0(2)
S(1)-Ce(1)-S(3)	99.68(8)	N(2)-Ce(1)-S(4)	85.2(2)
N(3)-Ce(1)-S(4)	78.7(2)	N(4)-Ce(1)-S(4)	56.1(2)
N(1)-Ce(1)-S(4)	83.3(2)	S(1)-Ce(1)-S(4)	110.75(8)
S(3)-Ce(1)-S(4)	135.06(8)	N(2)-Ce(1)-S(2)	56.5(2)
N(3)-Ce(1)-S(2)	126.9(2)	N(4)-Ce(1)-S(2)	77.8(2)
N(1)-Ce(1)-S(2)	142.1(2)	S(1)-Ce(1)-S(2)	88.29(7)
S(3)-Ce(1)-S(2)	85.08(8)	S(4)-Ce(1)-S(2)	126.73(8)
C(1)-S(1)-Ce(1)	82.7(3)	C(6)-S(2)-Ce(1)	81.9(3)
C(11)-S(3)-Ce(1)	83.1(3)	C(16)-S(4)-Ce(1)	82.7(3)
C(1)-N(1)-C(5)	119.9(8)	C(1)-N(1)-Ce(1)	103.1(6)
C(5)-N(1)-Ce(1)	136.8(6)	N(1)-C(1)-C(2)	120.5(8)
N(1)-C(1)-S(1)	117.5(7)	C(2)-C(1)-S(1)	122.0(7)
C(3)-C(2)-C(1)	117.9(9)	C(4)-C(3)-C(2)	120.5(10)
C(3)-C(4)-C(5)	118.9(10)	N(1)-C(5)-C(4)	122.3(9)
C(10)-N(2)-C(6)	118.2(8)	C(10)-N(2)-Ce(1)	136.4(7)
C(6)-N(2)-Ce(1)	105.4(6)	N(2)-C(6)-C(7)	120.7(8)
N(2)-C(6)-S(2)	116.1(7)	C(7)-C(6)-S(2)	123.1(7)
C(8)-C(7)-C(6)	120.2(9)	C(7)-C(8)-C(9)	119.3(10)
C(8)-C(9)-C(10)	117.9(10)	N(2)-C(10)-C(9)	123.6(9)
C(15)-N(3)-C(11)	118.1(8)	C(15)-N(3)-Ce(1)	136.8(7)
C(11)-N(3)-Ce(1)	104.3(6)	N(3)-C(11)-C(12)	121.0(9)
N(3)-C(11)-S(3)	115.4(7)	C(12)-C(11)-S(3)	123.6(8)

C(11)-C(12)-C(13)	119.4(10)	C(14)-C(13)-C(12)	119.6(10)
C(13)-C(14)-C(15)	117.7(10)	N(3)-C(15)-C(14)	124.2(10)
C(16)-N(4)-C(20)	119.7(8)	C(16)-N(4)-Ce(1)	105.5(6)
C(20)-N(4)-Ce(1)	134.6(6)	N(4)-C(16)-C(17)	121.8(9)
N(4)-C(16)-S(4)	115.7(7)	C(17)-C(16)-S(4)	122.5(8)
C(18)-C(17)-C(16)	118.5(9)	C(19)-C(18)-C(17)	121.8(9)
C(18)-C(19)-C(20)	117.0(9)	N(4)-C(20)-C(19)	121.1(9)
N(5)' -Ce(2)-N(5)	77.2(3)	N(5)' -Ce(2)-N(6)	131.1(2)
N(5)-Ce(2)-N(6)	121.0(2)	N(5)' -Ce(2)-N(6)'	121.0(2)
N(5)-Ce(2)-N(6)'	131.1(2)	N(6)-Ce(2)-N(6)'	82.8(3)
N(5)' -Ce(2)-S(5)	86.6(2)	N(5)-Ce(2)-S(5)	57.2(2)
N(6)-Ce(2)-S(5)	142.2(2)	N(6)' -Ce(2)-S(5)	77.7(2)
N(5)' -Ce(2)-S(5)'	57.2(2)	N(5)-Ce(2)-S(5)'	86.6(2)
N(6)-Ce(2)-S(5)'	77.7(2)	N(6)' -Ce(2)-S(5)'	142.2(2)
S(5)-Ce(2)-S(5)'	134.73(11)	N(5)' -Ce(2)-S(6)	149.4(2)
N(5)-Ce(2)-S(6)	75.9(2)	N(6)-Ce(2)-S(6)	56.1(2)
N(6)' -Ce(2)-S(6)	88.0(2)	S(5)-Ce(2)-S(6)	90.96(7)
S(5)' -Ce(2)-S(6)	106.68(7)	N(5)' -Ce(2)-S(6)'	75.9(2)
N(5)-Ce(2)-S(6)'	149.4(2)	N(6)-Ce(2)-S(6)'	88.0(2)
N(6)' -Ce(2)-S(6)'	56.1(2)	S(5)-Ce(2)-S(6)'	106.69(7)
S(5)' -Ce(2)-S(6)'	90.96(7)	S(6)-Ce(2)-S(6)'	133.49(11)
C(21)-S(5)-Ce(2)	82.1(3)	C(26)-S(6)-Ce(2)	83.1(3)
C(25)-N(5)-C(21)	119.0(8)	C(25)-N(5)-Ce(2)	136.4(6)
C(21)-N(5)-Ce(2)	103.3(5)	N(5)-C(21)-C(22)	119.9(8)
N(5)-C(21)-S(5)	116.5(7)	C(22)-C(21)-S(5)	123.5(7)
C(23)-C(22)-C(21)	120.7(9)	C(22)-C(23)-C(24)	118.0(9)
C(25)-C(24)-C(23)	119.3(9)	N(5)-C(25)-C(24)	123.1(9)
C(26)-N(6)-C(30)	118.8(8)	C(26)-N(6)-Ce(2)	104.9(6)
C(30)-N(6)-Ce(2)	135.8(7)	N(6)-C(26)-C(27)	120.4(9)
N(6)-C(26)-S(6)	115.8(7)	C(27)-C(26)-S(6)	123.8(8)
C(28)-C(27)-C(26)	120.6(9)	C(29)-C(28)-C(27)	118.1(9)
C(28)-C(29)-C(30)	119.7(10)	N(6)-C(30)-C(29)	122.5(10)
N(7)" -Ce(3)-N(7)	74.8(3)	N(7)" -Ce(3)-N(8)	173.7(2)
N(7)-Ce(3)-N(8)	101.7(2)	N(7)" -Ce(3)-N(8)"	101.7(2)
N(7)-Ce(3)-N(8)"	173.7(2)	N(8)-Ce(3)-N(8)"	82.3(3)
N(7)" -Ce(3)-S(8)	127.9(2)	N(7)-Ce(3)-S(8)	90.1(2)
N(8)-Ce(3)-S(8)	56.7(2)	N(8)" -Ce(3)-S(8)	87.9(2)
N(7)" -Ce(3)-S(8)"	90.1(2)	N(7)-Ce(3)-S(8)"	127.9(2)
N(8)-Ce(3)-S(8)"	87.9(2)	N(8)" -Ce(3)-S(8)"	56.7(2)
S(8)-Ce(3)-S(8)"	134.29(11)	N(7)" -Ce(3)-S(7)	85.7(2)
N(7)-Ce(3)-S(7)	55.3(2)	N(8)-Ce(3)-S(7)	88.0(2)
N(8)" -Ce(3)-S(7)	130.3(2)	S(8)-Ce(3)-S(7)	125.72(7)
S(8)" -Ce(3)-S(7)	74.45(7)	N(7)" -Ce(3)-S(7)"	55.3(2)
N(7)-Ce(3)-S(7)"	85.7(2)	N(8)-Ce(3)-S(7)"	130.3(2)
N(8)" -Ce(3)-S(7)"	88.0(2)	S(8)-Ce(3)-S(7)"	74.45(7)
S(8)" -Ce(3)-S(7)"	125.72(7)	S(7)-Ce(3)-S(7)"	132.04(11)
C(31)-S(7)-Ce(3)	82.7(3)	C(36)-S(8)-Ce(3)	82.8(3)
C(31)-N(7)-C(35)	118.5(9)	C(31)-N(7)-Ce(3)	106.3(6)
C(35)-N(7)-Ce(3)	133.8(7)	N(7)-C(31)-C(32)	120.6(9)
N(7)-C(31)-S(7)	114.7(7)	C(32)-C(31)-S(7)	124.7(8)
C(33)-C(32)-C(31)	119.6(11)	C(32)-C(33)-C(34)	120.7(11)
C(35)-C(34)-C(33)	117.1(11)	N(7)-C(35)-C(34)	123.4(11)
C(40)-N(8)-C(36)	118.6(8)	C(40)-N(8)-Ce(3)	137.9(6)
C(36)-N(8)-Ce(3)	103.1(6)	N(8)-C(36)-C(37)	120.0(9)
N(8)-C(36)-S(8)	116.7(7)	C(37)-C(36)-S(8)	123.3(7)
C(38)-C(37)-C(36)	120.3(9)	C(37)-C(38)-C(39)	119.4(10)
C(40)-C(39)-C(38)	117.5(9)	N(8)-C(40)-C(39)	124.0(9)
C(41)-P(1)-C(43)	109.3(5)	C(41)-P(1)-C(47)	109.6(5)
C(43)-P(1)-C(47)	110.5(5)	C(41)-P(1)-C(45)	112.9(5)
C(43)-P(1)-C(45)	105.0(5)	C(47)-P(1)-C(45)	109.5(5)
C(42)-C(41)-P(1)	115.6(7)	C(44)-C(43)-P(1)	112.5(7)
C(46)-C(45)-P(1)	113.7(8)	C(48)-C(47)-P(1)	114.1(7)
C(49)-P(2)-C(49)'"	108.1(6)	C(49)-P(2)-C(51)'"	111.5(4)
C(49)'"-P(2)-C(51)'"	108.0(4)	C(49)-P(2)-C(51)	108.0(4)
C(49)'"-P(2)-C(51)	111.5(4)	C(51)'"-P(2)-C(51)	109.9(6)
C(50)-C(49)-P(2)	113.0(7)	C(52)-C(51)-P(2)	113.3(6)
C(55)' -P(3)-C(55)	111.4(6)	C(55)' -P(3)-C(53)'	108.0(4)
C(55)-P(3)-C(53)'	109.6(4)	C(55)' -P(3)-C(53)	109.6(4)

C(55)-P(3)-C(53)	108.0(4)	C(53)' -P(3)-C(53)	110.2(6)
C(54)-C(53)-P(3)	114.8(7)	C(56)-C(55)-P(3)	115.0(7)

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

Table S4. Anisotropic displacement parameters (Uij, Å² x 10³) for [P(Et)4][Ce(Spy)4]. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$.

	U11	U22	U33	U23	U13	U12
Ce(1)	23(1)	22(1)	23(1)	-2(1)	-1(1)	-2(1)
S(1)	41(2)	36(2)	28(2)	7(1)	5(1)	4(1)
S(2)	36(2)	26(1)	24(2)	0(1)	6(1)	-4(1)
S(3)	50(2)	38(2)	37(2)	0(2)	-16(1)	-8(2)
S(4)	49(2)	25(2)	62(2)	-6(1)	-14(2)	-5(1)
N(1)	33(5)	24(5)	24(5)	6(4)	5(4)	4(4)
C(1)	27(5)	36(6)	21(5)	-1(5)	-4(4)	-7(5)
C(2)	29(5)	33(6)	28(6)	-2(5)	8(5)	-16(5)
C(3)	35(6)	44(7)	38(7)	-17(6)	1(5)	0(5)
C(4)	42(6)	29(6)	48(7)	-3(6)	2(6)	10(5)
C(5)	48(6)	39(6)	30(6)	6(5)	5(5)	6(5)
N(2)	25(4)	37(5)	26(5)	5(4)	-2(4)	-5(4)
C(6)	31(6)	32(6)	15(5)	-5(5)	-7(4)	-3(5)
C(7)	37(6)	24(5)	44(7)	7(5)	3(5)	7(5)
C(8)	33(6)	44(7)	44(7)	-5(6)	21(5)	3(5)
C(9)	37(6)	40(7)	40(7)	-3(6)	3(5)	-12(5)
C(10)	34(5)	30(6)	38(6)	7(5)	-5(5)	-3(5)
N(3)	43(5)	29(5)	30(5)	5(4)	0(4)	-9(4)
C(11)	31(5)	41(6)	25(6)	1(5)	3(5)	-1(5)
C(12)	40(6)	46(7)	41(7)	-9(6)	-13(5)	9(5)
C(13)	41(6)	55(7)	34(6)	15(6)	-1(5)	15(6)
C(14)	35(6)	43(6)	43(7)	14(6)	6(6)	12(5)
C(15)	39(6)	39(6)	34(7)	-2(5)	1(5)	-3(5)
N(4)	20(4)	36(5)	33(5)	4(4)	-4(4)	0(4)
C(16)	25(5)	27(6)	31(6)	-12(5)	3(5)	-10(5)
C(17)	34(6)	34(6)	43(6)	-19(5)	-8(5)	-4(5)
C(18)	30(6)	59(8)	39(6)	-5(6)	-4(5)	-6(6)
C(19)	31(6)	47(7)	30(6)	5(5)	-5(5)	-1(5)
C(20)	41(6)	34(6)	31(6)	2(5)	8(5)	-2(5)
Ce(2)	19(1)	24(1)	20(1)	0	1(1)	0
S(5)	21(1)	40(2)	34(2)	10(1)	-5(1)	-1(1)
S(6)	36(2)	39(2)	26(2)	-7(1)	9(1)	-9(1)
N(5)	18(4)	25(4)	16(4)	-6(4)	-2(3)	-6(4)
C(21)	21(5)	21(5)	19(5)	-10(4)	3(4)	-3(4)
C(22)	32(6)	32(6)	25(6)	0(5)	5(5)	-2(5)
C(23)	43(6)	35(6)	19(6)	-2(5)	7(5)	-4(5)
C(24)	46(6)	19(6)	27(6)	0(5)	-13(5)	10(5)
C(25)	31(6)	36(6)	36(7)	8(6)	-7(5)	7(5)
N(6)	32(5)	31(5)	27(5)	-4(4)	7(4)	-6(4)
C(26)	19(5)	24(5)	36(6)	-9(5)	-4(5)	10(4)
C(27)	35(6)	25(5)	29(6)	-2(5)	-8(5)	10(5)
C(28)	39(6)	23(5)	34(6)	-1(5)	-19(5)	2(5)
C(29)	40(6)	39(6)	52(7)	-4(6)	7(6)	-14(5)
C(30)	41(6)	52(7)	36(7)	3(6)	11(6)	-9(6)
Ce(3)	20(1)	25(1)	22(1)	0	-1(1)	0
S(7)	28(2)	34(2)	34(2)	5(1)	4(1)	-3(1)
S(8)	24(1)	45(2)	41(2)	-13(1)	4(1)	0(1)
N(7)	31(5)	42(5)	13(5)	-1(4)	5(4)	9(4)
C(31)	39(6)	29(6)	18(6)	-6(5)	-2(5)	-3(5)
C(32)	56(7)	44(7)	33(6)	10(6)	-9(5)	-2(6)
C(33)	72(8)	34(6)	40(7)	2(6)	-18(6)	2(6)
C(34)	79(8)	53(7)	46(7)	9(6)	-10(7)	27(7)
C(35)	52(7)	80(8)	36(7)	1(6)	7(6)	14(7)
N(8)	20(4)	31(5)	25(5)	1(4)	5(4)	-2(4)
C(36)	35(6)	21(5)	25(6)	2(5)	-3(5)	2(5)

C(37)	31(6)	35(6)	37(6)	9(5)	-4(5)	-3(5)
C(38)	48(7)	31(6)	33(6)	6(5)	1(5)	-8(6)
C(39)	62(7)	26(6)	20(6)	-4(5)	-2(6)	5(6)
C(40)	23(5)	28(6)	27(6)	8(5)	8(5)	7(5)
P(1)	45(2)	31(2)	32(2)	2(1)	10(1)	5(1)
C(41)	65(7)	43(7)	29(6)	-10(5)	-2(5)	5(6)
C(42)	49(6)	63(7)	28(6)	-8(6)	-1(5)	4(6)
C(43)	44(6)	61(7)	29(6)	-9(6)	-14(5)	-10(6)
C(44)	66(8)	109(10)	75(9)	-29(8)	5(7)	30(8)
C(45)	51(7)	36(6)	57(7)	2(6)	9(6)	10(5)
C(46)	70(7)	42(7)	73(8)	5(6)	28(7)	-2(6)
C(47)	62(7)	46(7)	38(7)	7(5)	7(6)	-7(6)
C(48)	98(9)	55(7)	54(8)	-6(6)	7(7)	-9(7)
P(2)	20(2)	33(2)	29(2)	0	2(2)	0
C(49)	35(5)	34(6)	30(6)	2(5)	5(5)	-6(5)
C(50)	40(6)	53(7)	52(7)	-8(6)	8(5)	-3(6)
C(51)	40(6)	26(6)	37(6)	-1(5)	-10(5)	0(5)
C(52)	36(6)	38(6)	35(6)	6(5)	-1(5)	8(5)
P(3)	22(2)	30(2)	25(2)	0	1(2)	0
C(53)	38(5)	34(6)	28(6)	2(5)	4(5)	-11(5)
C(54)	63(7)	40(6)	45(7)	16(6)	-7(6)	22(6)
C(55)	24(5)	38(6)	31(6)	-6(5)	4(5)	2(5)
C(56)	42(6)	54(7)	60(8)	-5(6)	7(6)	5(6)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [P(Et)4][Ce(Spy)4].

	x	y	z	U(eq)
H(2)	4978(6)	2302(6)	-1404(4)	36
H(3)	5618(6)	1030(6)	-1192(4)	47
H(4)	5140(6)	315(6)	-483(4)	47
H(5)	4015(6)	865(6)	4(4)	47
H(7)	589(6)	5193(6)	680(4)	42
H(8)	-324(6)	4562(6)	1274(4)	48
H(9)	-240(6)	3117(6)	1391(4)	47
H(10)	773(6)	2368(6)	914(4)	41
H(12)	4649(6)	2298(6)	1537(4)	51
H(13)	4370(7)	918(7)	1776(4)	52
H(14)	3211(6)	196(6)	1391(4)	48
H(15)	2450(6)	830(6)	734(4)	45
H(17)	67(6)	1209(6)	-893(4)	44
H(18)	-596(6)	2152(7)	-1434(4)	51
H(19)	-138(6)	3527(6)	-1458(3)	44
H(20)	1048(6)	3925(6)	-924(4)	43
H(22)	146(6)	5933(6)	3358(3)	36
H(23)	905(6)	5149(6)	3961(3)	39
H(24)	2470(6)	5232(5)	3985(4)	37
H(25)	3186(6)	6105(6)	3441(4)	42
H(27)	3499(6)	9744(6)	3957(4)	36
H(28)	4732(6)	10467(6)	3647(4)	39
H(29)	5179(7)	10221(6)	2818(4)	52
H(30)	4367(6)	9330(6)	2311(4)	52
H(32)	6652(7)	-11(6)	3779(4)	53
H(33)	7854(8)	-895(7)	3780(4)	59
H(34)	9088(8)	-599(7)	3281(4)	71
H(35)	9114(7)	654(8)	2849(4)	67
H(37)	9757(6)	4164(6)	3477(4)	41
H(38)	8950(7)	4936(6)	4045(4)	45
H(39)	7385(7)	4875(6)	4019(3)	43
H(40)	6723(6)	3983(6)	3446(3)	32
H(41A)	8046(7)	2924(6)	5609(4)	55
H(41B)	8760(7)	2285(6)	5395(4)	55
H(42A)	9346(6)	3633(7)	5391(4)	70
H(42B)	8554(6)	3946(7)	5036(4)	70
H(42C)	9270(6)	3305(7)	4821(4)	70

H(43A)	7672(6)	2000(7)	4016(4)	54
H(43B)	8399(6)	2690(7)	4146(4)	54
H(44A)	9105(7)	1403(8)	3984(5)	125
H(44B)	8554(7)	976(8)	4430(5)	125
H(44C)	9281(7)	1666(8)	4560(5)	125
H(45A)	7018(6)	3671(6)	4622(4)	57
H(45B)	6402(6)	2949(6)	4403(4)	57
H(46A)	5647(7)	3692(7)	5020(4)	93
H(46B)	6401(7)	3479(7)	5425(4)	93
H(46C)	5785(7)	2756(7)	5206(4)	93
H(47A)	7520(7)	1002(6)	5119(4)	58
H(47B)	6851(7)	1552(6)	5444(4)	58
H(48A)	6048(8)	622(7)	4928(4)	104
H(48B)	6501(8)	1002(7)	4433(4)	104
H(48C)	5831(8)	1553(7)	4758(4)	104
H(49A)	2338(6)	2149(6)	6851(3)	40
H(49B)	3113(6)	2791(6)	6725(3)	40
H(50A)	3718(6)	1458(6)	6869(4)	72
H(50B)	3294(6)	1439(6)	7423(4)	72
H(50C)	4069(6)	2081(6)	7295(4)	72
H(51A)	1809(6)	4007(5)	6954(4)	41
H(51B)	1103(6)	3372(5)	7183(4)	41
H(52A)	836(6)	4716(6)	7499(4)	54
H(52B)	1817(6)	4755(6)	7727(4)	54
H(52C)	1112(6)	4119(6)	7957(4)	54
H(53A)	3113(6)	2989(6)	3285(3)	40
H(53B)	2376(6)	2313(6)	3152(3)	40
H(54A)	3772(6)	1689(6)	3172(4)	74
H(54B)	4119(6)	2311(6)	2745(4)	74
H(54C)	3380(6)	1634(6)	2611(4)	74
H(55A)	1125(6)	3513(6)	2829(3)	38
H(55B)	1819(6)	4180(6)	3034(3)	38
H(56A)	780(6)	4828(6)	2511(4)	78
H(56B)	1041(6)	4228(6)	2052(4)	78
H(56C)	1738(6)	4896(6)	2258(4)	78

Table S6. Torsion angles [°] for [P(Et)4][Ce(Spy)4].

N(2)-Ce(1)-S(1)-C(1)	-175.7(4)	N(3)-Ce(1)-S(1)-C(1)	26.9(4)
N(4)-Ce(1)-S(1)-C(1)	-116.4(3)	N(1)-Ce(1)-S(1)-C(1)	1.1(3)
S(3)-Ce(1)-S(1)-C(1)	81.0(3)	S(4)-Ce(1)-S(1)-C(1)	-65.4(3)
S(2)-Ce(1)-S(1)-C(1)	165.7(3)	N(2)-Ce(1)-S(2)-C(6)	1.1(4)
N(3)-Ce(1)-S(2)-C(6)	-52.0(4)	N(4)-Ce(1)-S(2)-C(6)	81.9(3)
N(1)-Ce(1)-S(2)-C(6)	-171.2(4)	S(1)-Ce(1)-S(2)-C(6)	167.6(3)
S(3)-Ce(1)-S(2)-C(6)	-92.5(3)	S(4)-Ce(1)-S(2)-C(6)	52.8(3)
N(2)-Ce(1)-S(3)-C(11)	89.7(4)	N(3)-Ce(1)-S(3)-C(11)	4.7(4)
N(4)-Ce(1)-S(3)-C(11)	128.0(6)	N(1)-Ce(1)-S(3)-C(11)	-71.1(3)
S(1)-Ce(1)-S(3)-C(11)	-126.5(3)	S(4)-Ce(1)-S(3)-C(11)	6.3(3)
S(2)-Ce(1)-S(3)-C(11)	146.1(3)	N(2)-Ce(1)-S(4)-C(16)	77.7(3)
N(3)-Ce(1)-S(4)-C(16)	164.6(4)	N(4)-Ce(1)-S(4)-C(16)	1.7(4)
N(1)-Ce(1)-S(4)-C(16)	-118.0(3)	S(1)-Ce(1)-S(4)-C(16)	-67.5(3)
S(3)-Ce(1)-S(4)-C(16)	163.2(3)	S(2)-Ce(1)-S(4)-C(16)	36.6(3)
N(2)-Ce(1)-N(1)-C(1)	172.7(6)	N(3)-Ce(1)-N(1)-C(1)	-161.2(6)
N(4)-Ce(1)-N(1)-C(1)	68.7(6)	S(1)-Ce(1)-N(1)-C(1)	-1.5(5)
S(3)-Ce(1)-N(1)-C(1)	-105.1(5)	S(4)-Ce(1)-N(1)-C(1)	118.8(5)
S(2)-Ce(1)-N(1)-C(1)	-27.1(7)	N(2)-Ce(1)-N(1)-C(5)	-1.1(13)
N(3)-Ce(1)-N(1)-C(5)	25.0(9)	N(4)-Ce(1)-N(1)-C(5)	-105.1(9)
S(1)-Ce(1)-N(1)-C(5)	-175.2(10)	S(3)-Ce(1)-N(1)-C(5)	81.1(9)
S(4)-Ce(1)-N(1)-C(5)	-54.9(9)	S(2)-Ce(1)-N(1)-C(5)	159.2(8)
C(5)-N(1)-C(1)-C(2)	-1.9(13)	Ce(1)-N(1)-C(1)-C(2)	-177.0(7)
C(5)-N(1)-C(1)-S(1)	177.4(7)	Ce(1)-N(1)-C(1)-S(1)	2.3(7)
Ce(1)-S(1)-C(1)-N(1)	-2.0(6)	Ce(1)-S(1)-C(1)-C(2)	177.3(7)
N(1)-C(1)-C(2)-C(3)	-0.4(13)	S(1)-C(1)-C(2)-C(3)	-179.7(7)
C(1)-C(2)-C(3)-C(4)	1.3(13)	C(2)-C(3)-C(4)-C(5)	0(2)
C(1)-N(1)-C(5)-C(4)	3.5(14)	Ce(1)-N(1)-C(5)-C(4)	176.5(7)
C(3)-C(4)-C(5)-N(1)	-3(2)	N(3)-Ce(1)-N(2)-C(10)	-40.2(8)

N(4)-Ce(1)-N(2)-C(10)	95.0(9)	N(1)-Ce(1)-N(2)-C(10)	-14.8(13)
S(1)-Ce(1)-N(2)-C(10)	157.1(7)	S(3)-Ce(1)-N(2)-C(10)	-96.4(8)
S(4)-Ce(1)-N(2)-C(10)	38.8(8)	S(2)-Ce(1)-N(2)-C(10)	179.6(9)
N(3)-Ce(1)-N(2)-C(6)	138.8(6)	N(4)-Ce(1)-N(2)-C(6)	-86.1(6)
N(1)-Ce(1)-N(2)-C(6)	164.2(6)	S(1)-Ce(1)-N(2)-C(6)	-23.9(7)
S(3)-Ce(1)-N(2)-C(6)	82.5(5)	S(4)-Ce(1)-N(2)-C(6)	-142.2(5)
S(2)-Ce(1)-N(2)-C(6)	-1.4(5)	C(10)-N(2)-C(6)-C(7)	2.3(13)
Ce(1)-N(2)-C(6)-C(7)	-176.9(7)	C(10)-N(2)-C(6)-S(2)	-178.6(6)
Ce(1)-N(2)-C(6)-S(2)	2.2(7)	Ce(1)-S(2)-C(6)-N(2)	-1.9(6)
Ce(1)-S(2)-C(6)-C(7)	177.2(8)	N(2)-C(6)-C(7)-C(8)	0.3(14)
S(2)-C(6)-C(7)-C(8)	-178.7(7)	C(6)-C(7)-C(8)-C(9)	-2(2)
C(7)-C(8)-C(9)-C(10)	1(2)	C(6)-N(2)-C(10)-C(9)	-3.5(13)
Ce(1)-N(2)-C(10)-C(9)	175.4(6)	C(8)-C(9)-C(10)-N(2)	2(2)
N(2)-Ce(1)-N(3)-C(15)	91.7(9)	N(4)-Ce(1)-N(3)-C(15)	25.0(10)
N(1)-Ce(1)-N(3)-C(15)	-79.8(9)	S(1)-Ce(1)-N(3)-C(15)	-101.8(9)
S(3)-Ce(1)-N(3)-C(15)	-175.3(10)	S(4)-Ce(1)-N(3)-C(15)	5.9(9)
S(2)-Ce(1)-N(3)-C(15)	133.7(9)	N(2)-Ce(1)-N(3)-C(11)	-99.1(6)
N(4)-Ce(1)-N(3)-C(11)	-165.8(5)	N(1)-Ce(1)-N(3)-C(11)	89.3(6)
S(1)-Ce(1)-N(3)-C(11)	67.4(6)	S(3)-Ce(1)-N(3)-C(11)	-6.1(5)
S(4)-Ce(1)-N(3)-C(11)	175.0(6)	S(2)-Ce(1)-N(3)-C(11)	-57.2(6)
C(15)-N(3)-C(11)-C(12)	0.0(13)	Ce(1)-N(3)-C(11)-C(12)	-171.6(8)
C(15)-N(3)-C(11)-S(3)	-178.9(7)	Ce(1)-N(3)-C(11)-S(3)	9.5(7)
Ce(1)-S(3)-C(11)-N(3)	-8.3(6)	Ce(1)-S(3)-C(11)-C(12)	172.9(9)
N(3)-C(11)-C(12)-C(13)	1(2)	S(3)-C(11)-C(12)-C(13)	179.6(7)
C(11)-C(12)-C(13)-C(14)	-2(2)	C(12)-C(13)-C(14)-C(15)	3(2)
C(11)-N(3)-C(15)-C(14)	0.6(14)	Ce(1)-N(3)-C(15)-C(14)	168.7(7)
C(13)-C(14)-C(15)-N(3)	-2(2)	N(2)-Ce(1)-N(4)-C(16)	-96.1(6)
N(3)-Ce(1)-N(4)-C(16)	-25.1(7)	N(1)-Ce(1)-N(4)-C(16)	64.5(6)
S(1)-Ce(1)-N(4)-C(16)	116.5(6)	S(3)-Ce(1)-N(4)-C(16)	-135.9(6)
S(4)-Ce(1)-N(4)-C(16)	-2.3(5)	S(2)-Ce(1)-N(4)-C(16)	-154.3(6)
N(2)-Ce(1)-N(4)-C(20)	89.0(8)	N(3)-Ce(1)-N(4)-C(20)	160.0(7)
N(1)-Ce(1)-N(4)-C(20)	-110.4(8)	S(1)-Ce(1)-N(4)-C(20)	-58.4(8)
S(3)-Ce(1)-N(4)-C(20)	49.2(11)	S(4)-Ce(1)-N(4)-C(20)	-177.2(9)
S(2)-Ce(1)-N(4)-C(20)	30.8(8)	C(20)-N(4)-C(16)-C(17)	-0.5(13)
Ce(1)-N(4)-C(16)-C(17)	-176.4(7)	C(20)-N(4)-C(16)-S(4)	179.3(7)
Ce(1)-N(4)-C(16)-S(4)	3.5(7)	Ce(1)-S(4)-C(16)-N(4)	-3.0(6)
Ce(1)-S(4)-C(16)-C(17)	176.8(8)	N(4)-C(16)-C(17)-C(18)	1.0(14)
S(4)-C(16)-C(17)-C(18)	-178.8(7)	C(16)-C(17)-C(18)-C(19)	-1(2)
C(17)-C(18)-C(19)-C(20)	1(2)	C(16)-N(4)-C(20)-C(19)	0.0(13)
Ce(1)-N(4)-C(20)-C(19)	174.4(6)	C(18)-C(19)-C(20)-N(4)	0.0(14)
N(5)' -Ce(2)-S(5)-C(21)	81.9(3)	N(5)-Ce(2)-S(5)-C(21)	4.9(3)
N(6)-Ce(2)-S(5)-C(21)	-94.8(4)	N(6)' -Ce(2)-S(5)-C(21)	-155.4(3)
S(5)' -Ce(2)-S(5)-C(21)	47.3(3)	S(6)-Ce(2)-S(5)-C(21)	-67.6(3)
S(6)' -Ce(2)-S(5)-C(21)	156.0(3)	N(5)' -Ce(2)-S(6)-C(26)	113.1(4)
N(5)-Ce(2)-S(6)-C(26)	142.2(3)	N(6)-Ce(2)-S(6)-C(26)	-1.7(4)
N(6)' -Ce(2)-S(6)-C(26)	-84.4(3)	S(5)-Ce(2)-S(6)-C(26)	-162.0(3)
S(5)' -Ce(2)-S(6)-C(26)	60.2(3)	S(6)' -Ce(2)-S(6)-C(26)	-47.7(3)
N(5)' -Ce(2)-N(5)-C(25)	93.0(9)	N(6)-Ce(2)-N(5)-C(25)	-37.5(9)
N(6)' -Ce(2)-N(5)-C(25)	-146.9(8)	S(5)-Ce(2)-N(5)-C(25)	-172.8(9)
S(5)' -Ce(2)-N(5)-C(25)	35.9(8)	S(6)-Ce(2)-N(5)-C(25)	-72.3(8)
S(6)' -Ce(2)-N(5)-C(25)	121.9(8)	N(5)' -Ce(2)-N(5)-C(21)	-100.6(5)
N(6)-Ce(2)-N(5)-C(21)	128.8(5)	N(6)' -Ce(2)-N(5)-C(21)	19.5(6)
S(5)-Ce(2)-N(5)-C(21)	-6.4(4)	S(5)' -Ce(2)-N(5)-C(21)	-157.7(5)
S(6)-Ce(2)-N(5)-C(21)	94.1(5)	S(6)' -Ce(2)-N(5)-C(21)	-71.7(6)
C(25)-N(5)-C(21)-C(22)	2.1(12)	Ce(2)-N(5)-C(21)-C(22)	-167.2(7)
C(25)-N(5)-C(21)-S(5)	179.4(7)	Ce(2)-N(5)-C(21)-S(5)	10.1(7)
Ce(2)-S(5)-C(21)-N(5)	-8.8(6)	Ce(2)-S(5)-C(21)-C(22)	168.4(8)
N(5)-C(21)-C(22)-C(23)	-2.1(13)	S(5)-C(21)-C(22)-C(23)	-179.2(7)
C(21)-C(22)-C(23)-C(24)	0.4(14)	C(22)-C(23)-C(24)-C(25)	1.3(14)
C(21)-N(5)-C(25)-C(24)	-0.4(14)	Ce(2)-N(5)-C(25)-C(24)	164.5(7)
C(23)-C(24)-C(25)-N(5)	-1(2)	N(5)' -Ce(2)-N(6)-C(26)	-139.9(5)
N(5)-Ce(2)-N(6)-C(26)	-39.5(6)	N(6)' -Ce(2)-N(6)-C(26)	94.8(6)
S(5)-Ce(2)-N(6)-C(26)	35.7(7)	S(5)' -Ce(2)-N(6)-C(26)	-117.8(6)
S(6)-Ce(2)-N(6)-C(26)	2.3(5)	S(6)' -Ce(2)-N(6)-C(26)	150.8(5)
N(5)' -Ce(2)-N(6)-C(30)	31.3(10)	N(5)-Ce(2)-N(6)-C(30)	131.7(9)
N(6)' -Ce(2)-N(6)-C(30)	-94.1(9)	S(5)-Ce(2)-N(6)-C(30)	-153.2(8)
S(5)' -Ce(2)-N(6)-C(30)	53.4(9)	S(6)-Ce(2)-N(6)-C(30)	173.4(10)
S(6)' -Ce(2)-N(6)-C(30)	-38.0(9)	C(30)-N(6)-C(26)-C(27)	0.9(13)

Ce(2)-N(6)-C(26)-C(27)	173.8(7)	C(30)-N(6)-C(26)-S(6)	-176.5(7)
Ce(2)-N(6)-C(26)-S(6)	-3.6(7)	Ce(2)-S(6)-C(26)-N(6)	3.1(6)
Ce(2)-S(6)-C(26)-C(27)	-174.2(8)	N(6)-C(26)-C(27)-C(28)	-1.3(13)
S(6)-C(26)-C(27)-C(28)	175.9(7)	C(26)-C(27)-C(28)-C(29)	0.0(13)
C(27)-C(28)-C(29)-C(30)	1.6(14)	C(26)-N(6)-C(30)-C(29)	0.8(14)
Ce(2)-N(6)-C(30)-C(29)	-169.5(7)	C(28)-C(29)-C(30)-N(6)	-2(2)
N(7)* -Ce(3)-S(7)-C(31)	69.3(3)	N(7)-Ce(3)-S(7)-C(31)	-5.2(4)
N(8)-Ce(3)-S(7)-C(31)	-111.0(3)	N(8)* -Ce(3)-S(7)-C(31)	170.9(4)
S(8)-Ce(3)-S(7)-C(31)	-65.5(3)	S(8)* -Ce(3)-S(7)-C(31)	160.6(3)
S(7)* -Ce(3)-S(7)-C(31)	36.2(3)	N(7)* -Ce(3)-S(8)-C(36)	-170.2(4)
N(7)-Ce(3)-S(8)-C(36)	-99.5(3)	N(8)-Ce(3)-S(8)-C(36)	4.5(4)
N(8)* -Ce(3)-S(8)-C(36)	86.6(3)	S(8)* -Ce(3)-S(8)-C(36)	50.0(3)
S(7)-Ce(3)-S(8)-C(36)	-53.9(3)	S(7)* -Ce(3)-S(8)-C(36)	175.1(3)
N(7)* -Ce(3)-N(7)-C(31)	-88.3(6)	N(8)-Ce(3)-N(7)-C(31)	86.3(6)
N(8)* -Ce(3)-N(7)-C(31)	-146(2)	S(8)-Ce(3)-N(7)-C(31)	142.2(6)
S(8)* -Ce(3)-N(7)-C(31)	-10.3(7)	S(7)-Ce(3)-N(7)-C(31)	7.1(5)
S(7)* -Ce(3)-N(7)-C(31)	-143.4(6)	N(7)* -Ce(3)-N(7)-C(35)	77.5(9)
N(8)-Ce(3)-N(7)-C(35)	-107.9(9)	N(8)* -Ce(3)-N(7)-C(35)	20(3)
S(8)-Ce(3)-N(7)-C(35)	-52.0(9)	S(8)* -Ce(3)-N(7)-C(35)	155.5(8)
S(7)-Ce(3)-N(7)-C(35)	172.8(10)	S(7)* -Ce(3)-N(7)-C(35)	22.4(9)
C(35)-N(7)-C(31)-C(32)	2.6(14)	Ce(3)-N(7)-C(31)-C(32)	170.9(7)
C(35)-N(7)-C(31)-S(7)	-179.3(7)	Ce(3)-N(7)-C(31)-S(7)	-10.9(8)
Ce(3)-S(7)-C(31)-N(7)	9.2(6)	Ce(3)-S(7)-C(31)-C(32)	-172.7(9)
N(7)-C(31)-C(32)-C(33)	-1(2)	S(7)-C(31)-C(32)-C(33)	-179.2(8)
C(31)-C(32)-C(33)-C(34)	-2(2)	C(32)-C(33)-C(34)-C(35)	3(2)
C(31)-N(7)-C(35)-C(34)	-1(2)	Ce(3)-N(7)-C(35)-C(34)	-165.6(8)
C(33)-C(34)-C(35)-N(7)	-2(2)	N(7)* -Ce(3)-N(8)-C(40)	-39(3)
N(7)-Ce(3)-N(8)-C(40)	-95.4(9)	N(8)* -Ce(3)-N(8)-C(40)	89.7(9)
S(8)-Ce(3)-N(8)-C(40)	-177.7(9)	S(8)* -Ce(3)-N(8)-C(40)	33.0(8)
S(7)-Ce(3)-N(8)-C(40)	-41.5(8)	S(7)* -Ce(3)-N(8)-C(40)	170.4(8)
N(7)* -Ce(3)-N(8)-C(36)	132(2)	N(7)-Ce(3)-N(8)-C(36)	76.5(6)
N(8)* -Ce(3)-N(8)-C(36)	-98.5(6)	S(8)-Ce(3)-N(8)-C(36)	-5.9(5)
S(8)* -Ce(3)-N(8)-C(36)	-155.2(5)	S(7)-Ce(3)-N(8)-C(36)	130.3(5)
S(7)* -Ce(3)-N(8)-C(36)	-17.8(6)	C(40)-N(8)-C(36)-C(37)	3.2(13)
Ce(3)-N(8)-C(36)-C(37)	-170.6(7)	C(40)-N(8)-C(36)-S(8)	-177.0(6)
Ce(3)-N(8)-C(36)-S(8)	9.2(7)	Ce(3)-S(8)-C(36)-N(8)	-8.1(6)
Ce(3)-S(8)-C(36)-C(37)	171.7(8)	N(8)-C(36)-C(37)-C(38)	-2.2(14)
S(8)-C(36)-C(37)-C(38)	178.0(7)	C(36)-C(37)-C(38)-C(39)	-0.5(14)
C(37)-C(38)-C(39)-C(40)	1.9(14)	C(36)-N(8)-C(40)-C(39)	-1.7(13)
Ce(3)-N(8)-C(40)-C(39)	169.2(7)	C(38)-C(39)-C(40)-N(8)	-0.8(14)
C(43)-P(1)-C(41)-C(42)	51.4(9)	C(47)-P(1)-C(41)-C(42)	172.6(7)
C(45)-P(1)-C(41)-C(42)	-65.0(9)	C(41)-P(1)-C(43)-C(44)	62.4(9)
C(47)-P(1)-C(43)-C(44)	-58.3(9)	C(45)-P(1)-C(43)-C(44)	-176.2(8)
C(41)-P(1)-C(45)-C(46)	-72.0(9)	C(43)-P(1)-C(45)-C(46)	169.1(8)
C(47)-P(1)-C(45)-C(46)	50.5(10)	C(41)-P(1)-C(47)-C(48)	172.7(8)
C(43)-P(1)-C(47)-C(48)	-66.8(9)	C(45)-P(1)-C(47)-C(48)	48.3(9)
C(49)'*-P(2)-C(49)-C(50)	-53.1(6)	C(51)'*-P(2)-C(49)-C(50)	65.4(8)
C(51)-P(2)-C(49)-C(50)	-173.8(7)	C(49)-P(2)-C(51)-C(52)	-173.2(7)
C(49)'*-P(2)-C(51)-C(52)	68.2(8)	C(51)'*-P(2)-C(51)-C(52)	-51.4(6)
C(55)' -P(3)-C(53)-C(54)	-62.5(8)	C(55)-P(3)-C(53)-C(54)	176.0(7)
C(53)' -P(3)-C(53)-C(54)	56.3(6)	C(55)' -P(3)-C(55)-C(56)	54.6(6)
C(53)' -P(3)-C(55)-C(56)	-64.9(8)	C(53)-P(3)-C(55)-C(56)	175.0(7)

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

Table S7. Least-squares planes (x,y,z in crystal coordinates) and deviations from them for [P(Et)4][Ce(Spy)4]. (* indicates atom used to define plane)

10.561 (0.038) x + 7.359 (0.052) y + 14.522 (0.081) z = 4.939 (0.021)

*	-0.001 (0.006)	C1	*	-0.010 (0.006)	C2
*	0.008 (0.007)	C3	*	0.006 (0.007)	C4
*	-0.017 (0.007)	C5	*	0.015 (0.006)	N1
	-0.028 (0.012)	S1		-0.111 (0.014)	Ce1
	0.564 (0.022)	S2		-0.316 (0.023)	N2
	2.717 (0.014)	S3		0.782 (0.017)	N3
	-2.606 (0.014)	S4		-2.453 (0.018)	N4

Rms deviation of fitted atoms = 0.011

10.158 (0.038) x + 2.332 (0.059) y + 19.164 (0.063) z = 3.142 (0.021)
Angle to previous plane (with approximate esd) = 20.68 (0.43)

*	-0.004	(0.006)	C6	* -0.010 (0.007)	C7
*	0.012	(0.007)	C8	* 0.001 (0.007)	C9
*	-0.016	(0.006)	C10	* 0.017 (0.006)	N2
	0.002	(0.011)	S2	0.151 (0.013)	Ce1
	-0.446	(0.021)	S1	0.518 (0.023)	N1
	3.034	(0.013)	S3	1.844 (0.017)	N3
	-1.643	(0.016)	S4	-2.399 (0.013)	N4

Rms deviation of fitted atoms = 0.012

9.990 (0.042) x + 5.531 (0.056) y + 17.694 (0.071) z = 0.675 (0.024)
Angle to previous plane (with approximate esd) = 84.81 (0.22)

*	-0.002	(0.007)	C11	* -0.006 (0.007)	C12
*	0.012	(0.007)	C13	* -0.011 (0.007)	C14
*	0.004	(0.007)	C15	* 0.003 (0.006)	N3
	-0.034	(0.012)	S3	0.374 (0.014)	Ce1
	2.724	(0.020)	S1	2.805 (0.013)	N1
	-1.289	(0.022)	S2	-2.163 (0.016)	N2
	0.443	(0.017)	S4	0.092 (0.023)	N4

Rms deviation of fitted atoms = 0.008

9.848 (0.040) x + 3.722 (0.058) y + 19.153 (0.064) z = 1.345 (0.018)
Angle to previous plane (with approximate esd) = 7.19 (0.52)

*	0.004	(0.006)	C16	* -0.005 (0.007)	C17
*	0.004	(0.007)	C18	* 0.000 (0.007)	C19
*	-0.002	(0.006)	C20	* 0.000 (0.006)	N4
	0.024	(0.012)	S4	0.181 (0.013)	Ce1
	2.727	(0.014)	S1	2.481 (0.018)	N1
	-1.166	(0.016)	S2	-2.333 (0.014)	N2
	-0.266	(0.023)	S3	-0.475 (0.021)	N3

Rms deviation of fitted atoms = 0.003

- 1.193 (0.055) x + 12.191 (0.035) y + 17.175 (0.067) z = 12.960 (0.015)
Angle to previous plane (with approximate esd) = 45.94 (0.33)

*	-0.013	(0.006)	C21	* 0.007 (0.006)	C22
*	0.004	(0.006)	C23	* -0.011 (0.007)	C24
*	0.005	(0.007)	C25	* 0.007 (0.006)	N5
	0.008	(0.011)	S5	0.510 (0.013)	Ce2
	3.149	(0.010)	S6	2.434 (0.019)	N6

Rms deviation of fitted atoms = 0.009

- 9.032 (0.044) x + 11.998 (0.037) y - 7.844 (0.093) z = 5.409 (0.058)
Angle to previous plane (with approximate esd) = 65.37 (0.25)

*	-0.009	(0.006)	C26	* 0.006 (0.006)	C27
*	0.004	(0.006)	C28	* -0.011 (0.007)	C29
*	0.008	(0.007)	C30	* 0.002 (0.006)	N6
	-0.111	(0.012)	S6	-0.304 (0.013)	Ce2
	0.403	(0.022)	S5	-1.928 (0.019)	N5

Rms deviation of fitted atoms = 0.007

5.921 (0.057) x + 7.504 (0.053) y + 20.961 (0.063) z = 11.855 (0.035)
Angle to previous plane (with approximate esd) = 82.88 (0.27)

*	-0.014	(0.007)	C31	* -0.001 (0.007)	C32
*	0.015	(0.008)	C33	* -0.015 (0.008)	C34
*	0.001	(0.008)	C35	* 0.014 (0.006)	N7
	-0.015	(0.012)	S7	-0.421 (0.014)	Ce3
	1.492	(0.019)	S8	1.984 (0.019)	N8

Rms deviation of fitted atoms = 0.012

0.595 (0.054) x + 12.051 (0.037) y - 17.524 (0.069) z = 1.643 (0.057)
Angle to previous plane (with approximate esd) = 78.85 (0.23)

*	-0.017	(0.006)	C36	* 0.004 (0.006)	C37
*	0.010	(0.007)	C38	* -0.012 (0.006)	C39
*	0.000	(0.006)	C40	* 0.015 (0.006)	N8
	-0.076	(0.012)	S8	0.370 (0.013)	Ce3
	2.576	(0.015)	S7	2.895 (0.016)	N7

Rms deviation of fitted atoms = 0.011

Table S8. Crystal data and structure refinement for Yb(Spy)2(py)3.

Empirical formula	C25 H23 N5 S2 Yb
formula weight	630.64
Temperature	153(2) K
Radiation (type, wavelength)	MoKα, 0.71073 Å
Diffractometer, monochromator	CAD4, graphite
Stnd reflcns: no., interval, decay	3, 3600 s, < 1%
Crystal system, space group	Monoclinic, Cc
No. refls, Θ range for cell det'n	25, 17.6 to 18.7 °
Unit cell dimensions	a = 10.588(1) Å b = 16.810(3) Å c = 14.833(5) Å β = 109.12(2) °
Volume	2494.4(10) Å^3
Z	4
Density (calculated)	1.679 Mg/m^3
Absorption coefficient	3.939 mm^{-1}
F(000)	1240
Crystal color, description	green, plates
Crystal size	0.38 x 0.36 x 0.08 mm
Θ range for data collection	2 to 27 °
Index ranges	0<=h<=13, 0<=k<=21, -18<=l<=17
Reflections collected	2866
Transmission factors	0.290 to 0.729
Independent reflections	2760
Observed reflections	2722
Data / restraints / parameters	2759 / 182 / 321
Goodness-of-fit on all F^2 data	1.064
Final R(F), wR(F^2) [2722 I>2σ data]	0.026, 0.071
Final R(F), wR(F^2) [2759 I>0 data]	0.026, 0.072
Weights	$1/[\sigma^2(F_o^2)+(0.0626P)^2]$, where $P=(F_o^2+2F_c^2)/3$
Flack parameter	-0.001(11)
Largest diff. peak and hole	2.3 and -1.5 e·Å^{-3} within 0.8 Å of Yb; 0.7 and -0.6 e·Å^{-3} elsewhere

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Yb(Spy)2(py)3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb	1096(1)	1499(1)	2001(1)	17(1)
S(1)	2988(2)	1590(1)	1020(1)	25(1)
S(2)	-1630(2)	938(1)	1702(1)	24(1)
N(1)	3515(5)	1924(3)	2854(4)	23(1)
C(1)	4059(6)	1705(4)	2185(4)	21(1)
C(2)	5431(8)	1557(3)	2448(6)	25(2)
C(3)	6254(7)	1667(4)	3374(6)	31(2)
C(4)	5683(7)	1911(4)	4051(5)	33(2)
C(5)	4327(7)	2030(4)	3765(4)	29(1)
N(2)	-431(5)	1029(3)	398(4)	23(1)
C(6)	-1570(6)	786(4)	564(4)	22(1)
C(7)	-2613(6)	435(4)	-185(5)	28(1)
C(8)	-2503(7)	366(4)	-1087(4)	29(1)
C(9)	-1353(7)	638(4)	-1234(5)	31(1)
C(10)	-338(7)	950(4)	-473(5)	27(1)
N(3)	321(5)	2924(3)	1641(4)	23(1)
C(11)	1220(9)	3490(3)	1653(7)	31(2)
C(12)	880(8)	4282(4)	1443(5)	31(1)
C(13)	-448(8)	4497(4)	1217(5)	36(2)
C(14)	-1391(8)	3916(5)	1188(6)	39(2)
C(15)	-956(8)	3142(4)	1407(5)	32(2)

N(4)	920(6)	1772(3)	3668(4)	25(1)
C(16)	1150(7)	2476(4)	4103(4)	29(1)
C(17)	793(7)	2643(4)	4905(5)	30(1)
C(18)	185(7)	2062(4)	5266(5)	32(1)
C(19)	-46(8)	1322(5)	4818(5)	30(1)
C(20)	344(7)	1209(4)	4043(4)	27(1)
N(5)	1905(6)	109(3)	2660(4)	28(1)
C(21)	1083(8)	-513(4)	2393(5)	31(1)
C(22)	1418(8)	-1270(5)	2769(5)	32(1)
C(23)	2622(10)	-1385(5)	3457(7)	37(2)
C(24)	3470(9)	-748(5)	3756(7)	50(2)
C(25)	3075(8)	-18(4)	3336(6)	44(2)

Table S10. Bond lengths [Å] and angles [°] for Yb(Spy)2(py)3.

Yb-N(2)	2.524(5)	Yb-N(3)	2.533(5)
Yb-N(1)	2.560(5)	Yb-N(5)	2.568(5)
Yb-N(4)	2.582(5)	Yb-S(1)	2.839(2)
Yb-S(2)	2.929(2)	Yb-C(1)	3.078(6)
Yb-C(6)	3.163(6)	S(1)-C(1)	1.739(6)
S(2)-C(6)	1.729(6)	N(1)-C(1)	1.351(9)
N(1)-C(5)	1.354(8)	C(1)-C(2)	1.398(10)
C(2)-C(3)	1.376(11)	C(3)-C(4)	1.393(12)
C(4)-C(5)	1.372(10)	N(2)-C(10)	1.334(8)
N(2)-C(6)	1.370(8)	C(6)-C(7)	1.413(8)
C(7)-C(8)	1.385(9)	C(8)-C(9)	1.383(10)
C(9)-C(10)	1.382(9)	N(3)-C(15)	1.332(9)
N(3)-C(11)	1.342(9)	C(11)-C(12)	1.387(9)
C(12)-C(13)	1.382(11)	C(13)-C(14)	1.387(12)
C(14)-C(15)	1.384(11)	N(4)-C(16)	1.332(8)
N(4)-C(20)	1.342(9)	C(16)-C(17)	1.389(9)
C(17)-C(18)	1.370(11)	C(18)-C(19)	1.395(10)
C(19)-C(20)	1.356(10)	N(5)-C(25)	1.332(9)
N(5)-C(21)	1.335(9)	C(21)-C(22)	1.388(10)
C(22)-C(23)	1.361(12)	C(23)-C(24)	1.375(12)
C(24)-C(25)	1.377(11)		
N(2)-Yb-N(3)	92.0(2)	N(2)-Yb-N(1)	141.4(2)
N(3)-Yb-N(1)	92.4(2)	N(2)-Yb-N(5)	96.0(2)
N(3)-Yb-N(5)	170.2(2)	N(1)-Yb-N(5)	84.9(2)
N(2)-Yb-N(4)	137.1(2)	N(3)-Yb-N(4)	85.0(2)
N(1)-Yb-N(4)	81.4(2)	N(5)-Yb-N(4)	85.2(2)
N(2)-Yb-S(1)	82.89(13)	N(3)-Yb-S(1)	94.32(12)
N(1)-Yb-S(1)	58.56(12)	N(5)-Yb-S(1)	92.36(13)
N(4)-Yb-S(1)	139.96(13)	N(2)-Yb-S(2)	57.41(13)
N(3)-Yb-S(2)	92.13(12)	N(1)-Yb-S(2)	160.37(12)
N(5)-Yb-S(2)	87.39(13)	N(4)-Yb-S(2)	79.94(13)
S(1)-Yb-S(2)	139.97(5)	N(2)-Yb-C(1)	116.0(2)
N(3)-Yb-C(1)	99.4(2)	N(1)-Yb-C(1)	25.7(2)
N(5)-Yb-C(1)	82.3(2)	N(4)-Yb-C(1)	106.6(2)
S(1)-Yb-C(1)	33.87(12)	S(2)-Yb-C(1)	167.15(13)
N(2)-Yb-C(6)	24.8(2)	N(3)-Yb-C(6)	93.5(2)
N(1)-Yb-C(6)	165.2(2)	N(5)-Yb-C(6)	91.4(2)
N(4)-Yb-C(6)	112.6(2)	S(1)-Yb-C(6)	107.40(12)
S(2)-Yb-C(6)	32.69(12)	C(1)-Yb-C(6)	139.6(2)
C(1)-S(1)-Yb	80.6(2)	C(6)-S(2)-Yb	81.1(2)
C(1)-N(1)-C(5)	119.0(5)	C(1)-N(1)-Yb	99.1(4)
C(5)-N(1)-Yb	137.3(4)	N(1)-C(1)-C(2)	119.8(6)
N(1)-C(1)-S(1)	117.7(5)	C(2)-C(1)-S(1)	122.5(5)
N(1)-C(1)-Yb	55.2(3)	C(2)-C(1)-Yb	160.1(4)
S(1)-C(1)-Yb	65.5(2)	C(3)-C(2)-C(1)	121.0(7)
C(2)-C(3)-C(4)	118.5(7)	C(5)-C(4)-C(3)	118.5(6)
N(1)-C(5)-C(4)	123.2(6)	C(10)-N(2)-C(6)	119.5(5)
C(10)-N(2)-Yb	135.7(4)	C(6)-N(2)-Yb	104.7(4)
N(2)-C(6)-C(7)	119.4(6)	N(2)-C(6)-S(2)	116.6(4)
C(7)-C(6)-S(2)	124.1(5)	N(2)-C(6)-Yb	50.5(3)
C(7)-C(6)-Yb	169.3(5)	S(2)-C(6)-Yb	66.2(2)
C(8)-C(7)-C(6)	120.2(6)	C(9)-C(8)-C(7)	118.8(6)

C(10)-C(9)-C(8)	119.0(6)	N(2)-C(10)-C(9)	123.1(6)
C(15)-N(3)-C(11)	117.6(6)	C(15)-N(3)-Yb	123.1(4)
C(11)-N(3)-Yb	119.3(5)	N(3)-C(11)-C(12)	123.2(8)
C(13)-C(12)-C(11)	118.3(7)	C(12)-C(13)-C(14)	119.2(6)
C(15)-C(14)-C(13)	118.3(7)	N(3)-C(15)-C(14)	123.4(7)
C(16)-N(4)-C(20)	117.5(6)	C(16)-N(4)-Yb	124.3(4)
C(20)-N(4)-Yb	117.2(4)	N(4)-C(16)-C(17)	122.4(6)
C(18)-C(17)-C(16)	119.0(6)	C(17)-C(18)-C(19)	118.8(7)
C(20)-C(19)-C(18)	118.2(7)	N(4)-C(20)-C(19)	124.0(7)
C(25)-N(5)-C(21)	116.9(6)	C(25)-N(5)-Yb	123.0(4)
C(21)-N(5)-Yb	119.7(4)	N(5)-C(21)-C(22)	122.9(7)
C(23)-C(22)-C(21)	119.0(7)	C(22)-C(23)-C(24)	118.9(7)
C(23)-C(24)-C(25)	118.6(7)	N(5)-C(25)-C(24)	123.6(7)

Table S11. Anisotropic displacement parameters (Uij, Å² x 10³) for Yb(Spy)2(py)3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$.

	U11	U22	U33	U23	U13	U12
Yb	18(1)	18(1)	18(1)	0(1)	8(1)	-1(1)
S(1)	22(1)	32(1)	24(1)	1(1)	11(1)	-1(1)
S(2)	20(1)	28(1)	26(1)	0(1)	12(1)	-3(1)
N(1)	23(2)	21(2)	25(2)	0(2)	7(2)	-4(2)
C(1)	22(3)	17(2)	25(3)	4(2)	7(2)	-3(2)
C(2)	24(3)	16(3)	38(4)	-3(2)	14(3)	0(2)
C(3)	21(3)	28(3)	36(4)	6(3)	-1(3)	1(3)
C(4)	35(3)	30(3)	26(3)	6(2)	0(3)	-8(3)
C(5)	31(3)	31(3)	24(3)	0(2)	8(2)	-5(3)
N(2)	20(2)	27(2)	25(2)	-1(2)	9(2)	0(2)
C(6)	22(3)	16(2)	26(3)	-1(2)	7(2)	2(2)
C(7)	23(3)	26(3)	31(3)	0(2)	5(2)	-2(2)
C(8)	34(3)	25(3)	22(3)	-3(2)	2(2)	-2(2)
C(9)	35(3)	30(3)	27(3)	-4(2)	9(3)	5(3)
C(10)	26(3)	30(3)	28(3)	-1(2)	12(2)	0(2)
N(3)	22(2)	22(2)	27(2)	1(2)	10(2)	0(2)
C(11)	27(4)	25(4)	42(4)	1(2)	12(3)	-6(2)
C(12)	40(4)	25(3)	27(3)	3(2)	9(3)	-12(3)
C(13)	49(4)	24(3)	32(3)	1(2)	9(3)	4(3)
C(14)	35(4)	32(3)	48(4)	3(3)	12(3)	10(3)
C(15)	32(3)	29(3)	38(4)	2(3)	13(3)	0(3)
N(4)	29(3)	28(3)	24(2)	-5(2)	14(2)	-5(2)
C(16)	31(3)	29(3)	28(3)	-1(2)	11(2)	-6(3)
C(17)	35(3)	25(3)	30(3)	-5(2)	11(3)	8(3)
C(18)	35(3)	36(3)	27(3)	1(3)	14(3)	10(3)
C(19)	30(4)	33(3)	30(3)	2(3)	11(3)	-1(3)
C(20)	30(3)	30(3)	23(3)	-1(2)	12(2)	-6(3)
N(5)	33(3)	18(2)	31(3)	1(2)	9(2)	1(2)
C(21)	38(4)	29(3)	27(3)	0(2)	11(3)	5(3)
C(22)	33(4)	26(3)	34(3)	1(3)	7(3)	-5(3)
C(23)	44(4)	26(3)	38(4)	7(3)	12(3)	-2(3)
C(24)	40(4)	36(4)	56(4)	16(3)	-8(3)	-3(3)
C(25)	42(4)	26(3)	51(4)	11(3)	-2(3)	-7(3)

Table S12. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å² x 10³) for Yb(Spy)2(py)3.

	x	y	z	U(eq)
H(2)	5802(8)	1377(3)	1981(6)	27(21)
H(3)	7189(7)	1578(4)	3547(6)	3(15)
H(4)	6221(7)	1993(4)	4696(5)	90(42)
H(5)	3938(7)	2195(4)	4228(4)	24(18)
H(7)	-3391(6)	246(4)	-70(5)	48(26)

H(8)	-3205(7)	137(4)	-1596(4)	37(22)
H(9)	-1262(7)	611(4)	-1850(5)	26(19)
H(10)	462(7)	1116(4)	-574(5)	23(18)
H(11)	2132(9)	3342(3)	1813(7)	47(25)
H(12)	1542(8)	4666(4)	1454(5)	60(31)
H(13)	-711(8)	5036(4)	1084(5)	53(28)
H(14)	-2312(8)	4047(5)	1022(6)	59(30)
H(15)	-1601(8)	2744(4)	1388(5)	44(25)
H(16)	1573(7)	2880(4)	3856(4)	22(18)
H(17)	969(7)	3151(4)	5199(5)	22(19)
H(18)	-74(7)	2163(4)	5811(5)	36(22)
H(19)	-466(8)	907(5)	5050(5)	36(22)
H(20)	200(7)	700(4)	3748(4)	42(24)
H(21)	231(8)	-433(4)	1926(5)	46(25)
H(22)	816(8)	-1701(5)	2549(5)	180(106)
H(23)	2873(10)	-1897(5)	3726(7)	50(29)
H(24)	4311(9)	-809(5)	4242(7)	55(29)
H(25)	3671(8)	418(4)	3540(6)	53(31)

Table S13. Torsion angles [°] for Yb(Spy)2(py)3.

N(2)-Yb-S(1)-C(1)	-168.2(2)	N(3)-Yb-S(1)-C(1)	100.4(2)
N(1)-Yb-S(1)-C(1)	10.2(3)	N(5)-Yb-S(1)-C(1)	-72.4(3)
N(4)-Yb-S(1)-C(1)	13.0(3)	S(2)-Yb-S(1)-C(1)	-161.1(2)
C(6)-Yb-S(1)-C(1)	-164.6(2)	N(2)-Yb-S(2)-C(6)	2.1(2)
N(3)-Yb-S(2)-C(6)	93.1(2)	N(1)-Yb-S(2)-C(6)	-163.6(4)
N(5)-Yb-S(2)-C(6)	-96.8(2)	N(4)-Yb-S(2)-C(6)	177.6(2)
S(1)-Yb-S(2)-C(6)	-6.2(2)	C(1)-Yb-S(2)-C(6)	-60.4(6)
N(2)-Yb-N(1)-C(1)	-10.5(5)	N(3)-Yb-N(1)-C(1)	-106.7(4)
N(5)-Yb-N(1)-C(1)	82.8(4)	N(4)-Yb-N(1)-C(1)	168.7(4)
S(1)-Yb-N(1)-C(1)	-13.1(3)	S(2)-Yb-N(1)-C(1)	150.0(3)
C(6)-Yb-N(1)-C(1)	6.6(8)	N(2)-Yb-N(1)-C(5)	-164.4(6)
N(3)-Yb-N(1)-C(5)	99.4(6)	N(5)-Yb-N(1)-C(5)	-71.1(6)
N(4)-Yb-N(1)-C(5)	14.8(6)	S(1)-Yb-N(1)-C(5)	-167.0(7)
S(2)-Yb-N(1)-C(5)	-3.9(9)	C(1)-Yb-N(1)-C(5)	-153.9(9)
C(6)-Yb-N(1)-C(5)	-147.3(7)	C(5)-N(1)-C(1)-C(2)	2.9(9)
Yb-N(1)-C(1)-C(2)	-157.2(5)	C(5)-N(1)-C(1)-S(1)	-179.0(5)
Yb-N(1)-C(1)-S(1)	20.9(5)	C(5)-N(1)-C(1)-Yb	160.1(6)
Yb-S(1)-C(1)-N(1)	-18.8(5)	Yb-S(1)-C(1)-C(2)	159.3(5)
N(2)-Yb-C(1)-N(1)	172.7(4)	N(3)-Yb-C(1)-N(1)	75.9(4)
N(5)-Yb-C(1)-N(1)	-94.3(4)	N(4)-Yb-C(1)-N(1)	-11.7(4)
S(1)-Yb-C(1)-N(1)	159.7(5)	S(2)-Yb-C(1)-N(1)	-131.0(5)
C(6)-Yb-C(1)-N(1)	-177.4(3)	N(2)-Yb-C(1)-C(2)	-105.5(14)
N(3)-Yb-C(1)-C(2)	157.7(14)	N(1)-Yb-C(1)-C(2)	81.8(14)
N(5)-Yb-C(1)-C(2)	-12.5(14)	N(4)-Yb-C(1)-C(2)	70(2)
S(1)-Yb-C(1)-C(2)	-119(2)	S(2)-Yb-C(1)-C(2)	-49(2)
C(6)-Yb-C(1)-C(2)	-95.6(14)	N(2)-Yb-C(1)-S(1)	13.1(3)
N(3)-Yb-C(1)-S(1)	-83.8(2)	N(1)-Yb-C(1)-S(1)	-159.7(5)
N(5)-Yb-C(1)-S(1)	106.1(2)	N(4)-Yb-C(1)-S(1)	-171.3(2)
S(2)-Yb-C(1)-S(1)	69.3(6)	C(6)-Yb-C(1)-S(1)	22.9(4)
N(1)-C(1)-C(2)-C(3)	-3.1(9)	S(1)-C(1)-C(2)-C(3)	178.9(5)
Yb-C(1)-C(2)-C(3)	-73(2)	C(1)-C(2)-C(3)-C(4)	1.6(10)
C(2)-C(3)-C(4)-C(5)	0.0(10)	C(1)-N(1)-C(5)-C(4)	-1.2(10)
Yb-N(1)-C(5)-C(4)	149.0(5)	C(3)-C(4)-C(5)-N(1)	-0.2(11)
N(3)-Yb-N(2)-C(10)	89.0(6)	N(1)-Yb-N(2)-C(10)	-7.4(7)
N(5)-Yb-N(2)-C(10)	-96.8(6)	N(4)-Yb-N(2)-C(10)	173.8(6)
S(1)-Yb-N(2)-C(10)	-5.1(6)	S(2)-Yb-N(2)-C(10)	-179.8(7)
C(1)-Yb-N(2)-C(10)	-12.4(7)	C(6)-Yb-N(2)-C(10)	-177.0(8)
N(3)-Yb-N(2)-C(6)	-94.0(4)	N(1)-Yb-N(2)-C(6)	169.6(3)
N(5)-Yb-N(2)-C(6)	80.3(4)	N(4)-Yb-N(2)-C(6)	-9.2(5)
S(1)-Yb-N(2)-C(6)	171.9(4)	S(2)-Yb-N(2)-C(6)	-2.7(3)
C(1)-Yb-N(2)-C(6)	164.6(3)	C(10)-N(2)-C(6)-C(7)	1.8(8)
Yb-N(2)-C(6)-C(7)	-175.8(4)	C(10)-N(2)-C(6)-S(2)	-178.0(5)
Yb-N(2)-C(6)-S(2)	4.4(5)	C(10)-N(2)-C(6)-Yb	177.6(7)
Yb-S(2)-C(6)-N(2)	-3.7(4)	Yb-S(2)-C(6)-C(7)	176.5(5)
N(3)-Yb-C(6)-N(2)	87.2(4)	N(1)-Yb-C(6)-N(2)	-26.0(8)

N(5)-Yb-C(6)-N(2)	-101.4(4)	N(4)-Yb-C(6)-N(2)	173.2(4)
S(1)-Yb-C(6)-N(2)	-8.4(4)	S(2)-Yb-C(6)-N(2)	175.7(5)
C(1)-Yb-C(6)-N(2)	-21.6(5)	N(2)-Yb-C(6)-C(7)	20(2)
N(3)-Yb-C(6)-C(7)	107(2)	N(1)-Yb-C(6)-C(7)	-6(3)
N(5)-Yb-C(6)-C(7)	-81(2)	N(4)-Yb-C(6)-C(7)	-167(2)
S(1)-Yb-C(6)-C(7)	12(2)	S(2)-Yb-C(6)-C(7)	-164(2)
C(1)-Yb-C(6)-C(7)	-2(2)	N(2)-Yb-C(6)-S(2)	-175.7(5)
N(3)-Yb-C(6)-S(2)	-88.6(2)	N(1)-Yb-C(6)-S(2)	158.2(5)
N(5)-Yb-C(6)-S(2)	82.9(2)	N(4)-Yb-C(6)-S(2)	-2.5(3)
S(1)-Yb-C(6)-S(2)	175.8(2)	C(1)-Yb-C(6)-S(2)	162.7(2)
N(2)-C(6)-C(7)-C(8)	-2.5(9)	S(2)-C(6)-C(7)-C(8)	177.3(5)
Yb-C(6)-C(7)-C(8)	-20(3)	C(6)-C(7)-C(8)-C(9)	0.7(9)
C(7)-C(8)-C(9)-C(10)	1.7(10)	C(6)-N(2)-C(10)-C(9)	0.7(9)
Yb-N(2)-C(10)-C(9)	177.4(5)	C(8)-C(9)-C(10)-N(2)	-2.5(10)
N(2)-Yb-N(3)-C(15)	56.6(5)	N(1)-Yb-N(3)-C(15)	-161.8(5)
N(5)-Yb-N(3)-C(15)	-87.8(11)	N(4)-Yb-N(3)-C(15)	-80.6(5)
S(1)-Yb-N(3)-C(15)	139.6(5)	S(2)-Yb-N(3)-C(15)	-0.9(5)
C(1)-Yb-N(3)-C(15)	173.4(5)	C(6)-Yb-N(3)-C(15)	31.8(5)
N(2)-Yb-N(3)-C(11)	-121.1(6)	N(1)-Yb-N(3)-C(11)	20.6(6)
N(5)-Yb-N(3)-C(11)	94.5(12)	N(4)-Yb-N(3)-C(11)	101.8(6)
S(1)-Yb-N(3)-C(11)	-38.1(6)	S(2)-Yb-N(3)-C(11)	-178.5(6)
C(1)-Yb-N(3)-C(11)	-4.3(6)	C(6)-Yb-N(3)-C(11)	-145.8(6)
C(15)-N(3)-C(11)-C(12)	0.6(12)	Yb-N(3)-C(11)-C(12)	178.4(6)
N(3)-C(11)-C(12)-C(13)	0.5(13)	C(11)-C(12)-C(13)-C(14)	-1.4(11)
C(12)-C(13)-C(14)-C(15)	1.3(12)	C(11)-N(3)-C(15)-C(14)	-0.8(11)
Yb-N(3)-C(15)-C(14)	-178.5(6)	C(13)-C(14)-C(15)-N(3)	-0.2(12)
N(2)-Yb-N(4)-C(16)	-119.9(5)	N(3)-Yb-N(4)-C(16)	-32.4(5)
N(1)-Yb-N(4)-C(16)	60.8(5)	N(5)-Yb-N(4)-C(16)	146.3(5)
S(1)-Yb-N(4)-C(16)	58.4(6)	S(2)-Yb-N(4)-C(16)	-125.5(5)
C(1)-Yb-N(4)-C(16)	65.9(6)	C(6)-Yb-N(4)-C(16)	-124.1(5)
N(2)-Yb-N(4)-C(20)	48.3(6)	N(3)-Yb-N(4)-C(20)	135.8(5)
N(1)-Yb-N(4)-C(20)	-131.0(5)	N(5)-Yb-N(4)-C(20)	-45.5(5)
S(1)-Yb-N(4)-C(20)	-133.5(4)	S(2)-Yb-N(4)-C(20)	42.7(5)
C(1)-Yb-N(4)-C(20)	-126.0(5)	C(6)-Yb-N(4)-C(20)	44.1(5)
C(20)-N(4)-C(16)-C(17)	-1.2(10)	Yb-N(4)-C(16)-C(17)	166.9(5)
N(4)-C(16)-C(17)-C(18)	0.1(10)	C(16)-C(17)-C(18)-C(19)	0.5(10)
C(17)-C(18)-C(19)-C(20)	0.0(11)	C(16)-N(4)-C(20)-C(19)	1.8(10)
Yb-N(4)-C(20)-C(19)	-167.2(6)	C(18)-C(19)-C(20)-N(4)	-1.2(11)
N(2)-Yb-N(5)-C(25)	154.5(6)	N(3)-Yb-N(5)-C(25)	-61.3(13)
N(1)-Yb-N(5)-C(25)	13.3(6)	N(4)-Yb-N(5)-C(25)	-68.5(7)
S(1)-Yb-N(5)-C(25)	71.4(6)	S(2)-Yb-N(5)-C(25)	-148.6(6)
C(1)-Yb-N(5)-C(25)	39.0(6)	C(6)-Yb-N(5)-C(25)	178.9(6)
N(2)-Yb-N(5)-C(21)	-32.2(5)	N(3)-Yb-N(5)-C(21)	112.0(10)
N(1)-Yb-N(5)-C(21)	-173.5(5)	N(4)-Yb-N(5)-C(21)	104.7(5)
S(1)-Yb-N(5)-C(21)	-115.3(5)	S(2)-Yb-N(5)-C(21)	24.6(5)
C(1)-Yb-N(5)-C(21)	-147.7(5)	C(6)-Yb-N(5)-C(21)	-7.8(5)
C(25)-N(5)-C(21)-C(22)	-1.8(11)	Yb-N(5)-C(21)-C(22)	-175.5(6)
N(5)-C(21)-C(22)-C(23)	1.7(12)	C(21)-C(22)-C(23)-C(24)	-0.2(14)
C(22)-C(23)-C(24)-C(25)	-1(2)	C(21)-N(5)-C(25)-C(24)	0.6(13)
Yb-N(5)-C(25)-C(24)	174.0(8)	C(23)-C(24)-C(25)-N(5)	1(2)

Table S14. Least-squares planes (x,y,z in crystal coordinates) and deviations from them for Yb(Spy)2(py)3. (* indicates atom used to define plane)

```
 2.270 (0.027) x + 16.081 (0.014) y - 3.806 (0.037) z = 2.816 (0.015)
*   -0.009 (0.004)  N1          *    0.016 (0.004)  C1
*   -0.011 (0.004)  C2          *    0.001 (0.005)  C3
*    0.006 (0.005)  C4          *   -0.002 (0.005)  C5
     0.031 (0.008)  S1              -0.918 (0.009)  Yb
    -2.324 (0.016)  S2              -1.410 (0.016)  N2
     1.335 (0.013)  N3              -1.153 (0.013)  N4
    -3.220 (0.009)  N5
Rms deviation of fitted atoms =   0.009
- 3.663 (0.027) x + 15.243 (0.019) y - 1.695 (0.039) z = 1.663 (0.003)
Angle to previous plane (with approximate esd) = 32.78 ( 0.16 )
*   -0.004 (0.004)  N2          *    0.015 (0.004)  C6
```

*	-0.011 (0.004)	C7	*	-0.003 (0.004)	C8
*	0.015 (0.005)	C9	*	-0.011 (0.004)	C10
	0.076 (0.008)	S2		-0.120 (0.010)	Yb
	-0.507 (0.012)	S1		-0.502 (0.016)	N1
	2.398 (0.011)	N3		0.079 (0.016)	N4
	-2.645 (0.011)	N5			

Rms deviation of fitted atoms = 0.011

- 2.098 (0.038) x + 2.895 (0.044) y + 14.486 (0.011) z = 3.151 (0.016)

Angle to previous plane (with approximate esd) = 89.56 (0.22)

*	0.006 (0.005)	N3	*	-0.002 (0.006)	C11
*	-0.006 (0.006)	C12	*	0.008 (0.005)	C13
*	-0.004 (0.006)	C14	*	-0.003 (0.005)	C15
	-0.049 (0.011)	Yb		-1.840 (0.015)	S1
	-0.072 (0.014)	S2		0.803 (0.016)	N1
	-2.186 (0.013)	N2		2.483 (0.012)	N4
	0.335 (0.019)	N5			

Rms deviation of fitted atoms = 0.005

7.893 (0.021) x - 5.282 (0.047) y + 4.616 (0.040) z = 1.491 (0.020)

Angle to previous plane (with approximate esd) = 68.57 (0.25)

*	-0.008 (0.004)	N4	*	0.002 (0.005)	C16
*	0.003 (0.005)	C17	*	-0.004 (0.005)	C18
*	-0.002 (0.005)	C19	*	0.008 (0.005)	C20
	-0.494 (0.011)	Yb		0.499 (0.018)	S1
	-2.488 (0.010)	S2		1.585 (0.013)	N1
	-2.191 (0.017)	N2		-2.025 (0.013)	N3
	1.182 (0.014)	N5			

Rms deviation of fitted atoms = 0.005

- 7.176 (0.031) x + 3.554 (0.057) y + 13.163 (0.026) z = 2.181 (0.014)

Angle to previous plane (with approximate esd) = 80.93 (0.21)

*	-0.007 (0.005)	N5	*	0.010 (0.005)	C21
*	-0.005 (0.006)	C22	*	-0.004 (0.007)	C23
*	0.008 (0.007)	C24	*	-0.002 (0.007)	C25
	0.199 (0.013)	Yb		-2.417 (0.015)	S1
	1.563 (0.016)	S2		-0.263 (0.017)	N1
	-0.982 (0.018)	N2		0.789 (0.022)	N3
	2.618 (0.013)	N4			

Rms deviation of fitted atoms = 0.007

Table S15. Crystal data and structure refinement for Yb(Spy)3(py)3.

Empirical formula	C30 H27 N6 S3 Yb
formula weight	740.80
Temperature	153(2) K
Radiation (type, wavelength)	MoKα, 0.71073 Å
Diffractometer, monochromator	CAD4, graphite
Stnd reflcns: no., interval, decay	3, 3600 s, < 1%
Crystal system, space group	Monoclinic, $P2_1/n$
No. refls, Θ range for cell det'n	25, 17.0 to 19.0 °
Unit cell dimensions	a = 9.672(2) Å
	b = 16.293(4) Å
	c = 19.214(3) Å
	β = 101.51(1) °
Volume	2967.0(11) $Å^3$
Z	4
Density (calculated)	1.658 Mg/m^3
Absorption coefficient	3.394 mm^{-1}
F(000)	1468
Crystal color, description	colourless, lathe
Crystal size	0.34 x 0.32 x 0.30 mm
Θ range for data collection	2 to 26 °
Index ranges	0<=h<=11, 0<=k<=20, -23<=l<=23
Reflections collected	6396
Transmission factors	0.351 to 0.449
Independent reflections	5799 [R(int) = 0.034]
Observed reflections	4248
Data / restraints / parameters	5097 / 216 / 388
Goodness-of-fit on all F^2 data	1.044

Final R(F), wR(F^2) [4248 I>2σ data]	0.033, 0.075
Final R(F), wR(F^2) [5097 I>0 data]	0.046, 0.081
Weights	$1/[\sigma^2(F_o^2)+(0.04P)^2+4.63P]$, where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	2.2 and -0.9 e·Å^{-3} within 0.8 Å of Yb; 0.6 and -0.4 e·Å^{-3} elsewhere

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for Yb(Spy)3(py)3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Yb	2172(1)	2451(1)	795(1)	19(1)
S(1)	4662(1)	2551(1)	1771(1)	26(1)
S(2)	-696(1)	2463(1)	784(1)	29(1)
S(3)	1142(1)	2076(1)	-619(1)	28(1)
N(1)	2322(4)	1839(2)	1947(2)	23(1)
C(1)	3674(5)	1988(3)	2274(3)	22(1)
C(2)	4203(6)	1712(3)	2968(3)	30(1)
C(3)	3317(6)	1277(3)	3310(3)	34(1)
C(4)	1944(6)	1121(3)	2974(3)	30(1)
C(5)	1488(5)	1409(3)	2299(3)	26(1)
N(2)	1218(4)	3397(2)	1552(2)	26(1)
C(6)	-153(6)	3178(3)	1460(3)	28(1)
C(7)	-1036(6)	3526(3)	1877(3)	32(1)
C(8)	-490(7)	4103(3)	2377(3)	38(1)
C(9)	921(6)	4336(3)	2464(3)	35(1)
C(10)	1740(6)	3959(3)	2044(3)	31(1)
N(3)	3773(4)	2382(2)	-39(2)	24(1)
C(11)	2888(5)	2245(3)	-668(3)	25(1)
C(12)	3385(6)	2267(3)	-1305(3)	33(1)
C(13)	4794(6)	2467(3)	-1283(3)	34(1)
C(14)	5671(6)	2637(3)	-635(3)	32(1)
C(15)	5134(5)	2574(3)	-25(3)	28(1)
N(4)	2568(5)	955(2)	728(2)	25(1)
C(16)	3779(6)	578(3)	698(3)	30(1)
C(17)	3890(7)	-264(3)	637(3)	38(1)
C(18)	2702(7)	-735(3)	622(3)	42(2)
C(19)	1456(6)	-360(3)	680(3)	37(1)
C(20)	1417(6)	478(3)	724(3)	29(1)
N(5)	2375(5)	3855(2)	334(2)	24(1)
C(21)	3446(6)	4362(3)	605(3)	25(1)
C(22)	3554(6)	5149(3)	364(3)	29(1)
C(23)	2541(6)	5437(3)	-192(3)	34(1)
C(24)	1439(7)	4925(3)	-472(3)	41(2)
C(25)	1406(6)	4144(3)	-195(3)	36(1)
N(6)	-3913(5)	4868(3)	2113(3)	46(1)
C(26)	-3229(6)	5584(4)	2116(4)	41(2)
C(27)	-2591(6)	5983(4)	2727(4)	43(2)
C(28)	-2650(6)	5639(4)	3368(4)	38(1)
C(29)	-3329(6)	4889(4)	3381(4)	40(1)
C(30)	-3945(6)	4544(4)	2746(4)	41(2)

Table S17. Bond lengths [Å] and angles [°] for Yb(Spy)3(py)3.

Yb-N(1)	2.405(4)	Yb-N(2)	2.424(4)
Yb-N(3)	2.442(4)	Yb-N(4)	2.474(4)
Yb-N(5)	2.476(4)	Yb-S(1)	2.746(1)
Yb-S(3)	2.768(1)	Yb-S(2)	2.770(1)
Yb-C(1)	3.017(5)	Yb-C(6)	3.040(5)
Yb-C(11)	3.045(5)	S(1)-C(1)	1.748(5)
S(2)-C(6)	1.747(6)	S(3)-C(11)	1.732(5)
N(1)-C(5)	1.348(6)	N(1)-C(1)	1.356(6)
C(1)-C(2)	1.404(7)	C(2)-C(3)	1.376(7)
C(3)-C(4)	1.380(7)	C(4)-C(5)	1.367(7)
N(2)-C(10)	1.342(7)	N(2)-C(6)	1.350(7)

C(6)-C(7)	1.402(7)	C(7)-C(8)	1.372(8)
C(8)-C(9)	1.394(8)	C(9)-C(10)	1.382(7)
N(3)-C(15)	1.348(6)	N(3)-C(11)	1.354(6)
C(11)-C(12)	1.403(7)	C(12)-C(13)	1.393(8)
C(13)-C(14)	1.387(8)	C(14)-C(15)	1.378(7)
N(4)-C(16)	1.334(7)	N(4)-C(20)	1.356(7)
C(16)-C(17)	1.383(7)	C(17)-C(18)	1.377(9)
C(18)-C(19)	1.376(8)	C(19)-C(20)	1.369(7)
N(5)-C(25)	1.324(7)	N(5)-C(21)	1.345(6)
C(21)-C(22)	1.374(7)	C(22)-C(23)	1.379(8)
C(23)-C(24)	1.376(8)	C(24)-C(25)	1.382(7)
N(6)-C(30)	1.332(8)	N(6)-C(26)	1.340(8)
C(26)-C(27)	1.376(9)	C(27)-C(28)	1.365(9)
C(28)-C(29)	1.391(8)	C(29)-C(30)	1.367(9)
N(1)-Yb-N(2)	70.83(14)	N(1)-Yb-N(3)	130.90(13)
N(2)-Yb-N(3)	142.13(13)	N(1)-Yb-N(4)	70.00(14)
N(2)-Yb-N(4)	137.62(14)	N(3)-Yb-N(4)	78.23(14)
N(1)-Yb-N(5)	135.86(14)	N(2)-Yb-N(5)	72.16(14)
N(3)-Yb-N(5)	72.65(13)	N(4)-Yb-N(5)	150.2(2)
N(1)-Yb-S(1)	60.84(10)	N(2)-Yb-S(1)	86.52(11)
N(3)-Yb-S(1)	82.30(10)	N(4)-Yb-S(1)	88.30(11)
N(5)-Yb-S(1)	93.88(11)	N(1)-Yb-S(3)	139.05(10)
N(2)-Yb-S(3)	128.56(11)	N(3)-Yb-S(3)	59.85(10)
N(4)-Yb-S(3)	76.17(11)	N(5)-Yb-S(3)	83.78(11)
S(1)-Yb-S(3)	141.08(4)	N(1)-Yb-S(2)	83.49(10)
N(2)-Yb-S(2)	59.98(11)	N(3)-Yb-S(2)	139.49(10)
N(4)-Yb-S(2)	99.90(11)	N(5)-Yb-S(2)	98.12(10)
S(1)-Yb-S(2)	138.20(4)	S(3)-Yb-S(2)	80.22(4)
N(1)-Yb-C(1)	25.95(13)	N(2)-Yb-C(1)	76.31(13)
N(3)-Yb-C(1)	110.90(13)	N(4)-Yb-C(1)	75.67(13)
N(5)-Yb-C(1)	120.65(14)	S(1)-Yb-C(1)	34.90(9)
S(3)-Yb-C(1)	151.68(9)	S(2)-Yb-C(1)	107.62(10)
N(1)-Yb-C(6)	71.85(13)	N(2)-Yb-C(6)	25.57(14)
N(3)-Yb-C(6)	155.85(13)	N(4)-Yb-C(6)	122.75(14)
N(5)-Yb-C(6)	84.73(13)	S(1)-Yb-C(6)	108.13(11)
S(3)-Yb-C(6)	110.31(11)	S(2)-Yb-C(6)	34.60(11)
C(1)-Yb-C(6)	87.66(13)	N(1)-Yb-C(11)	145.16(13)
N(2)-Yb-C(11)	143.89(13)	N(3)-Yb-C(11)	25.69(14)
N(4)-Yb-C(11)	77.13(13)	N(5)-Yb-C(11)	73.92(13)
S(1)-Yb-C(11)	107.87(10)	S(3)-Yb-C(11)	34.25(10)
S(2)-Yb-C(11)	113.92(10)	C(1)-Yb-C(11)	133.33(13)
C(6)-Yb-C(11)	139.01(14)	C(1)-S(1)-Yb	81.1(2)
C(6)-S(2)-Yb	81.2(2)	C(11)-S(3)-Yb	81.6(2)
C(5)-N(1)-C(1)	118.7(4)	C(5)-N(1)-Yb	138.2(3)
C(1)-N(1)-Yb	103.1(3)	N(1)-C(1)-C(2)	121.1(4)
N(1)-C(1)-S(1)	114.9(4)	C(2)-C(1)-S(1)	123.9(4)
N(1)-C(1)-Yb	50.9(2)	C(2)-C(1)-Yb	172.0(4)
S(1)-C(1)-Yb	64.0(2)	C(3)-C(2)-C(1)	118.4(5)
C(2)-C(3)-C(4)	120.2(5)	C(5)-C(4)-C(3)	118.7(5)
N(1)-C(5)-C(4)	122.9(5)	C(10)-N(2)-C(6)	119.6(5)
C(10)-N(2)-Yb	136.3(4)	C(6)-N(2)-Yb	103.6(3)
N(2)-C(6)-C(7)	120.9(5)	N(2)-C(6)-S(2)	114.5(4)
C(7)-C(6)-S(2)	124.6(4)	N(2)-C(6)-Yb	50.8(2)
C(7)-C(6)-Yb	169.7(4)	S(2)-C(6)-Yb	64.2(2)
C(8)-C(7)-C(6)	118.9(5)	C(7)-C(8)-C(9)	120.1(5)
C(10)-C(9)-C(8)	118.1(5)	N(2)-C(10)-C(9)	122.4(5)
C(15)-N(3)-C(11)	119.8(4)	C(15)-N(3)-Yb	136.2(3)
C(11)-N(3)-Yb	102.9(3)	N(3)-C(11)-C(12)	120.7(5)
N(3)-C(11)-S(3)	115.3(4)	C(12)-C(11)-S(3)	124.0(4)
N(3)-C(11)-Yb	51.4(2)	C(12)-C(11)-Yb	169.7(4)
S(3)-C(11)-Yb	64.1(2)	C(13)-C(12)-C(11)	118.9(5)
C(14)-C(13)-C(12)	119.6(5)	C(15)-C(14)-C(13)	118.8(5)
N(3)-C(15)-C(14)	122.2(5)	C(16)-N(4)-C(20)	117.5(4)
C(16)-N(4)-Yb	127.1(3)	C(20)-N(4)-Yb	115.4(3)
N(4)-C(16)-C(17)	123.0(5)	C(18)-C(17)-C(16)	118.4(5)
C(17)-C(18)-C(19)	119.5(5)	C(20)-C(19)-C(18)	118.9(5)
N(4)-C(20)-C(19)	122.6(5)	C(25)-N(5)-C(21)	116.8(4)
C(25)-N(5)-Yb	120.6(3)	C(21)-N(5)-Yb	122.6(3)

N(5)-C(21)-C(22)	123.2(5)	C(21)-C(22)-C(23)	119.2(5)
C(24)-C(23)-C(22)	118.2(5)	C(23)-C(24)-C(25)	118.9(5)
N(5)-C(25)-C(24)	123.7(5)	C(30)-N(6)-C(26)	116.2(6)
N(6)-C(26)-C(27)	123.5(6)	C(28)-C(27)-C(26)	118.9(6)
C(27)-C(28)-C(29)	118.8(6)	C(30)-C(29)-C(28)	117.9(6)
N(6)-C(30)-C(29)	124.6(6)		

Table S18. Anisotropic displacement parameters (Uij, Å² x 10³) for Yb(Spy)3(py)3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$.

	U11	U22	U33	U23	U13	U12
Yb	20(1)	16(1)	22(1)	1(1)	3(1)	0(1)
S(1)	21(1)	26(1)	30(1)	2(1)	2(1)	-5(1)
S(2)	22(1)	29(1)	35(1)	1(1)	2(1)	2(1)
S(3)	31(1)	25(1)	26(1)	0(1)	2(1)	-4(1)
N(1)	19(2)	20(2)	29(2)	-2(2)	6(2)	-2(2)
C(1)	21(2)	21(2)	24(3)	-5(2)	3(2)	-1(2)
C(2)	24(3)	35(3)	28(3)	-6(2)	2(2)	-4(2)
C(3)	36(3)	40(3)	23(3)	5(2)	-2(2)	1(2)
C(4)	29(3)	32(3)	29(3)	4(2)	9(2)	-2(2)
C(5)	23(3)	24(2)	29(3)	-3(2)	4(2)	0(2)
N(2)	26(2)	19(2)	32(2)	-1(2)	6(2)	2(2)
C(6)	28(3)	25(3)	29(3)	10(2)	6(2)	6(2)
C(7)	30(3)	36(3)	31(3)	13(2)	11(2)	11(2)
C(8)	43(3)	39(3)	36(3)	7(3)	19(3)	17(3)
C(9)	47(4)	26(3)	33(3)	-1(2)	10(3)	2(2)
C(10)	34(3)	27(3)	32(3)	-2(2)	10(2)	-3(2)
N(3)	24(2)	21(2)	30(2)	1(2)	8(2)	-3(2)
C(11)	33(3)	15(2)	30(3)	1(2)	10(2)	-5(2)
C(12)	48(3)	23(2)	29(3)	-3(2)	13(3)	-5(2)
C(13)	51(3)	22(2)	33(3)	2(2)	20(2)	-1(3)
C(14)	37(3)	15(2)	49(3)	0(2)	21(3)	0(2)
C(15)	31(3)	20(2)	34(3)	0(2)	10(2)	1(2)
N(4)	27(2)	21(2)	26(2)	1(2)	3(2)	3(2)
C(16)	27(3)	28(3)	35(3)	6(2)	8(2)	1(2)
C(17)	41(3)	29(3)	45(4)	5(3)	12(3)	12(2)
C(18)	53(4)	21(3)	52(4)	1(3)	10(3)	5(3)
C(19)	37(3)	22(3)	50(4)	0(2)	2(3)	-3(2)
C(20)	28(3)	23(2)	36(3)	-2(2)	4(2)	-2(2)
N(5)	29(2)	17(2)	28(2)	1(2)	7(2)	-1(2)
C(21)	28(3)	21(2)	25(3)	-1(2)	5(2)	-1(2)
C(22)	33(3)	22(2)	35(3)	-3(2)	13(3)	-7(2)
C(23)	50(3)	19(2)	35(3)	1(2)	11(3)	-1(2)
C(24)	45(4)	27(3)	43(4)	9(2)	-9(3)	2(2)
C(25)	38(3)	23(3)	38(3)	6(2)	-9(3)	-6(2)
N(6)	34(3)	34(3)	62(4)	-9(3)	-4(3)	7(2)
C(26)	32(3)	39(3)	53(4)	10(3)	6(3)	9(3)
C(27)	27(3)	28(3)	71(5)	-2(3)	5(3)	-3(2)
C(28)	21(3)	39(3)	53(4)	-15(3)	2(3)	4(2)
C(29)	29(3)	41(3)	52(4)	7(3)	13(3)	9(3)
C(30)	27(3)	28(3)	69(5)	-3(3)	9(3)	-1(2)

Table S19. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å² x 10³) for Yb(Spy)3(py)3.

	x	y	z	U(eq)
H(2)	5149(6)	1822(3)	3196(3)	57(20)
H(3)	3652(6)	1084(3)	3780(3)	37(16)
H(4)	1328(6)	820(3)	3207(3)	28(14)
H(5)	542(5)	1301(3)	2068(3)	31(15)

H(7)	-1997(6)	3366(3)	1814(3)	18(13)
H(8)	-1074(7)	4344(3)	2664(3)	11(12)
H(9)	1309(6)	4742(3)	2802(3)	34(16)
H(10)	2709(6)	4104(3)	2106(3)	25(14)
H(12)	2772(6)	2148(3)	-1745(3)	36(16)
H(13)	5151(6)	2488(3)	-1709(3)	50(19)
H(14)	6625(6)	2793(3)	-613(3)	47(18)
H(15)	5743(5)	2669(3)	420(3)	29(15)
H(16)	4602(6)	902(3)	719(3)	8(11)
H(17)	4765(7)	-512(3)	606(3)	32(15)
H(18)	2743(7)	-1314(3)	572(3)	82(26)
H(19)	636(6)	-677(3)	690(3)	53(20)
H(20)	549(6)	736(3)	753(3)	20(13)
H(21)	4162(6)	4166(3)	980(3)	31(16)
H(22)	4317(6)	5491(3)	578(3)	26(14)
H(23)	2603(6)	5973(3)	-376(3)	37(16)
H(24)	713(7)	5106(3)	-849(3)	53(20)
H(25)	645(6)	3794(3)	-396(3)	45(18)
H(26)	-3181(6)	5828(4)	1672(4)	50(20)
H(27)	-2118(6)	6490(4)	2703(4)	57(20)
H(28)	-2234(6)	5908(4)	3798(4)	37(17)
H(29)	-3364(6)	4624(4)	3818(4)	68(24)
H(30)	-4430(6)	4039(4)	2757(4)	62(21)

Table S20. Torsion angles [°] for Yb(Spy)3(py)3.

N(1)-Yb-S(1)-C(1)	0.9(2)	N(2)-Yb-S(1)-C(1)	70.9(2)
N(3)-Yb-S(1)-C(1)	-145.4(2)	N(4)-Yb-S(1)-C(1)	-67.0(2)
N(5)-Yb-S(1)-C(1)	142.7(2)	S(3)-Yb-S(1)-C(1)	-132.4(2)
S(2)-Yb-S(1)-C(1)	36.0(2)	C(6)-Yb-S(1)-C(1)	57.0(2)
C(11)-Yb-S(1)-C(1)	-142.9(2)	N(1)-Yb-S(2)-C(6)	67.2(2)
N(2)-Yb-S(2)-C(6)	-4.4(2)	N(3)-Yb-S(2)-C(6)	-141.0(2)
N(4)-Yb-S(2)-C(6)	135.6(2)	N(5)-Yb-S(2)-C(6)	-68.3(2)
S(1)-Yb-S(2)-C(6)	36.9(2)	S(3)-Yb-S(2)-C(6)	-150.5(2)
C(1)-Yb-S(2)-C(6)	57.6(2)	C(11)-Yb-S(2)-C(6)	-144.2(2)
N(1)-Yb-S(3)-C(11)	-122.2(2)	N(2)-Yb-S(3)-C(11)	131.7(2)
N(3)-Yb-S(3)-C(11)	-3.1(2)	N(4)-Yb-S(3)-C(11)	-87.4(2)
N(5)-Yb-S(3)-C(11)	70.4(2)	S(1)-Yb-S(3)-C(11)	-18.1(2)
S(2)-Yb-S(3)-C(11)	169.8(2)	C(1)-Yb-S(3)-C(11)	-81.1(3)
C(6)-Yb-S(3)-C(11)	152.4(2)	N(2)-Yb-N(1)-C(5)	84.2(5)
N(3)-Yb-N(1)-C(5)	-132.2(4)	N(4)-Yb-N(1)-C(5)	-79.2(5)
N(5)-Yb-N(1)-C(5)	118.8(5)	S(1)-Yb-N(1)-C(5)	-178.9(5)
S(3)-Yb-N(1)-C(5)	-43.1(5)	S(2)-Yb-N(1)-C(5)	23.8(5)
C(1)-Yb-N(1)-C(5)	-177.6(7)	C(6)-Yb-N(1)-C(5)	57.2(5)
C(11)-Yb-N(1)-C(5)	-99.6(5)	N(2)-Yb-N(1)-C(1)	-98.1(3)
N(3)-Yb-N(1)-C(1)	45.4(3)	N(4)-Yb-N(1)-C(1)	98.4(3)
N(5)-Yb-N(1)-C(1)	-63.6(3)	S(1)-Yb-N(1)-C(1)	-1.2(2)
S(3)-Yb-N(1)-C(1)	134.5(2)	S(2)-Yb-N(1)-C(1)	-158.6(3)
C(6)-Yb-N(1)-C(1)	-125.1(3)	C(11)-Yb-N(1)-C(1)	78.0(4)
C(5)-N(1)-C(1)-C(2)	-0.7(7)	Yb-N(1)-C(1)-C(2)	-178.9(4)
C(5)-N(1)-C(1)-S(1)	-180.0(3)	Yb-N(1)-C(1)-S(1)	1.8(4)
C(5)-N(1)-C(1)-Yb	178.2(5)	Yb-S(1)-C(1)-N(1)	-1.6(3)
Yb-S(1)-C(1)-C(2)	179.2(4)	N(2)-Yb-C(1)-N(1)	74.2(3)
N(3)-Yb-C(1)-N(1)	-144.8(3)	N(4)-Yb-C(1)-N(1)	-73.6(3)
N(5)-Yb-C(1)-N(1)	133.5(3)	S(1)-Yb-C(1)-N(1)	178.1(4)
S(3)-Yb-C(1)-N(1)	-79.9(3)	S(2)-Yb-C(1)-N(1)	22.4(3)
C(6)-Yb-C(1)-N(1)	51.1(3)	C(11)-Yb-C(1)-N(1)	-129.8(3)
N(1)-Yb-C(1)-C(2)	7(2)	N(2)-Yb-C(1)-C(2)	81(3)
N(3)-Yb-C(1)-C(2)	-138(3)	N(4)-Yb-C(1)-C(2)	-67(3)
N(5)-Yb-C(1)-C(2)	140(3)	S(1)-Yb-C(1)-C(2)	-175(3)
S(3)-Yb-C(1)-C(2)	-73(3)	S(2)-Yb-C(1)-C(2)	29(3)
C(6)-Yb-C(1)-C(2)	58(3)	C(11)-Yb-C(1)-C(2)	-123(3)
N(1)-Yb-C(1)-S(1)	-178.1(4)	N(2)-Yb-C(1)-S(1)	-103.9(2)
N(3)-Yb-C(1)-S(1)	37.1(2)	N(4)-Yb-C(1)-S(1)	108.2(2)
N(5)-Yb-C(1)-S(1)	-44.6(2)	S(3)-Yb-C(1)-S(1)	101.9(2)
S(2)-Yb-C(1)-S(1)	-155.75(11)	C(6)-Yb-C(1)-S(1)	-127.1(2)
C(11)-Yb-C(1)-S(1)	52.1(2)	N(1)-C(1)-C(2)-C(3)	0.5(7)

S(1)-C(1)-C(2)-C(3)	179.7(4)	Yb-C(1)-C(2)-C(3)	-6(3)
C(1)-C(2)-C(3)-C(4)	0.0(8)	C(2)-C(3)-C(4)-C(5)	-0.2(8)
C(1)-N(1)-C(5)-C(4)	0.5(7)	Yb-N(1)-C(5)-C(4)	177.9(4)
C(3)-C(4)-C(5)-N(1)	0.0(8)	N(1)-Yb-N(2)-C(10)	83.6(5)
N(3)-Yb-N(2)-C(10)	-49.5(6)	N(4)-Yb-N(2)-C(10)	106.9(5)
N(5)-Yb-N(2)-C(10)	-71.9(5)	S(1)-Yb-N(2)-C(10)	23.3(5)
S(3)-Yb-N(2)-C(10)	-138.2(5)	S(2)-Yb-N(2)-C(10)	177.1(5)
C(1)-Yb-N(2)-C(10)	57.1(5)	C(6)-Yb-N(2)-C(10)	171.4(7)
C(11)-Yb-N(2)-C(10)	-92.7(5)	N(1)-Yb-N(2)-C(6)	-87.8(3)
N(3)-Yb-N(2)-C(6)	139.1(3)	N(4)-Yb-N(2)-C(6)	-64.5(4)
N(5)-Yb-N(2)-C(6)	116.7(3)	S(1)-Yb-N(2)-C(6)	-148.1(3)
S(3)-Yb-N(2)-C(6)	50.4(3)	S(2)-Yb-N(2)-C(6)	5.7(3)
C(1)-Yb-N(2)-C(6)	-114.3(3)	C(11)-Yb-N(2)-C(6)	95.9(4)
C(10)-N(2)-C(6)-C(7)	-0.5(7)	Yb-N(2)-C(6)-C(7)	172.6(4)
C(10)-N(2)-C(6)-S(2)	178.2(4)	Yb-N(2)-C(6)-S(2)	-8.7(4)
C(10)-N(2)-C(6)-Yb	-173.2(5)	Yb-S(2)-C(6)-N(2)	7.5(3)
Yb-S(2)-C(6)-C(7)	-173.9(4)	N(1)-Yb-C(6)-N(2)	83.4(3)
N(3)-Yb-C(6)-N(2)	-79.0(5)	N(4)-Yb-C(6)-N(2)	133.7(3)
N(5)-Yb-C(6)-N(2)	-58.7(3)	S(1)-Yb-C(6)-N(2)	33.7(3)
S(3)-Yb-C(6)-N(2)	-140.0(3)	S(2)-Yb-C(6)-N(2)	-171.2(4)
C(1)-Yb-C(6)-N(2)	62.4(3)	C(11)-Yb-C(6)-N(2)	-116.7(3)
N(1)-Yb-C(6)-C(7)	45(2)	N(2)-Yb-C(6)-C(7)	-38(2)
N(3)-Yb-C(6)-C(7)	-117(2)	N(4)-Yb-C(6)-C(7)	96(2)
N(5)-Yb-C(6)-C(7)	-97(2)	S(1)-Yb-C(6)-C(7)	-4(2)
S(3)-Yb-C(6)-C(7)	-178(2)	S(2)-Yb-C(6)-C(7)	151(2)
C(1)-Yb-C(6)-C(7)	24(2)	C(11)-Yb-C(6)-C(7)	-155(2)
N(1)-Yb-C(6)-S(2)	-105.4(2)	N(2)-Yb-C(6)-S(2)	171.2(4)
N(3)-Yb-C(6)-S(2)	92.3(3)	N(4)-Yb-C(6)-S(2)	-55.1(2)
N(5)-Yb-C(6)-S(2)	112.6(2)	S(1)-Yb-C(6)-S(2)	-155.07(12)
S(3)-Yb-C(6)-S(2)	31.2(2)	C(1)-Yb-C(6)-S(2)	-126.4(2)
C(11)-Yb-C(6)-S(2)	54.6(3)	N(2)-C(6)-C(7)-C(8)	0.7(7)
S(2)-C(6)-C(7)-C(8)	-177.9(4)	Yb-C(6)-C(7)-C(8)	35(2)
C(6)-C(7)-C(8)-C(9)	0.2(8)	C(7)-C(8)-C(9)-C(10)	-1.2(8)
C(6)-N(2)-C(10)-C(9)	-0.5(8)	Yb-N(2)-C(10)-C(9)	-170.9(4)
C(8)-C(9)-C(10)-N(2)	1.4(8)	N(1)-Yb-N(3)-C(15)	-58.5(5)
N(2)-Yb-N(3)-C(15)	55.4(5)	N(4)-Yb-N(3)-C(15)	-108.5(5)
N(5)-Yb-N(3)-C(15)	77.9(5)	S(1)-Yb-N(3)-C(15)	-18.7(4)
S(3)-Yb-N(3)-C(15)	170.7(5)	S(2)-Yb-N(3)-C(15)	159.9(4)
C(1)-Yb-N(3)-C(15)	-39.0(5)	C(6)-Yb-N(3)-C(15)	99.1(5)
C(11)-Yb-N(3)-C(15)	166.7(6)	N(1)-Yb-N(3)-C(11)	134.7(3)
N(2)-Yb-N(3)-C(11)	-111.3(3)	N(4)-Yb-N(3)-C(11)	84.7(3)
N(5)-Yb-N(3)-C(11)	-88.9(3)	S(1)-Yb-N(3)-C(11)	174.6(3)
S(3)-Yb-N(3)-C(11)	4.0(2)	S(2)-Yb-N(3)-C(11)	-6.8(4)
C(1)-Yb-N(3)-C(11)	154.2(3)	C(6)-Yb-N(3)-C(11)	-67.6(5)
C(15)-N(3)-C(11)-C(12)	2.6(7)	Yb-N(3)-C(11)-C(12)	172.0(4)
C(15)-N(3)-C(11)-S(3)	-175.6(3)	Yb-N(3)-C(11)-S(3)	-6.2(4)
C(15)-N(3)-C(11)-Yb	-169.4(5)	Yb-S(3)-C(11)-N(3)	5.3(3)
Yb-S(3)-C(11)-C(12)	-172.7(4)	N(1)-Yb-C(11)-N(3)	-70.0(4)
N(2)-Yb-C(11)-N(3)	103.9(3)	N(4)-Yb-C(11)-N(3)	-89.6(3)
N(5)-Yb-C(11)-N(3)	83.3(3)	S(1)-Yb-C(11)-N(3)	-5.6(3)
S(3)-Yb-C(11)-N(3)	-173.8(4)	S(2)-Yb-C(11)-N(3)	175.2(3)
C(1)-Yb-C(11)-N(3)	-33.9(3)	C(6)-Yb-C(11)-N(3)	144.8(3)
N(1)-Yb-C(11)-C(12)	-112(2)	N(2)-Yb-C(11)-C(12)	62(2)
N(3)-Yb-C(11)-C(12)	-42(2)	N(4)-Yb-C(11)-C(12)	-132(2)
N(5)-Yb-C(11)-C(12)	41(2)	S(1)-Yb-C(11)-C(12)	-48(2)
S(3)-Yb-C(11)-C(12)	144(2)	S(2)-Yb-C(11)-C(12)	133(2)
C(1)-Yb-C(11)-C(12)	-76(2)	C(6)-Yb-C(11)-C(12)	103(2)
N(1)-Yb-C(11)-S(3)	103.8(2)	N(2)-Yb-C(11)-S(3)	-82.3(3)
N(3)-Yb-C(11)-S(3)	173.8(4)	N(4)-Yb-C(11)-S(3)	84.3(2)
N(5)-Yb-C(11)-S(3)	-102.9(2)	S(1)-Yb-C(11)-S(3)	168.19(12)
S(2)-Yb-C(11)-S(3)	-11.0(2)	C(1)-Yb-C(11)-S(3)	139.9(2)
C(6)-Yb-C(11)-S(3)	-41.4(3)	N(3)-C(11)-C(12)-C(13)	-2.7(7)
S(3)-C(11)-C(12)-C(13)	175.3(4)	Yb-C(11)-C(12)-C(13)	35(2)
C(11)-C(12)-C(13)-C(14)	0.2(8)	C(12)-C(13)-C(14)-C(15)	2.2(7)
C(11)-N(3)-C(15)-C(14)	0.0(7)	Yb-N(3)-C(15)-C(14)	-165.0(3)
C(13)-C(14)-C(15)-N(3)	-2.4(7)	N(1)-Yb-N(4)-C(16)	-102.6(5)
N(2)-Yb-N(4)-C(16)	-126.0(4)	N(3)-Yb-N(4)-C(16)	39.4(4)
N(5)-Yb-N(4)-C(16)	51.8(6)	S(1)-Yb-N(4)-C(16)	-43.1(4)

S(3)-Yb-N(4)-C(16)	100.9(4)	S(2)-Yb-N(4)-C(16)	178.2(4)
C(1)-Yb-N(4)-C(16)	-76.0(4)	C(6)-Yb-N(4)-C(16)	-153.6(4)
C(11)-Yb-N(4)-C(16)	65.7(4)	N(1)-Yb-N(4)-C(20)	77.3(4)
N(2)-Yb-N(4)-C(20)	53.8(5)	N(3)-Yb-N(4)-C(20)	-140.8(4)
N(5)-Yb-N(4)-C(20)	-128.4(4)	S(1)-Yb-N(4)-C(20)	136.8(4)
S(3)-Yb-N(4)-C(20)	-79.3(4)	S(2)-Yb-N(4)-C(20)	-2.0(4)
C(1)-Yb-N(4)-C(20)	103.8(4)	C(6)-Yb-N(4)-C(20)	26.2(4)
C(11)-Yb-N(4)-C(20)	-114.5(4)	C(20)-N(4)-C(16)-C(17)	2.4(8)
Yb-N(4)-C(16)-C(17)	-177.7(4)	N(4)-C(16)-C(17)-C(18)	-1.4(9)
C(16)-C(17)-C(18)-C(19)	-1.1(10)	C(17)-C(18)-C(19)-C(20)	2.5(10)
C(16)-N(4)-C(20)-C(19)	-0.9(8)	Yb-N(4)-C(20)-C(19)	179.2(5)
C(18)-C(19)-C(20)-N(4)	-1.5(9)	N(1)-Yb-N(5)-C(25)	-130.9(4)
N(2)-Yb-N(5)-C(25)	-96.7(4)	N(3)-Yb-N(5)-C(25)	97.6(4)
N(4)-Yb-N(5)-C(25)	84.9(5)	S(1)-Yb-N(5)-C(25)	178.3(4)
S(3)-Yb-N(5)-C(25)	37.3(4)	S(2)-Yb-N(5)-C(25)	-41.9(4)
C(1)-Yb-N(5)-C(25)	-158.0(4)	C(6)-Yb-N(5)-C(25)	-73.9(4)
C(11)-Yb-N(5)-C(25)	70.8(4)	N(1)-Yb-N(5)-C(21)	48.5(5)
N(2)-Yb-N(5)-C(21)	82.8(4)	N(3)-Yb-N(5)-C(21)	-83.0(4)
N(4)-Yb-N(5)-C(21)	-95.7(5)	S(1)-Yb-N(5)-C(21)	-2.3(4)
S(3)-Yb-N(5)-C(21)	-143.3(4)	S(2)-Yb-N(5)-C(21)	137.5(4)
C(1)-Yb-N(5)-C(21)	21.4(4)	C(6)-Yb-N(5)-C(21)	105.6(4)
C(11)-Yb-N(5)-C(21)	-109.8(4)	C(25)-N(5)-C(21)-C(22)	0.9(8)
Yb-N(5)-C(21)-C(22)	-178.5(4)	N(5)-C(21)-C(22)-C(23)	-1.5(8)
C(21)-C(22)-C(23)-C(24)	1.6(8)	C(22)-C(23)-C(24)-C(25)	-1.1(9)
C(21)-N(5)-C(25)-C(24)	-0.5(9)	Yb-N(5)-C(25)-C(24)	179.0(5)
C(23)-C(24)-C(25)-N(5)	0.6(10)	C(30)-N(6)-C(26)-C(27)	-0.5(9)
N(6)-C(26)-C(27)-C(28)	0.0(9)	C(26)-C(27)-C(28)-C(29)	1.2(8)
C(27)-C(28)-C(29)-C(30)	-2.0(8)	C(26)-N(6)-C(30)-C(29)	-0.4(9)
C(28)-C(29)-C(30)-N(6)	1.6(9)		

Table S21. Least-squares planes (x,y,z in crystal coordinates) and deviations from them for Yb(Spy)3(py)3. (* indicates atom used to define plane)

```
- 3.599 (0.019) x + 13.891 (0.018) y + 8.335 (0.034) z = 3.338 (0.010)
*    0.003 (0.003)  N1                *   -0.003 (0.003)  C1
*    0.001 (0.004)  C2                *    0.002 (0.004)  C3
*   -0.002 (0.004)  C4                *   -0.001 (0.003)  C5
     0.004 (0.006)  S1                    -0.053 (0.007)  Yb
     0.987 (0.009)  S2                    -1.381 (0.012)  S3
     2.235 (0.007)  N2                    -1.419 (0.011)  N3
    -2.328 (0.007)  N4                     1.441 (0.011)  N5
Rms deviation of fitted atoms =   0.002

- 1.100 (0.020) x + 11.781 (0.024) y - 12.392 (0.031) z = 1.946 (0.014)
Angle to previous plane (with approximate esd) = 65.87 ( 0.14 )
*   -0.001 (0.003)  N2                *    0.006 (0.003)  C6
*   -0.003 (0.004)  C7                *   -0.004 (0.004)  C8
*    0.008 (0.004)  C9                *   -0.006 (0.004)  C10
     0.062 (0.007)  S2                    -0.283 (0.008)  Yb
    -1.648 (0.009)  S1                     1.141 (0.012)  S3
    -2.447 (0.007)  N1                     0.494 (0.013)  N3
    -2.005 (0.012)  N4                     1.921 (0.008)  N5
Rms deviation of fitted atoms =   0.005

- 2.221 (0.018) x + 15.795 (0.010) y - 0.751 (0.037) z = 2.936 (0.010)
Angle to previous plane (with approximate esd) = 38.18 ( 0.17 )
*   -0.008 (0.003)  N3                *    0.018 (0.003)  C11
*   -0.009 (0.004)  C12               *   -0.007 (0.004)  C13
*    0.017 (0.003)  C14               *   -0.009 (0.003)  C15
     0.136 (0.006)  S3                     0.392 (0.007)  Yb
     1.050 (0.011)  S2                    -0.075 (0.009)  S1
     2.041 (0.011)  N2                    -0.694 (0.012)  N1
    -2.052 (0.008)  N4                     2.601 (0.007)  N5
Rms deviation of fitted atoms =   0.012

 0.320 (0.024) x - 1.141 (0.038) y + 18.644 (0.013) z = 1.342 (0.006)
Angle to previous plane (with approximate esd) = 80.68 ( 0.18 )
```

*	-0.012 (0.004)	N4	*	0.013 (0.004)	C16
*	-0.001 (0.004)	C17	*	-0.013 (0.005)	C18
*	0.014 (0.004)	C19	*	-0.002 (0.004)	C20
	-0.070 (0.009)	Yb		1.817 (0.010)	S1
	-0.185 (0.012)	S2		-2.696 (0.007)	S3
	2.152 (0.008)	N1		1.202 (0.014)	N2
	-1.565 (0.010)	N3		-1.083 (0.014)	N5

Rms deviation of fitted atoms = 0.011

- 6.483 (0.018) x - 5.607 (0.033) y - 14.949 (0.029) z = 1.121 (0.017)

Angle to previous plane (with approximate esd) = 52.47 (0.17)

*	0.001 (0.004)	N5	*	-0.005 (0.004)	C21
*	0.007 (0.004)	C22	*	-0.006 (0.004)	C23
*	0.003 (0.004)	C24	*	0.000 (0.004)	C25
	0.034 (0.008)	Yb		-0.065 (0.011)	S1
	1.883 (0.011)	S2		-1.622 (0.010)	S3
	1.316 (0.013)	N1		2.314 (0.008)	N2
	-2.288 (0.008)	N3		-1.161 (0.013)	N4

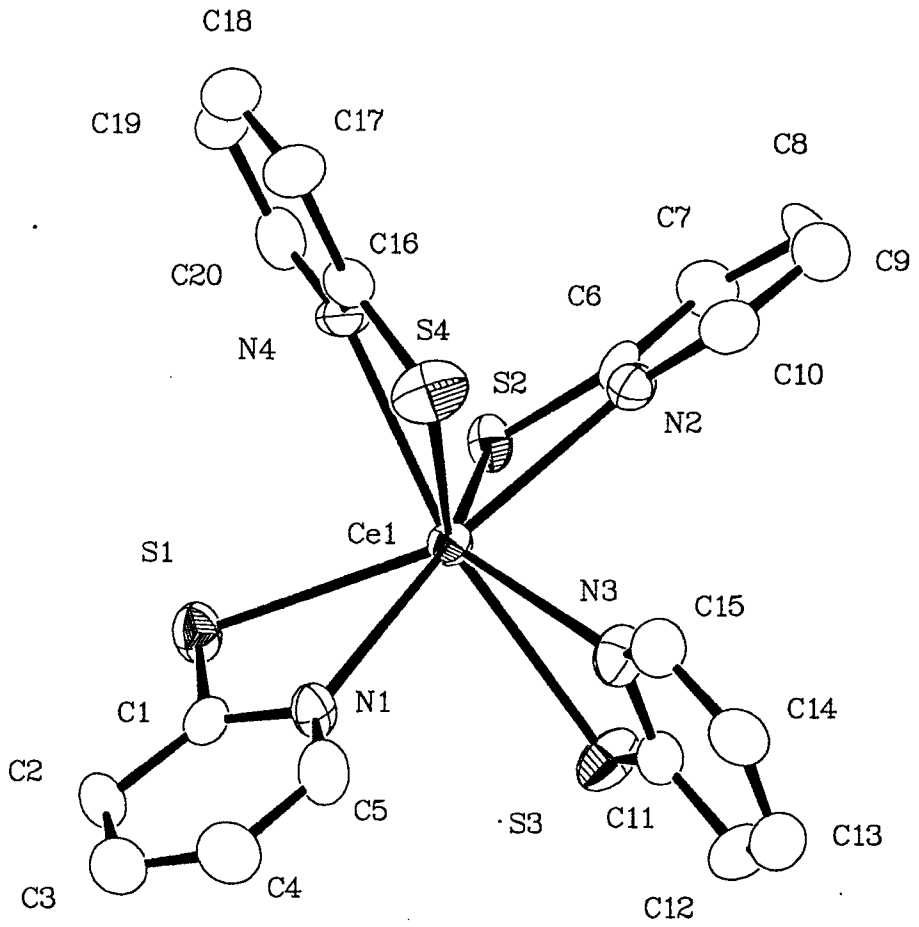
Rms deviation of fitted atoms = 0.004

- 8.441 (0.011) x - 7.950 (0.033) y - 3.655 (0.042) z = 7.942 (0.016)

Angle to previous plane (with approximate esd) = 40.21 (0.21)

*	0.003 (0.004)	N6	*	-0.004 (0.004)	C26
*	-0.002 (0.004)	C27	*	0.009 (0.004)	C28
*	-0.010 (0.004)	C29	*	0.004 (0.004)	C30
	-7.537 (0.009)	Yb		-9.202 (0.005)	S1
	-5.110 (0.010)	S2		-7.482 (0.014)	S3
	-7.729 (0.007)	N1		-5.703 (0.007)	N2
	-9.247 (0.012)	N3		-9.084 (0.011)	N4
	-6.760 (0.011)	N5			

Rms deviation of fitted atoms = 0.006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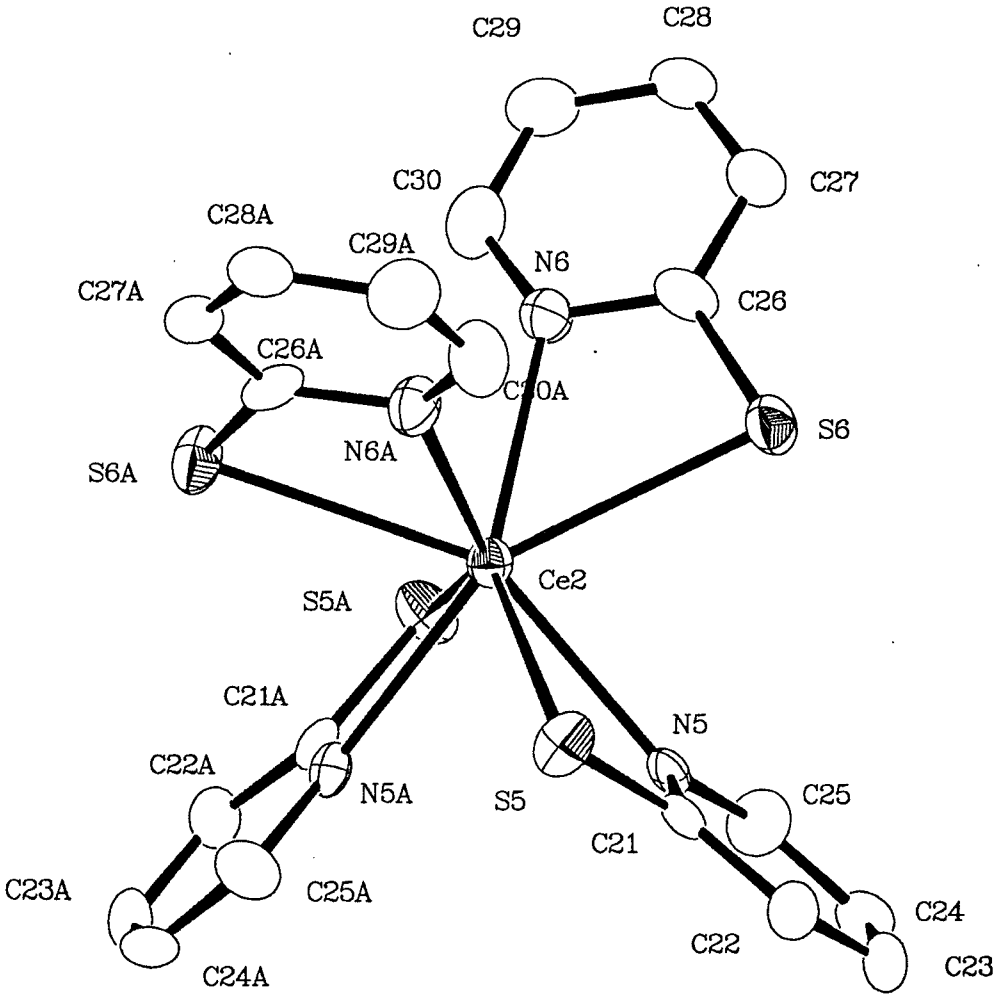
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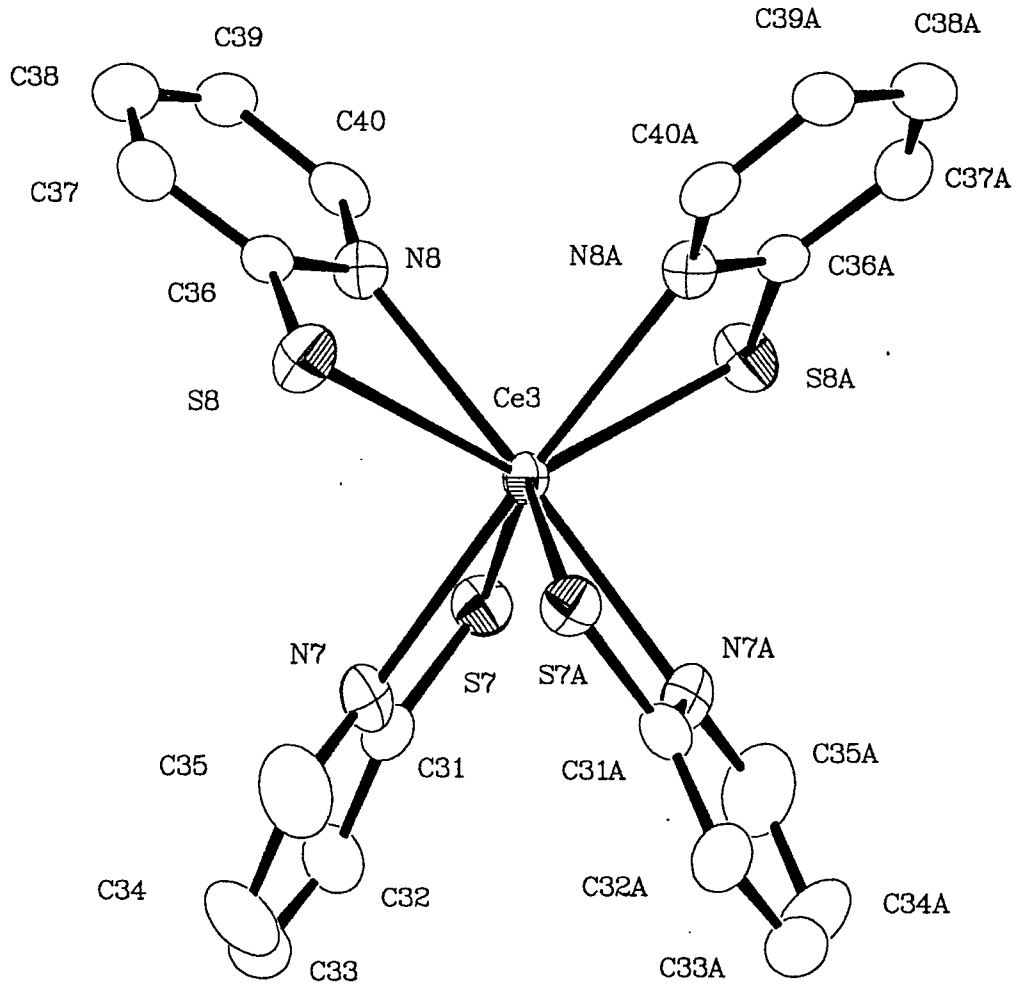
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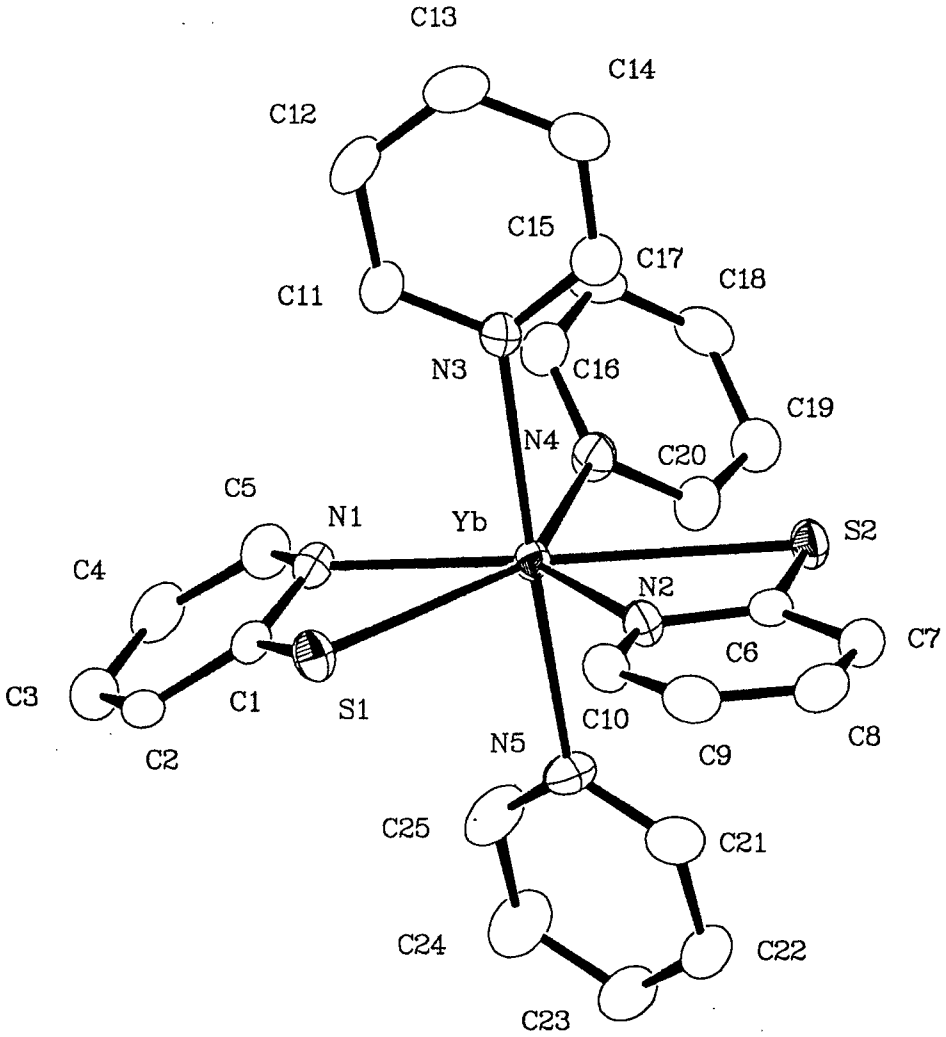
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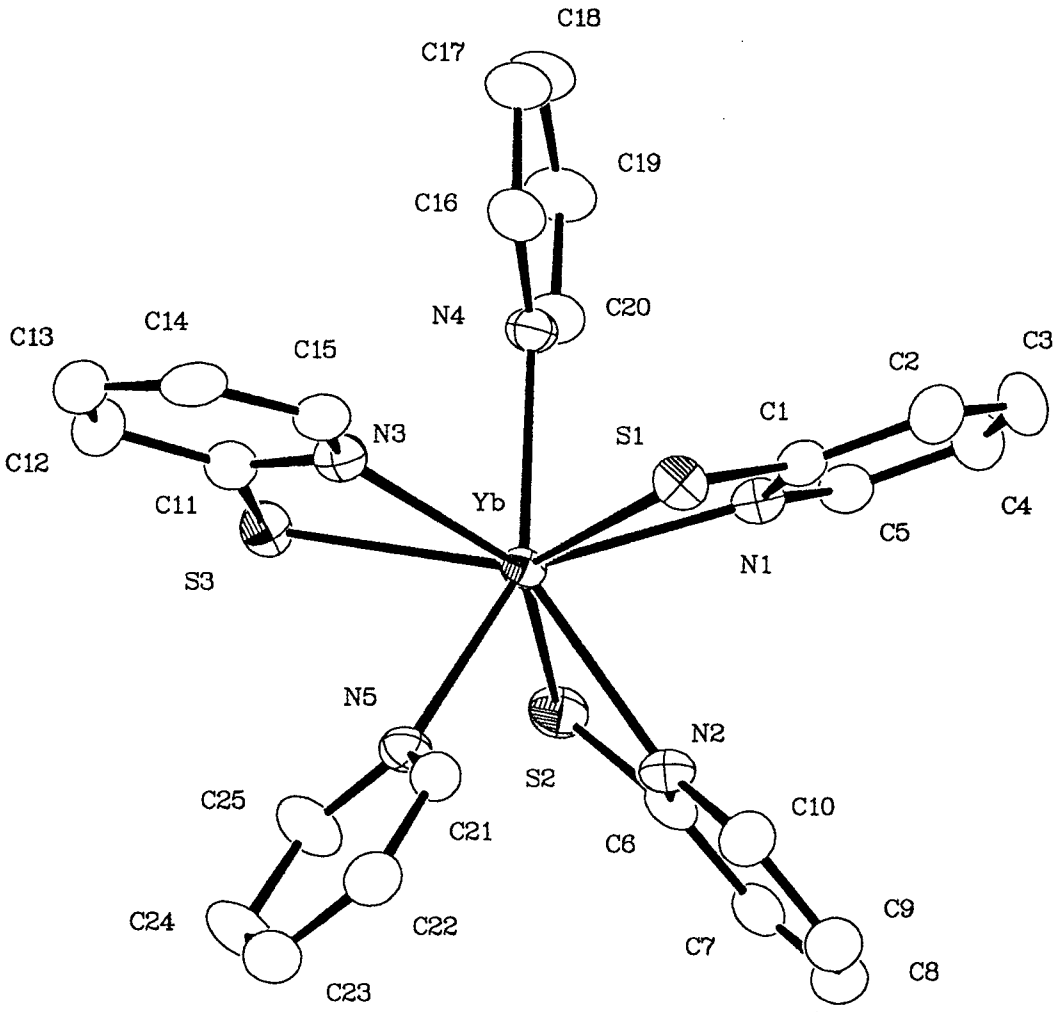
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