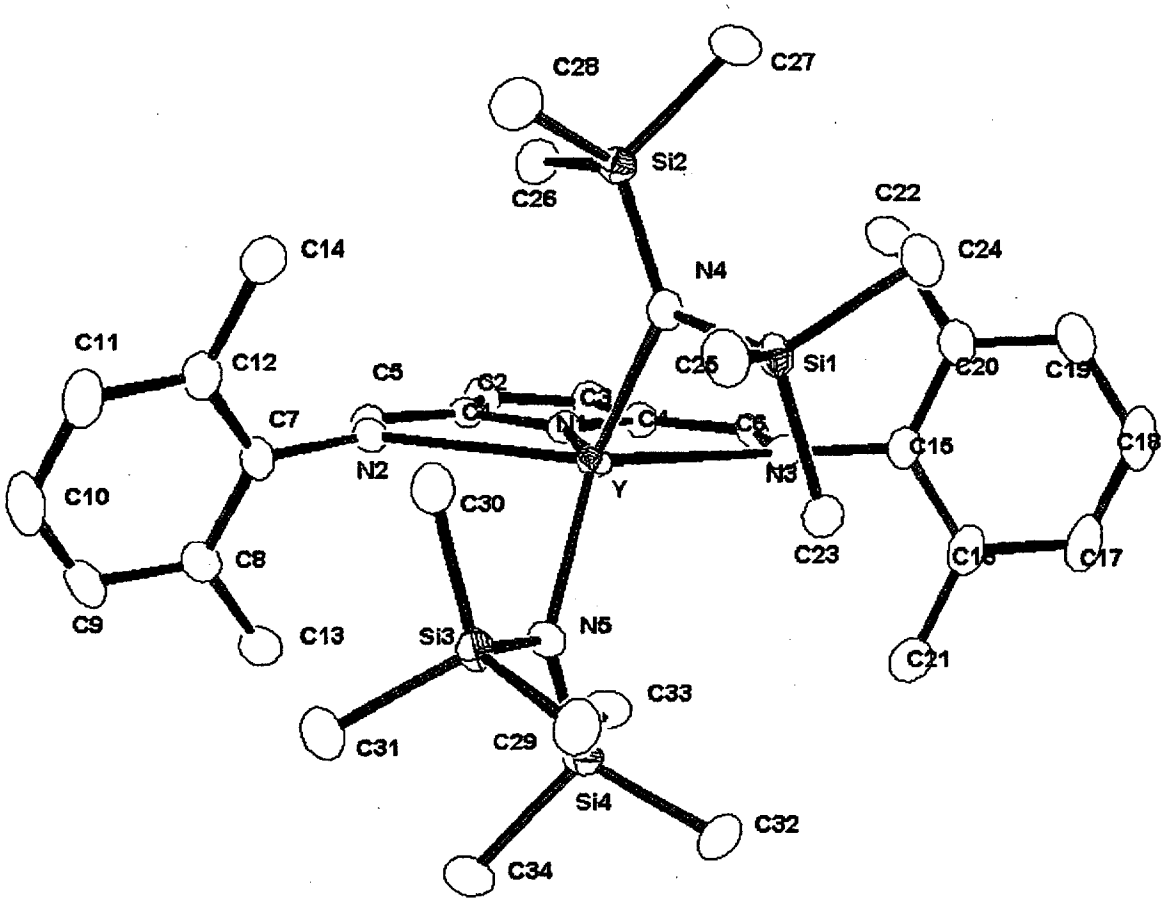

Figure S1. Molecular Structure of $Y(Xyl_2\text{-}pyr)\{N(SiMe_3)_2\}_2$ (**3d**) with a labeling scheme. Hydrogen atoms are omitted for clarity.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 3d.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	Y	z	U(eq)
Y	2630(1)	574(1)	2500	15(1)
Si(1)	3656(1)	-828(1)	3722(1)	19(1)
Si(2)	4215(1)	-870(1)	2010(1)	21(1)
Si(3)	3105(1)	2469(1)	3749(1)	19(1)
Si(4)	1433(1)	2113(1)	3560(1)	20(1)
N(1)	1941(2)	364(2)	1357(2)	16(1)
N(2)	2924(2)	1916(2)	1340(2)	17(1)
N(3)	1613(2)	-1000(2)	2494(2)	19(1)
N(4)	3599(2)	-479(2)	2738(2)	18(1)
N(5)	2356(2)	1834(2)	3329(2)	19(1)
C(1)	1986(2)	940(3)	695(2)	15(1)
C(2)	1478(2)	596(3)	113(2)	20(1)
C(3)	1109(2)	-219(3)	434(2)	22(1)
C(4)	1411(2)	-344(3)	1204(2)	17(1)
C(5)	2503(2)	1754(3)	722(2)	17(1)
C(6)	1268(2)	-1060(3)	1815(2)	19(1)
C(7)	3319(2)	2853(3)	1317(2)	19(1)
C(8)	2892(3)	3734(3)	1361(3)	24(1)
C(9)	3280(3)	4638(3)	1305(3)	29(1)
C(10)	4062(3)	4668(3)	1218(3)	32(1)
C(11)	4471(3)	3796(3)	1176(3)	29(1)
C(12)	4111(2)	2875(3)	1231(2)	22(1)
C(13)	2049(3)	3715(3)	1489(3)	28(1)
C(14)	1566(2)	1935(3)	1180(3)	28(1)
C(15)	1490(2)	-1838(3)	3013(2)	19(1)
C(16)	971(2)	-1750(3)	3645(3)	25(1)
C(17)	896(3)	-2563(4)	4151(3)	29(1)
C(18)	1312(3)	-3421(4)	4042(3)	32(1)
C(19)	1802(3)	-3498(3)	3411(3)	27(1)
C(20)	1894(2)	-2712(3)	2878(3)	23(1)
C(21)	504(3)	-833(4)	3758(3)	35(1)
C(22)	2418(3)	-2798(3)	2171(3)	31(1)
C(23)	2746(2)	-461(3)	4233(3)	23(1)
C(24)	3759(3)	-2198(3)	3891(3)	29(1)
C(25)	4450(3)	-239(3)	4293(3)	27(1)
C(26)	3785(3)	-580(3)	1014(3)	27(1)
C(27)	4443(3)	-2234(4)	1976(3)	35(1)
C(28)	5185(2)	-297(4)	2101(3)	32(1)
C(29)	3171(3)	2273(4)	4855(3)	30(1)
C(30)	4009(2)	2035(3)	3276(3)	24(1)
C(31)	3106(3)	3844(3)	3572(3)	30(1)
C(32)	1133(3)	1620(4)	4559(3)	32(1)
C(33)	820(2)	1564(3)	2756(3)	28(1)
C(34)	1215(3)	3476(3)	3615(3)	31(1)

Table S2. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 3d.

	x	Y	z	U(eq)
H(2)	1402	870	-402	24
H(3)	729	-613	186	27
H(5)	2538	2187	276	21
H(6)	917	-1583	1722	22
H(9)	3002	5242	1327	35
H(10)	4316	5288	1186	38
H(11)	5007	3823	1109	35
H(13A)	1873	3025	1507	42
H(13B)	1796	4063	1050	42
H(13C)	1927	4045	1993	42
H(14A)	4226	1362	1230	42
H(14B)	4941	1921	1610	42
H(14C)	4827	1907	665	42
H(17)	548	-2526	4583	35
H(18)	1260	-3958	4404	39
H(19)	2081	-4093	3335	32
H(21A)	177	-914	4226	53
H(21B)	188	-724	3286	53
H(21C)	840	-262	3838	53
H(22A)	2654	-3457	2168	47
H(22B)	2813	-2288	2206	47
H(22C)	2127	-2706	1679	47
H(23A)	2661	252	4163	34
H(23B)	2783	-615	4802	34
H(23C)	2322	-831	3999	34
H(24A)	3359	-2552	3601	43
H(24B)	3716	-2341	4462	43
H(24C)	4257	-2418	3699	43
H(25A)	4123	484	4234	41
H(25B)	4937	-479	4088	41
H(25C)	4404	-413	4858	41
H(26A)	3281	-884	978	41
H(26B)	4111	-846	591	41
H(26C)	3740	141	952	41
H(27A)	3972	-2615	1926	52
H(27B)	4707	-2426	2466	52
H(27C)	4771	-2371	1516	52
H(28A)	5398	-453	2626	48
H(28B)	5144	425	2041	48
H(28C)	5517	-563	1685	48
H(29A)	2700	2498	5108	45
H(29B)	3600	2654	5067	45
H(29C)	3247	1566	4966	45
H(30A)	4056	1314	3339	36
H(30B)	4442	2362	3532	36
H(30C)	4004	2201	2707	36
H(31A)	2647	4137	3804	44
H(31B)	3115	3974	2998	44
H(31C)	3555	4139	3821	44
H(32A)	1226	903	4580	47
H(32B)	591	1750	4640	47
H(32C)	1426	1950	4979	47
H(33A)	920	850	2715	42
H(33B)	937	1884	2246	42
H(33C)	284	1671	2887	42
H(34A)	1358	3794	3111	47
H(34B)	1504	3776	4052	47
H(34C)	671	3570	3709	47

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for 3d.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Y	18(1)	15(1)	14(1)	-1(1)	-2(1)	2(1)
Si(1)	19(1)	17(1)	20(1)	5(1)	-4(1)	0(1)
Si(2)	19(1)	20(1)	23(1)	2(1)	3(1)	4(1)
Si(3)	25(1)	17(1)	16(1)	0(1)	-2(1)	-2(1)
Si(4)	20(1)	19(1)	20(1)	-2(1)	3(1)	4(1)
N(1)	18(2)	17(1)	14(2)	-1(1)	1(1)	0(1)
N(2)	20(2)	15(2)	15(2)	0(1)	-1(1)	0(1)
N(3)	20(1)	18(1)	19(1)	0(2)	2(2)	0(1)
N(4)	18(2)	18(2)	19(2)	4(1)	-1(1)	0(1)
N(5)	21(2)	16(2)	19(2)	0(1)	0(1)	2(1)
C(1)	20(2)	14(2)	12(2)	-1(1)	0(1)	2(2)
C(2)	25(2)	18(2)	17(2)	0(2)	-4(2)	2(2)
C(3)	23(2)	22(2)	21(2)	-1(2)	-6(2)	0(2)
C(4)	18(2)	16(2)	18(2)	0(1)	-2(1)	-2(1)
C(5)	18(2)	16(2)	18(2)	2(2)	6(1)	4(2)
C(6)	22(2)	13(2)	21(2)	-3(2)	-2(2)	0(2)
C(7)	29(2)	17(2)	13(2)	0(1)	-2(2)	-5(2)
C(8)	35(2)	20(2)	16(2)	2(2)	-1(2)	3(2)
C(9)	52(3)	15(2)	20(2)	3(2)	-3(2)	1(2)
C(10)	43(3)	24(2)	27(2)	5(2)	-11(2)	-14(2)
C(11)	28(2)	32(2)	27(2)	5(2)	-6(2)	-12(2)
C(12)	27(2)	24(2)	14(2)	3(2)	-5(2)	-4(2)
C(13)	34(2)	24(2)	26(2)	2(2)	4(2)	6(2)
C(14)	23(2)	32(2)	29(2)	6(2)	1(2)	1(2)
C(15)	22(2)	19(2)	17(2)	0(2)	-3(1)	-7(2)
C(16)	27(2)	28(2)	20(2)	1(2)	-2(2)	-12(2)
C(17)	29(2)	38(2)	20(2)	10(2)	-4(2)	-10(2)
C(18)	34(2)	36(3)	27(2)	14(2)	-12(2)	-14(2)
C(19)	31(2)	19(2)	30(2)	3(2)	-10(2)	-4(2)
C(20)	26(2)	20(2)	24(2)	2(2)	-6(2)	-5(2)
C(21)	39(3)	32(2)	35(3)	2(2)	14(2)	-3(2)
C(22)	39(2)	24(2)	31(2)	-2(2)	7(2)	9(2)
C(23)	23(2)	24(2)	20(2)	2(2)	2(2)	0(2)
C(24)	33(2)	22(2)	31(2)	7(2)	-3(2)	2(2)
C(25)	29(2)	28(2)	25(2)	4(2)	-10(2)	-1(2)
C(26)	27(2)	29(2)	25(2)	2(2)	3(2)	-1(2)
C(27)	33(2)	29(2)	43(3)	1(2)	7(2)	12(2)
C(28)	19(2)	42(3)	35(2)	9(2)	-3(2)	5(2)
C(29)	40(3)	31(2)	19(2)	1(2)	-4(2)	-9(2)
C(30)	22(2)	25(2)	27(2)	4(2)	-3(2)	-3(2)
C(31)	44(3)	21(2)	24(2)	-1(2)	-6(2)	-5(2)
C(32)	33(2)	36(2)	26(2)	4(2)	12(2)	-1(2)
C(33)	21(2)	32(2)	31(2)	-7(2)	-1(2)	5(2)
C(34)	29(2)	25(2)	40(3)	-3(2)	5(2)	8(2)

Table S4. Bond lengths [A] and angles [deg] for **3d**.

Y-N(5)	2.246(3)	C(15)-C(20)	1.394(6)
Y-N(4)	2.254(3)	C(15)-C(16)	1.406(6)
Y-N(1)	2.288(3)	C(16)-C(17)	1.391(6)
Y-N(2)	2.707(3)	C(16)-C(21)	1.497(6)
Y-N(3)	2.776(3)	C(17)-C(18)	1.382(7)
Y-Si(1)	3.3221(11)	C(17)-H(17)	0.9500
Y-Si(3)	3.4070(12)	C(18)-C(19)	1.369(7)
Si(1)-N(4)	1.721(3)	C(18)-H(18)	0.9500
Si(1)-C(25)	1.872(4)	C(19)-C(20)	1.395(6)
Si(1)-C(24)	1.876(4)	C(19)-H(19)	0.9500
Si(1)-C(23)	1.884(4)	C(20)-C(22)	1.507(6)
Si(2)-N(4)	1.717(3)	C(21)-H(21A)	0.9800
Si(2)-C(26)	1.878(5)	C(21)-H(21B)	0.9800
Si(2)-C(28)	1.880(5)	C(21)-H(21C)	0.9800
Si(2)-C(27)	1.880(5)	C(22)-H(22A)	0.9800
Si(3)-N(5)	1.723(3)	C(22)-H(22B)	0.9800
Si(3)-C(30)	1.874(4)	C(22)-H(22C)	0.9800
Si(3)-C(31)	1.876(4)	C(23)-H(23A)	0.9800
Si(3)-C(29)	1.879(4)	C(23)-H(23B)	0.9800
Si(4)-N(5)	1.714(3)	C(23)-H(23C)	0.9800
Si(4)-C(34)	1.877(4)	C(24)-H(24A)	0.9800
Si(4)-C(32)	1.879(4)	C(24)-H(24B)	0.9800
Si(4)-C(33)	1.881(4)	C(24)-H(24C)	0.9800
N(1)-C(1)	1.358(5)	C(25)-H(25A)	0.9800
N(1)-C(4)	1.359(5)	C(25)-H(25B)	0.9800
N(2)-C(5)	1.295(5)	C(25)-H(25C)	0.9800
N(2)-C(7)	1.442(5)	C(26)-H(26A)	0.9800
N(3)-C(6)	1.295(5)	C(26)-H(26B)	0.9800
N(3)-C(15)	1.442(5)	C(26)-H(26C)	0.9800
C(1)-C(2)	1.403(5)	C(27)-H(27A)	0.9800
C(1)-C(5)	1.425(5)	C(27)-H(27B)	0.9800
C(2)-C(3)	1.386(6)	C(27)-H(27C)	0.9800
C(2)-H(2)	0.9500	C(28)-H(28A)	0.9800
C(3)-C(4)	1.409(5)	C(28)-H(28B)	0.9800
C(3)-H(3)	0.9500	C(28)-H(28C)	0.9800
C(4)-C(6)	1.431(5)	C(29)-H(29A)	0.9800
C(5)-H(5)	0.9500	C(29)-H(29B)	0.9800
C(6)-H(6)	0.9500	C(29)-H(29C)	0.9800
C(7)-C(12)	1.401(6)	C(30)-H(30A)	0.9800
C(7)-C(8)	1.406(6)	C(30)-H(30B)	0.9800
C(8)-C(9)	1.399(6)	C(30)-H(30C)	0.9800
C(8)-C(13)	1.501(6)	C(31)-H(31A)	0.9800
C(9)-C(10)	1.386(7)	C(31)-H(31B)	0.9800
C(9)-H(9)	0.9500	C(31)-H(31C)	0.9800
C(10)-C(11)	1.379(7)	C(32)-H(32A)	0.9800
C(10)-H(10)	0.9500	C(32)-H(32B)	0.9800
C(11)-C(12)	1.396(6)	C(32)-H(32C)	0.9800
C(11)-H(11)	0.9500	C(33)-H(33A)	0.9800
C(12)-C(14)	1.501(6)	C(33)-H(33B)	0.9800
C(13)-H(13A)	0.9800	C(33)-H(33C)	0.9800
C(13)-H(13B)	0.9800	C(34)-H(34A)	0.9800
C(13)-H(13C)	0.9800	C(34)-H(34B)	0.9800
C(14)-H(14A)	0.9800	C(34)-H(34C)	0.9800
C(14)-H(14B)	0.9800		
C(14)-H(14C)	0.9800		

N(5)-Y-N(4)	121.89(12)
N(5)-Y-N(1)	119.92(11)
N(4)-Y-N(1)	118.16(11)
N(5)-Y-N(2)	89.00(11)
N(4)-Y-N(2)	113.78(11)
N(1)-Y-N(2)	65.19(10)
N(5)-Y-N(3)	116.12(11)
N(4)-Y-N(3)	90.47(10)
N(1)-Y-N(3)	63.91(11)
N(2)-Y-N(3)	129.10(11)
N(5)-Y-Si(1)	99.42(9)
N(4)-Y-Si(1)	28.54(8)
N(1)-Y-Si(1)	137.39(8)
N(2)-Y-Si(1)	136.05(7)
N(3)-Y-Si(1)	85.36(7)
N(5)-Y-Si(3)	26.61(8)
N(4)-Y-Si(3)	100.19(9)
N(1)-Y-Si(3)	137.65(8)
N(2)-Y-Si(3)	84.04(7)
N(3)-Y-Si(3)	137.09(8)
Si(1)-Y-Si(3)	84.96(3)
N(4)-Si(1)-C(25)	114.89(19)
N(4)-Si(1)-C(24)	114.83(19)
C(25)-Si(1)-C(24)	105.5(2)
N(4)-Si(1)-C(23)	108.42(18)
C(25)-Si(1)-C(23)	106.9(2)
C(24)-Si(1)-C(23)	105.7(2)
N(4)-Si(1)-Y	38.73(11)
C(25)-Si(1)-Y	118.80(14)
C(24)-Si(1)-Y	134.86(15)
C(23)-Si(1)-Y	70.72(13)
N(4)-Si(2)-C(26)	108.34(19)
N(4)-Si(2)-C(28)	113.0(2)
C(26)-Si(2)-C(28)	110.7(2)
N(4)-Si(2)-C(27)	117.16(19)
C(26)-Si(2)-C(27)	105.2(2)
C(28)-Si(2)-C(27)	102.1(2)
N(5)-Si(3)-C(30)	108.75(18)
N(5)-Si(3)-C(31)	115.18(19)
C(30)-Si(3)-C(31)	103.9(2)
N(5)-Si(3)-C(29)	112.52(19)
C(30)-Si(3)-C(29)	108.8(2)
C(31)-Si(3)-C(29)	107.2(2)
N(5)-Si(3)-Y	35.73(11)
C(30)-Si(3)-Y	73.35(14)
C(31)-Si(3)-Y	129.91(15)
C(29)-Si(3)-Y	121.24(15)
N(5)-Si(4)-C(34)	114.79(19)
N(5)-Si(4)-C(32)	113.0(2)
C(34)-Si(4)-C(32)	104.2(2)
N(5)-Si(4)-C(33)	107.15(18)
C(34)-Si(4)-C(33)	107.6(2)
C(32)-Si(4)-C(33)	109.9(2)
C(1)-N(1)-C(4)	106.6(3)
C(1)-N(1)-Y	125.8(2)
C(4)-N(1)-Y	127.6(3)
C(5)-N(2)-C(7)	113.8(3)
C(5)-N(2)-Y	110.8(2)
C(7)-N(2)-Y	134.1(2)
C(6)-N(3)-C(15)	114.4(3)
C(6)-N(3)-Y	110.7(3)
C(15)-N(3)-Y	133.8(2)
Si(2)-N(4)-Si(1)	124.2(2)
Si(2)-N(4)-Y	123.08(17)
Si(1)-N(4)-Y	112.73(17)
Si(4)-N(5)-Si(3)	121.6(2)
Si(4)-N(5)-Y	120.69(17)
Si(3)-N(5)-Y	117.66(17)
N(1)-C(1)-C(2)	110.2(3)
N(1)-C(1)-C(5)	116.7(3)
C(2)-C(1)-C(5)	133.0(4)
C(3)-C(2)-C(1)	106.9(4)
C(3)-C(2)-H(2)	126.6
C(1)-C(2)-H(2)	126.6
C(2)-C(3)-C(4)	105.9(4)
C(2)-C(3)-H(3)	127.1
C(4)-C(3)-H(3)	127.1
N(1)-C(4)-C(3)	110.5(3)
N(1)-C(4)-C(6)	117.3(3)
C(3)-C(4)-C(6)	132.2(4)
N(2)-C(5)-C(1)	121.4(3)
N(2)-C(5)-H(5)	119.3
C(1)-C(5)-H(5)	119.3
N(3)-C(6)-C(4)	120.4(3)
N(3)-C(6)-H(6)	119.8
C(4)-C(6)-H(6)	119.8
C(12)-C(7)-C(8)	121.3(4)
C(12)-C(7)-N(2)	120.1(3)
C(8)-C(7)-N(2)	118.6(4)
C(9)-C(8)-C(7)	118.0(4)
C(9)-C(8)-C(13)	120.5(4)
C(7)-C(8)-C(13)	121.5(4)
C(10)-C(9)-C(8)	121.1(4)
C(10)-C(9)-H(9)	119.4
C(8)-C(9)-H(9)	119.4
C(11)-C(10)-C(9)	120.0(4)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	121.0(4)
C(10)-C(11)-H(11)	119.5
C(12)-C(11)-H(11)	119.5
C(11)-C(12)-C(7)	118.5(4)
C(11)-C(12)-C(14)	120.2(4)
C(7)-C(12)-C(14)	121.3(4)
C(8)-C(13)-H(13A)	109.5
C(8)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(8)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(20)-C(15)-C(16)	121.7(4)
C(20)-C(15)-N(3)	119.1(3)
C(16)-C(15)-N(3)	119.2(4)
C(17)-C(16)-C(15)	117.2(4)
C(17)-C(16)-C(21)	121.2(4)
C(15)-C(16)-C(21)	121.6(4)
C(18)-C(17)-C(16)	121.7(4)
C(18)-C(17)-H(17)	119.1
C(16)-C(17)-H(17)	119.1
C(19)-C(18)-C(17)	120.0(4)
C(19)-C(18)-H(18)	120.0

C(17)-C(18)-H(18)	120.0
C(18)-C(19)-C(20)	120.9(4)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(15)-C(20)-C(19)	118.4(4)
C(15)-C(20)-C(22)	120.4(4)
C(19)-C(20)-C(22)	121.2(4)
C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
Si(1)-C(23)-H(23A)	109.5
Si(1)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
Si(1)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
Si(1)-C(24)-H(24A)	109.5
Si(1)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
Si(1)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
Si(1)-C(25)-H(25A)	109.5
Si(1)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
Si(1)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(2)-C(26)-H(26A)	109.5
Si(2)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(2)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(2)-C(27)-H(27A)	109.5
Si(2)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(2)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(2)-C(28)-H(28A)	109.5
Si(2)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(2)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
Si(3)-C(29)-H(29A)	109.5
Si(3)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
Si(3)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
Si(3)-C(30)-H(30A)	109.5
Si(3)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(3)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si(3)-C(31)-H(31A)	109.5
Si(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
Si(4)-C(32)-H(32A)	109.5
Si(4)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
Si(4)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
Si(4)-C(33)-H(33A)	109.5
Si(4)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
Si(4)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
Si(4)-C(34)-H(34A)	109.5
Si(4)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
Si(4)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5

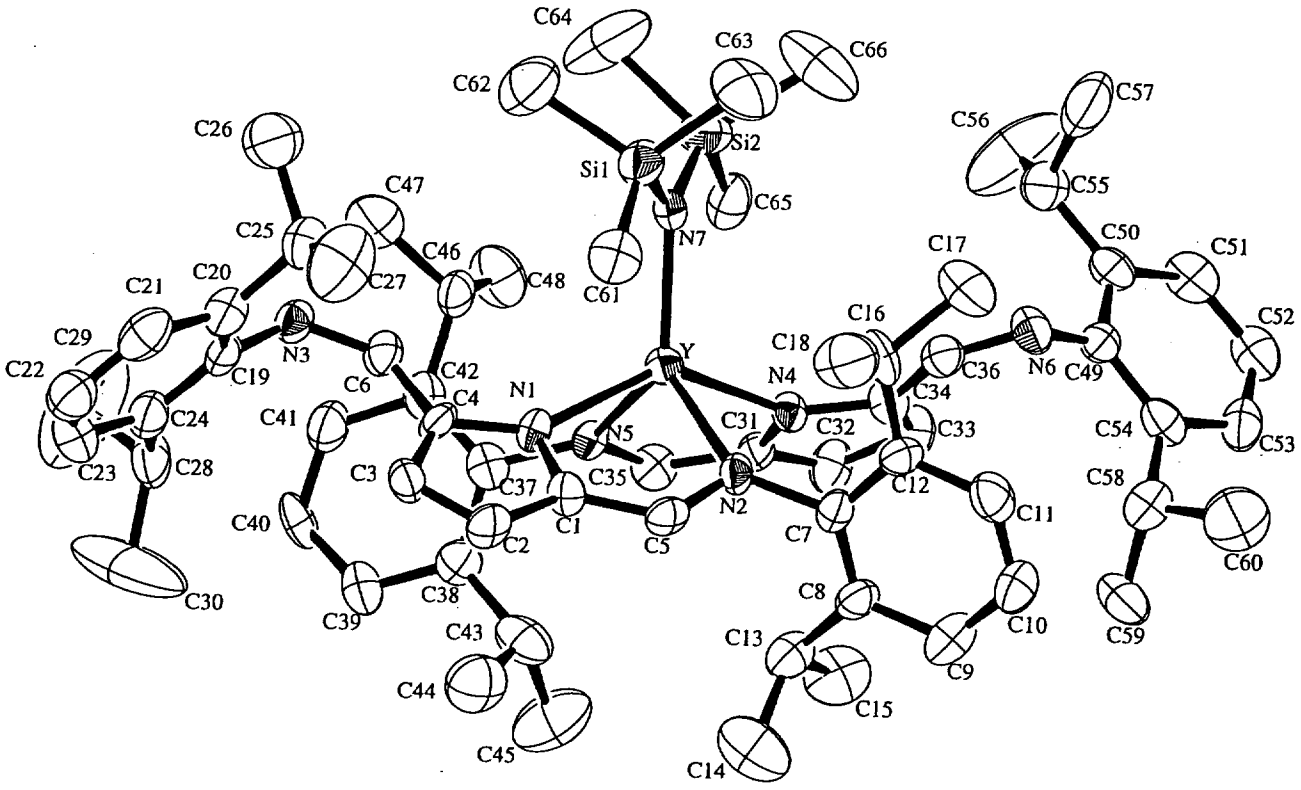

Figure S2. Molecular Structure of $Y(DIP_2\text{-}pyr)_2N(SiMe_3)_2$ (**4e**) with a labeling scheme. Hydrogen atoms are omitted for clarity.

Table S5. Positional Parameters and B(eq) for 4e.

atom	x	y	z	B(eq)
Y	0.05542(5)	0.13392(3)	0.20944(3)	2.30(1)
Si(1)	-0.1228(1)	0.18695(8)	0.28018(9)	3.66(5)
Si(2)	-0.1936(1)	0.10822(8)	0.1706(1)	4.20(6)
N(1)	0.1641(3)	0.1446(2)	0.3201(2)	2.2(1)
N(2)	0.1586(3)	0.2056(2)	0.1979(2)	2.4(1)
N(3)	0.1116(3)	0.0711(2)	0.4665(2)	2.8(1)
N(4)	0.0555(3)	0.1153(2)	0.0898(2)	2.2(1)
N(5)	0.1303(3)	0.0516(2)	0.2048(2)	2.2(1)
N(6)	-0.0789(3)	0.2044(2)	-0.0369(2)	3.2(1)
N(7)	-0.0983(3)	0.1431(2)	0.2207(2)	2.7(1)
C(1)	0.2271(4)	0.1838(2)	0.3199(3)	2.3(1)
C(2)	0.2850(4)	0.1906(2)	0.3868(3)	3.2(2)
C(3)	0.2570(4)	0.1562(2)	0.4304(3)	2.7(2)
C(4)	0.1821(4)	0.1295(3)	0.3888(3)	2.6(1)
C(5)	0.2242(4)	0.2127(2)	0.2575(3)	2.7(2)
C(6)	0.1208(4)	0.0899(2)	0.4076(3)	2.9(2)
C(7)	0.1712(4)	0.2355(2)	0.1374(3)	2.6(2)
C(8)	0.2462(4)	0.2233(3)	0.1047(3)	3.0(2)
C(9)	0.2634(5)	0.2553(3)	0.0495(3)	4.1(2)
C(10)	0.2036(5)	0.2963(3)	0.0297(3)	4.4(2)
C(11)	0.1265(5)	0.3057(2)	0.0611(3)	3.7(2)
C(12)	0.1074(4)	0.2750(3)	0.1152(3)	2.9(2)
C(13)	0.3098(5)	0.1771(3)	0.1216(3)	3.9(2)
C(14)	0.4156(5)	0.1893(3)	0.1552(4)	6.7(2)
C(15)	0.3052(5)	0.1439(3)	0.0571(4)	5.6(2)
C(16)	0.0193(5)	0.2860(2)	0.1466(3)	3.0(2)
C(17)	-0.0722(5)	0.3031(3)	0.0924(3)	5.2(2)
C(18)	0.0447(5)	0.3260(3)	0.2046(4)	5.8(2)
C(19)	0.1715(4)	0.0876(2)	0.5350(3)	2.7(2)
C(20)	0.1406(4)	0.1301(3)	0.5670(3)	3.4(2)
C(21)	0.1907(5)	0.1384(3)	0.6377(3)	4.2(2)
C(22)	0.2660(5)	0.1088(3)	0.6713(3)	4.6(2)
C(23)	0.2942(5)	0.0691(3)	0.6366(4)	4.5(2)
C(24)	0.2462(5)	0.0567(3)	0.5686(3)	3.4(2)
C(25)	0.0566(5)	0.1636(3)	0.5320(3)	3.7(2)
C(26)	-0.0379(5)	0.1480(3)	0.5529(4)	6.5(2)
C(27)	0.0808(6)	0.2184(3)	0.5435(4)	7.2(3)
C(28)	0.2768(5)	0.0117(3)	0.5302(3)	4.3(2)
C(29)	0.2354(9)	-0.0356(3)	0.5527(5)	13.3(4)
C(30)	0.3871(6)	0.0073(4)	0.5383(5)	13.1(4)
C(31)	0.0925(4)	0.0692(2)	0.0803(3)	2.8(2)
C(32)	0.0790(5)	0.0565(2)	0.0086(3)	3.4(2)
C(33)	0.0295(5)	0.0964(2)	-0.0285(3)	3.2(2)
C(34)	0.0181(4)	0.1320(3)	0.0219(3)	2.7(1)
C(35)	0.1327(4)	0.0387(2)	0.1405(3)	3.0(2)
C(36)	-0.0314(4)	0.1802(2)	0.0159(3)	2.8(2)
C(37)	0.1791(5)	0.0184(2)	0.2616(3)	2.7(2)
C(38)	0.2819(5)	0.0177(3)	0.2791(3)	3.1(2)
C(39)	0.3278(5)	-0.0174(3)	0.3299(3)	4.1(2)
C(40)	0.2730(5)	-0.0495(2)	0.3605(3)	3.7(2)
C(41)	0.1725(5)	-0.0463(2)	0.3449(3)	3.7(2)
C(42)	0.1215(5)	-0.0123(2)	0.2948(3)	2.9(2)
C(43)	0.3466(5)	0.0542(3)	0.2487(4)	4.3(2)
C(44)	0.4127(5)	0.0843(3)	0.3084(4)	5.6(2)

C(45)	0.4080(5)	0.0288(3)	0.2021(4)	7.2(3)
C(46)	0.0107(5)	-0.0105(2)	0.2761(3)	3.2(2)
C(47)	-0.0377(5)	-0.0206(2)	0.3393(3)	4.6(2)
C(48)	-0.0293(5)	-0.0471(3)	0.2152(3)	5.2(2)
C(49)	-0.0943(4)	0.1856(2)	-0.1076(3)	2.8(2)
C(50)	-0.1787(5)	0.1572(2)	-0.1342(3)	3.3(2)
C(51)	-0.1990(4)	0.1457(2)	-0.2076(3)	3.5(2)
C(52)	-0.1409(5)	0.1615(3)	-0.2525(3)	4.0(2)
C(53)	-0.0577(5)	0.1889(3)	-0.2247(3)	3.7(2)
C(54)	-0.0321(5)	0.2008(2)	-0.1521(3)	3.3(2)
C(55)	-0.2439(5)	0.1398(3)	-0.0873(3)	3.6(2)
C(56)	-0.2812(7)	0.0884(3)	-0.1010(5)	10.4(4)
C(57)	-0.3275(6)	0.1763(3)	-0.0892(4)	7.7(3)
C(58)	0.0626(5)	0.2298(3)	-0.1228(3)	4.3(2)
C(59)	0.1535(5)	0.1996(3)	-0.1306(4)	7.1(3)
C(60)	0.0623(5)	0.2814(3)	-0.1560(4)	6.5(3)
C(61)	-0.0111(4)	0.2236(2)	0.3241(3)	3.9(2)
C(62)	-0.1699(5)	0.1592(3)	0.3559(3)	6.0(2)
C(63)	-0.2147(5)	0.2348(3)	0.2360(3)	6.2(2)
C(64)	-0.2624(6)	0.0708(3)	0.2278(4)	8.9(3)
C(65)	-0.1481(4)	0.0622(2)	0.1121(3)	4.2(2)
C(66)	-0.2876(5)	0.1456(3)	0.1089(4)	8.0(3)
C(67)	0.459(1)	0.0104(7)	0.9749(9)	20.4(3)
C(68)	0.443(1)	0.0457(6)	0.9464(9)	22.9(3)
C(69)	0.3640(9)	0.0682(5)	0.8944(7)	18.4(4)
H(1)	0.3349	0.2154	0.4003	3.6985
H(2)	0.2848	0.1515	0.4798	3.1566
H(3)	0.2721	0.2383	0.2592	3.1938
H(4)	0.0790	0.0752	0.3672	3.4038
H(5)	0.3158	0.2481	0.0264	4.9444
H(6)	0.2162	0.3182	-0.0064	5.2447
H(7)	0.0847	0.3336	0.0462	4.2905
H(8)	0.2840	0.1583	0.1555	4.5876
H(9)	0.4512	0.1590	0.1662	8.2009
H(10)	0.4433	0.2078	0.1221	8.2009
H(11)	0.4182	0.2080	0.1969	8.2009
H(12)	0.2385	0.1355	0.0380	6.5094
H(13)	0.3312	0.1619	0.0227	6.5094
H(14)	0.3428	0.1150	0.0711	6.5094
H(15)	0.0031	0.2563	0.1680	3.7033
H(16)	-0.0573	0.3323	0.0701	6.1870
H(17)	-0.0915	0.2773	0.0587	6.1870
H(18)	-0.1234	0.3091	0.1173	6.1870
H(19)	0.0991	0.3142	0.2399	6.9575
H(20)	0.0622	0.3556	0.1842	6.9575
H(21)	-0.0104	0.3309	0.2250	6.9575
H(22)	0.1719	0.1659	0.6628	5.0771
H(23)	0.2987	0.1163	0.7191	5.7142
H(24)	0.3487	0.0491	0.6607	5.1926
H(25)	0.0468	0.1580	0.4822	4.3345
H(26)	-0.0323	0.1532	0.6025	8.0567
H(27)	-0.0915	0.1671	0.5271	8.0567
H(28)	-0.0501	0.1136	0.5423	8.0567
H(29)	0.0899	0.2262	0.5929	8.5734
H(30)	0.1393	0.2260	0.5278	8.5734
H(31)	0.0278	0.2381	0.5175	8.5734
H(32)	0.2489	0.0160	0.4810	5.0358
H(33)	0.1676	-0.0332	0.5467	16.4407
H(34)	0.2529	-0.0624	0.5248	16.4407

H(35)	0.2658	-0.0418	0.6016	16.4407
H(36)	0.4161	0.0023	0.5859	16.0852
H(37)	0.3994	-0.0197	0.5096	16.0852
H(38)	0.4099	0.0375	0.5210	16.0852
H(39)	0.0988	0.0266	-0.0111	4.0192
H(40)	0.0076	0.0991	-0.0784	3.7799
H(41)	0.1621	0.0073	0.1329	3.4573
H(42)	-0.0265	0.1970	0.0602	3.3889
H(43)	0.3979	-0.0186	0.3435	4.8360
H(44)	0.3051	-0.0744	0.3926	4.4520
H(45)	0.1356	-0.0678	0.3692	4.3618
H(46)	0.3033	0.0769	0.2196	5.1848
H(47)	0.4544	0.0626	0.3393	6.8280
H(48)	0.4494	0.1076	0.2880	6.8280
H(49)	0.3710	0.1018	0.3341	6.8280
H(50)	0.4507	0.0056	0.2287	8.7282
H(51)	0.3647	0.0128	0.1631	8.7282
H(52)	0.4448	0.0538	0.1834	8.7282
H(53)	-0.0083	0.0224	0.2597	3.7716
H(54)	-0.0153	0.0035	0.3751	5.4940
H(55)	-0.1071	-0.0183	0.3235	5.4940
H(56)	-0.0198	-0.0529	0.3568	5.4940
H(57)	-0.0996	-0.0439	0.2026	6.1297
H(58)	-0.0021	-0.0393	0.1760	6.1297
H(59)	-0.0127	-0.0800	0.2313	6.1297
H(60)	-0.2561	0.1262	-0.2266	4.0843
H(61)	-0.1575	0.1538	-0.3018	4.8190
H(62)	-0.0170	0.1997	-0.2554	4.4110
H(63)	-0.2053	0.1404	-0.0399	4.2721
H(64)	-0.3181	0.0801	-0.0655	12.2256
H(65)	-0.3219	0.0865	-0.1462	12.2256
H(66)	-0.2270	0.0663	-0.0963	12.2256
H(67)	-0.3013	0.2085	-0.0773	9.1590
H(68)	-0.3681	0.1766	-0.1358	9.1590
H(69)	-0.3654	0.1661	-0.0560	9.1590
H(70)	0.0661	0.2344	-0.0733	5.1737
H(71)	0.1534	0.1687	-0.1078	8.5543
H(72)	0.1532	0.1956	-0.1793	8.5543
H(73)	0.2113	0.2182	-0.1083	8.5543
H(74)	0.1216	0.2982	-0.1346	7.9739
H(75)	0.0592	0.2779	-0.2057	7.9739
H(76)	0.0073	0.2996	-0.1485	7.9739
H(77)	0.0358	0.2020	0.3511	4.7038
H(78)	0.0155	0.2397	0.2886	4.7038
H(79)	-0.0306	0.2481	0.3543	4.7038
H(80)	-0.1854	0.1852	0.3848	7.3330
H(81)	-0.2280	0.1405	0.3368	7.3330
H(82)	-0.1213	0.1381	0.3823	7.3330
H(83)	-0.2251	0.2585	0.2707	7.4810
H(84)	-0.1896	0.2515	0.2001	7.4810
H(85)	-0.2750	0.2190	0.2156	7.4810
H(86)	-0.2886	0.0944	0.2570	10.3916
H(87)	-0.3157	0.0547	0.1974	10.3916
H(88)	-0.2198	0.0490	0.2556	10.3916
H(89)	-0.2033	0.0438	0.0861	4.9608
H(90)	-0.1174	0.0794	0.0800	4.9608
H(91)	-0.1035	0.0401	0.1406	4.9608
H(92)	-0.3142	0.1694	0.1358	10.0225
H(93)	-0.2577	0.1611	0.0754	10.0225

H(94)	-0.3384	0.1236	0.0858	10.0225
H(95)	0.4143	0.0090	1.0010	23.5499
H(98)	0.4425	0.0737	0.9729	32.9255
H(99)	0.4798	0.0497	0.9102	32.9255
H(100)	0.3879	0.1038	0.8815	27.1077
H(101)	0.3439	0.0534	0.8498	27.1077
H(102)	0.3067	0.0776	0.9125	27.1077
H(103)	0.4650	-0.0111	0.9422	23.5499

Table S6. Anisotropic Displacement Parameters for 4e.

atom	U11	U22	U33	U12	U13	U23
Y	0.0303(3)	0.0290(4)	0.0280(3)	0.0015(4)	0.0064(2)	-0.0004(4)
Si(1)	0.048(1)	0.049(2)	0.046(1)	0.010(1)	0.020(1)	0.005(1)
Si(2)	0.036(1)	0.072(2)	0.052(1)	-0.002(1)	0.011(1)	-0.002(1)
N(1)	0.041(3)	0.021(4)	0.022(2)	-0.002(3)	0.010(2)	-0.001(2)
N(2)	0.036(3)	0.029(4)	0.028(3)	0.007(3)	0.008(3)	0.008(3)
N(3)	0.042(3)	0.030(4)	0.038(3)	0.005(3)	0.015(3)	0.009(3)
N(4)	0.033(3)	0.023(3)	0.029(3)	0.009(3)	0.008(2)	0.003(2)
N(5)	0.034(3)	0.025(3)	0.024(3)	-0.001(3)	0.008(2)	0.000(3)
N(6)	0.043(3)	0.045(4)	0.030(3)	0.013(3)	0.002(3)	0.001(3)
N(7)	0.035(3)	0.039(4)	0.030(3)	0.007(3)	0.006(2)	0.012(3)
C(1)	0.036(4)	0.025(4)	0.023(3)	-0.006(3)	0.000(3)	-0.006(3)
C(2)	0.041(4)	0.035(5)	0.044(4)	-0.018(4)	0.007(3)	0.003(4)
C(3)	0.034(4)	0.037(5)	0.030(3)	0.000(3)	-0.001(3)	0.006(3)
C(4)	0.033(4)	0.040(5)	0.027(3)	-0.010(4)	0.014(3)	0.004(4)
C(5)	0.034(4)	0.026(4)	0.044(4)	-0.008(3)	0.012(3)	0.003(4)
C(6)	0.045(4)	0.041(5)	0.025(4)	0.002(4)	0.010(3)	0.000(3)
C(7)	0.036(4)	0.036(5)	0.024(3)	-0.014(4)	0.003(3)	0.001(3)
C(8)	0.035(4)	0.041(5)	0.040(4)	-0.008(4)	0.013(3)	0.003(4)
C(9)	0.064(5)	0.052(6)	0.048(4)	-0.007(4)	0.028(4)	0.000(4)
C(10)	0.059(5)	0.059(6)	0.049(4)	-0.006(5)	0.015(4)	0.021(4)
C(11)	0.046(5)	0.037(5)	0.054(4)	0.003(4)	0.002(4)	0.011(4)
C(12)	0.033(4)	0.040(5)	0.040(4)	-0.005(4)	0.011(3)	0.002(4)
C(13)	0.052(5)	0.050(6)	0.050(4)	-0.004(4)	0.020(4)	0.005(4)
C(14)	0.070(6)	0.078(7)	0.098(6)	0.015(5)	-0.002(5)	-0.018(5)
C(15)	0.080(6)	0.052(6)	0.084(5)	0.003(5)	0.029(4)	-0.013(5)
C(16)	0.053(5)	0.018(4)	0.036(4)	0.007(4)	-0.010(3)	-0.001(3)
C(17)	0.057(5)	0.066(6)	0.068(5)	0.017(5)	-0.002(4)	-0.001(4)
C(18)	0.065(5)	0.092(6)	0.065(5)	-0.012(5)	0.016(4)	-0.015(5)
C(19)	0.040(4)	0.036(5)	0.028(4)	-0.007(4)	0.011(3)	0.006(3)
C(20)	0.053(4)	0.041(5)	0.039(4)	0.001(5)	0.016(3)	0.004(4)
C(21)	0.067(5)	0.057(5)	0.040(4)	-0.013(5)	0.024(4)	-0.011(5)
C(22)	0.052(5)	0.077(7)	0.046(5)	-0.014(5)	0.006(4)	0.004(5)
C(23)	0.050(5)	0.070(7)	0.044(5)	0.006(5)	-0.004(4)	0.008(4)
C(24)	0.047(5)	0.045(5)	0.035(4)	-0.007(4)	0.008(3)	0.009(4)
C(25)	0.059(5)	0.039(5)	0.044(4)	0.002(4)	0.014(4)	0.005(4)
C(26)	0.071(6)	0.075(7)	0.109(6)	0.019(5)	0.032(5)	0.037(5)
C(27)	0.140(8)	0.040(6)	0.102(7)	0.007(6)	0.047(6)	0.008(5)
C(28)	0.068(6)	0.051(6)	0.043(4)	0.020(5)	0.011(4)	0.018(4)
C(29)	0.35(2)	0.045(7)	0.150(9)	-0.009(9)	0.15(1)	-0.018(7)
C(30)	0.055(6)	0.26(1)	0.165(9)	0.063(8)	-0.004(6)	-0.100(9)
C(31)	0.036(4)	0.045(5)	0.027(4)	0.011(4)	0.013(3)	0.005(4)
C(32)	0.064(5)	0.027(5)	0.041(4)	0.005(4)	0.017(4)	0.004(4)
C(33)	0.060(5)	0.036(5)	0.027(4)	0.002(4)	0.009(3)	-0.005(4)
C(34)	0.039(4)	0.030(4)	0.032(3)	0.002(4)	0.003(3)	-0.003(4)
C(35)	0.046(4)	0.021(5)	0.047(4)	0.006(4)	0.014(4)	-0.003(4)
C(36)	0.037(4)	0.042(5)	0.029(4)	-0.004(4)	0.007(3)	-0.005(4)
C(37)	0.044(4)	0.027(5)	0.032(4)	0.006(4)	0.006(3)	-0.007(3)
C(38)	0.037(4)	0.041(5)	0.038(4)	-0.011(4)	0.005(3)	-0.006(4)
C(39)	0.051(5)	0.057(6)	0.045(4)	0.007(4)	0.001(4)	0.017(4)
C(40)	0.055(5)	0.031(5)	0.047(4)	0.016(4)	-0.007(4)	0.015(4)
C(41)	0.056(5)	0.045(5)	0.042(4)	-0.004(4)	0.012(4)	0.013(4)
C(42)	0.049(5)	0.022(4)	0.039(4)	0.001(4)	0.008(3)	0.002(3)
C(43)	0.045(5)	0.054(6)	0.062(5)	0.018(4)	0.005(4)	-0.009(4)
C(44)	0.071(6)	0.060(6)	0.084(6)	-0.007(5)	0.020(5)	0.003(5)

C(45)	0.100(7)	0.099(7)	0.092(6)	-0.017(6)	0.058(5)	-0.027(6)
C(46)	0.049(5)	0.035(5)	0.038(4)	0.001(4)	0.011(3)	0.012(4)
C(47)	0.057(5)	0.045(5)	0.069(5)	-0.009(4)	0.004(4)	-0.001(4)
C(48)	0.069(5)	0.055(6)	0.063(5)	-0.001(5)	-0.004(4)	-0.005(5)
C(49)	0.037(4)	0.030(5)	0.040(4)	0.012(4)	0.014(3)	0.008(4)
C(50)	0.036(4)	0.038(5)	0.048(4)	0.013(4)	0.007(4)	0.005(4)
C(51)	0.049(4)	0.034(5)	0.047(4)	-0.002(4)	0.001(3)	-0.015(4)
C(52)	0.057(5)	0.057(6)	0.036(4)	0.017(4)	0.003(4)	-0.012(4)
C(53)	0.062(5)	0.045(5)	0.037(4)	0.017(5)	0.017(4)	0.009(4)
C(54)	0.039(4)	0.035(5)	0.047(4)	0.005(4)	-0.003(4)	0.005(4)
C(55)	0.049(4)	0.034(5)	0.054(4)	0.001(4)	0.011(3)	0.004(4)
C(56)	0.19(1)	0.075(8)	0.168(9)	-0.079(7)	0.116(8)	-0.044(7)
C(57)	0.113(7)	0.118(9)	0.082(6)	0.038(6)	0.062(6)	0.052(6)
C(58)	0.055(5)	0.064(6)	0.048(4)	-0.002(5)	0.018(4)	0.009(4)
C(59)	0.041(5)	0.121(8)	0.100(6)	0.009(5)	-0.003(5)	0.059(6)
C(60)	0.077(6)	0.067(7)	0.097(7)	-0.025(5)	0.010(5)	0.007(5)
C(61)	0.064(5)	0.033(5)	0.054(4)	0.008(4)	0.017(4)	-0.007(4)
C(62)	0.080(6)	0.092(7)	0.064(5)	-0.009(5)	0.033(4)	0.000(5)
C(63)	0.076(6)	0.076(6)	0.083(6)	0.035(5)	0.018(5)	-0.011(5)
C(64)	0.109(7)	0.151(9)	0.098(7)	-0.069(7)	0.066(6)	-0.043(6)
C(65)	0.065(5)	0.054(5)	0.040(4)	-0.020(4)	0.007(4)	0.006(4)
C(66)	0.071(5)	0.114(8)	0.099(6)	0.034(6)	-0.029(5)	-0.029(6)

Table S7. Intramolecular Distances Involving the Nonhydrogen Atoms for 4e.

atom	atom	distance	atom	atom	distance
Y	N(1)	2.347(4)	C(1)	C(5)	1.421(7)
Y	N(2)	2.437(5)	C(2)	C(3)	1.358(7)
Y	N(4)	2.355(4)	C(3)	C(4)	1.371(7)
Y	N(5)	2.449(5)	C(4)	C(6)	1.453(7)
Y	N(7)	2.204(4)	C(7)	C(8)	1.367(7)
Si(1)	N(7)	1.723(4)	C(7)	C(12)	1.387(8)
Si(1)	C(61)	1.876(6)	C(8)	C(9)	1.425(8)
Si(1)	C(62)	1.873(6)	C(8)	C(13)	1.516(8)
Si(1)	C(63)	1.880(7)	C(9)	C(10)	1.381(8)
Si(2)	N(7)	1.735(4)	C(10)	C(11)	1.360(8)
Si(2)	C(64)	1.891(7)	C(11)	C(12)	1.397(7)
Si(2)	C(65)	1.870(6)	C(12)	C(16)	1.503(7)
Si(2)	C(66)	1.857(7)	C(13)	C(14)	1.508(8)
N(1)	C(1)	1.368(6)	C(13)	C(15)	1.516(8)
N(1)	C(4)	1.352(6)	C(16)	C(17)	1.530(7)
N(2)	C(5)	1.315(6)	C(16)	C(18)	1.533(8)
N(2)	C(7)	1.454(6)	C(19)	C(20)	1.407(8)
N(3)	C(6)	1.270(6)	C(19)	C(24)	1.376(7)
N(3)	C(19)	1.466(6)	C(20)	C(21)	1.404(7)
N(4)	C(31)	1.365(6)	C(20)	C(25)	1.510(8)
N(4)	C(34)	1.374(6)	C(21)	C(22)	1.359(8)
N(5)	C(35)	1.290(6)	C(22)	C(23)	1.359(8)
N(5)	C(37)	1.459(6)	C(23)	C(24)	1.375(8)
N(6)	C(36)	1.264(6)	C(24)	C(28)	1.521(8)
N(6)	C(49)	1.422(6)	C(25)	C(26)	1.510(8)
C(1)	C(2)	1.376(6)	C(25)	C(27)	1.515(8)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms cont.

atom	atom	distance	atom	atom	distance
C(28)	C(29)	1.49(1)	C(54)	C(58)	1.527(8)
C(28)	C(30)	1.509(9)	C(55)	C(56)	1.476(9)
C(31)	C(32)	1.394(7)	C(55)	C(57)	1.512(8)
C(31)	C(35)	1.429(7)	C(58)	C(59)	1.532(9)
C(32)	C(33)	1.384(7)	C(58)	C(60)	1.524(9)
C(33)	C(34)	1.392(7)	C(67)	C(67)	1.43(3)
C(34)	C(36)	1.456(8)	C(67)	C(68)	1.09(2)
C(37)	C(38)	1.393(7)	C(68)	C(69)	1.45(2)
C(37)	C(42)	1.395(7)			
C(38)	C(39)	1.406(8)			
C(38)	C(43)	1.528(8)			
C(39)	C(40)	1.364(8)			
C(40)	C(41)	1.366(8)			
C(41)	C(42)	1.401(7)			
C(42)	C(46)	1.503(8)			
C(43)	C(44)	1.538(9)			
C(43)	C(45)	1.523(8)			
C(46)	C(47)	1.533(7)			
C(46)	C(48)	1.537(8)			
C(49)	C(50)	1.399(7)			
C(49)	C(54)	1.401(7)			
C(50)	C(51)	1.413(7)			
C(50)	C(55)	1.483(7)			
C(51)	C(52)	1.368(8)			
C(52)	C(53)	1.376(8)			
C(53)	C(54)	1.401(7)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S8. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for 4e.

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Y	N(2)	73.2(2)	Y	N(2)	C(7)	132.9(4)
N(1)	Y	N(4)	141.0(1)	C(5)	N(2)	C(7)	116.1(5)
N(1)	Y	N(5)	87.0(1)	C(6)	N(3)	C(19)	122.3(5)
N(1)	Y	N(7)	110.1(1)	Y	N(4)	C(31)	113.7(4)
N(2)	Y	N(4)	87.4(1)	Y	N(4)	C(34)	141.3(4)
N(2)	Y	N(5)	116.5(1)	C(31)	N(4)	C(34)	104.2(5)
N(2)	Y	N(7)	121.4(2)	Y	N(5)	C(35)	112.0(4)
N(4)	Y	N(5)	71.6(1)	Y	N(5)	C(37)	131.0(3)
N(4)	Y	N(7)	108.9(1)	C(35)	N(5)	C(37)	116.7(5)
N(5)	Y	N(7)	122.2(2)	C(36)	N(6)	C(49)	122.1(5)
N(7)	Si(1)	C(61)	113.3(2)	Y	N(7)	Si(1)	118.3(2)
N(7)	Si(1)	C(62)	113.4(3)	Y	N(7)	Si(2)	121.6(2)
N(7)	Si(1)	C(63)	112.1(3)	Si(1)	N(7)	Si(2)	120.1(2)
C(61)	Si(1)	C(62)	104.5(3)	N(1)	C(1)	C(2)	110.2(5)
C(61)	Si(1)	C(63)	105.1(3)	N(1)	C(1)	C(5)	121.4(5)
C(62)	Si(1)	C(63)	107.8(3)	C(2)	C(1)	C(5)	128.4(6)
N(7)	Si(2)	C(64)	112.5(3)	C(1)	C(2)	C(3)	107.5(5)
N(7)	Si(2)	C(65)	112.0(3)	C(2)	C(3)	C(4)	106.1(5)
N(7)	Si(2)	C(66)	114.3(3)	N(1)	C(4)	C(3)	111.8(5)
C(64)	Si(2)	C(65)	106.1(3)	N(1)	C(4)	C(6)	117.8(5)
C(64)	Si(2)	C(66)	106.6(4)	C(3)	C(4)	C(6)	130.4(5)
C(65)	Si(2)	C(66)	104.7(3)	N(2)	C(5)	C(1)	123.0(5)
Y	N(1)	C(1)	112.1(3)	N(3)	C(6)	C(4)	133.5(5)
Y	N(1)	C(4)	142.8(4)	N(2)	C(7)	C(8)	118.0(6)
C(1)	N(1)	C(4)	104.5(5)	N(2)	C(7)	C(12)	119.2(6)
Y	N(2)	C(5)	110.2(4)	C(8)	C(7)	C(12)	122.8(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont.

atom	atom	atom	angle	atom	atom	atom	angle
C(7)	C(8)	C(9)	117.6(6)	C(23)	C(24)	C(28)	121.7(6)
C(7)	C(8)	C(13)	124.3(6)	C(20)	C(25)	C(26)	110.5(6)
C(9)	C(8)	C(13)	118.1(6)	C(20)	C(25)	C(27)	112.7(6)
C(8)	C(9)	C(10)	119.9(6)	C(26)	C(25)	C(27)	114.0(6)
C(9)	C(10)	C(11)	120.6(6)	C(24)	C(28)	C(29)	111.6(6)
C(10)	C(11)	C(12)	121.0(6)	C(24)	C(28)	C(30)	113.3(7)
C(7)	C(12)	C(11)	117.9(6)	C(29)	C(28)	C(30)	110.3(8)
C(7)	C(12)	C(16)	123.2(6)	N(4)	C(31)	C(32)	112.3(5)
C(11)	C(12)	C(16)	118.9(6)	N(4)	C(31)	C(35)	120.1(5)
C(8)	C(13)	C(14)	112.5(6)	C(32)	C(31)	C(35)	127.5(6)
C(8)	C(13)	C(15)	112.5(6)	C(31)	C(32)	C(33)	105.4(5)
C(14)	C(13)	C(15)	110.1(6)	C(32)	C(33)	C(34)	106.9(5)
C(12)	C(16)	C(17)	114.4(5)	N(4)	C(34)	C(33)	111.1(6)
C(12)	C(16)	C(18)	110.5(5)	N(4)	C(34)	C(36)	116.1(5)
C(17)	C(16)	C(18)	108.3(5)	C(33)	C(34)	C(36)	132.5(5)
N(3)	C(19)	C(20)	118.1(6)	N(5)	C(35)	C(31)	122.5(6)
N(3)	C(19)	C(24)	117.7(6)	N(6)	C(36)	C(34)	132.4(5)
C(20)	C(19)	C(24)	123.5(6)	N(5)	C(37)	C(38)	118.4(6)
C(19)	C(20)	C(21)	114.7(6)	N(5)	C(37)	C(42)	119.0(6)
C(19)	C(20)	C(25)	124.4(6)	C(38)	C(37)	C(42)	122.6(6)
C(21)	C(20)	C(25)	120.8(7)	C(37)	C(38)	C(39)	117.7(6)
C(20)	C(21)	C(22)	122.6(7)	C(37)	C(38)	C(43)	123.7(6)
C(21)	C(22)	C(23)	119.8(7)	C(39)	C(38)	C(43)	118.5(6)
C(22)	C(23)	C(24)	121.7(7)	C(38)	C(39)	C(40)	120.6(6)
C(19)	C(24)	C(23)	117.6(7)	C(39)	C(40)	C(41)	120.2(6)
C(19)	C(24)	C(28)	120.7(6)	C(40)	C(41)	C(42)	122.3(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont.

atom	atom	atom	angle	atom	atom	atom	angle
C(37)	C(42)	C(41)	116.3(6)	C(59)	C(58)	C(60)	111.5(6)
C(37)	C(42)	C(46)	121.9(6)	C(67)	C(67)	C(68)	137(3)
C(41)	C(42)	C(46)	121.7(6)	C(67)	C(68)	C(69)	139(2)
C(38)	C(43)	C(44)	110.9(5)				
C(38)	C(43)	C(45)	112.8(6)				
C(44)	C(43)	C(45)	110.8(6)				
C(42)	C(46)	C(47)	113.8(5)				
C(42)	C(46)	C(48)	110.2(5)				
C(47)	C(46)	C(48)	110.0(6)				
N(6)	C(49)	C(50)	119.0(6)				
N(6)	C(49)	C(54)	119.7(6)				
C(50)	C(49)	C(54)	120.9(6)				
C(49)	C(50)	C(51)	117.1(6)				
C(49)	C(50)	C(55)	121.5(6)				
C(51)	C(50)	C(55)	121.5(6)				
C(50)	C(51)	C(52)	123.0(6)				
C(51)	C(52)	C(53)	118.6(6)				
C(52)	C(53)	C(54)	121.4(6)				
C(49)	C(54)	C(53)	119.0(6)				
C(49)	C(54)	C(58)	121.1(6)				
C(53)	C(54)	C(58)	119.9(6)				
C(50)	C(55)	C(56)	114.9(6)				
C(50)	C(55)	C(57)	110.3(6)				
C(56)	C(55)	C(57)	111.3(7)				
C(54)	C(58)	C(59)	111.0(6)				
C(54)	C(58)	C(60)	112.4(6)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

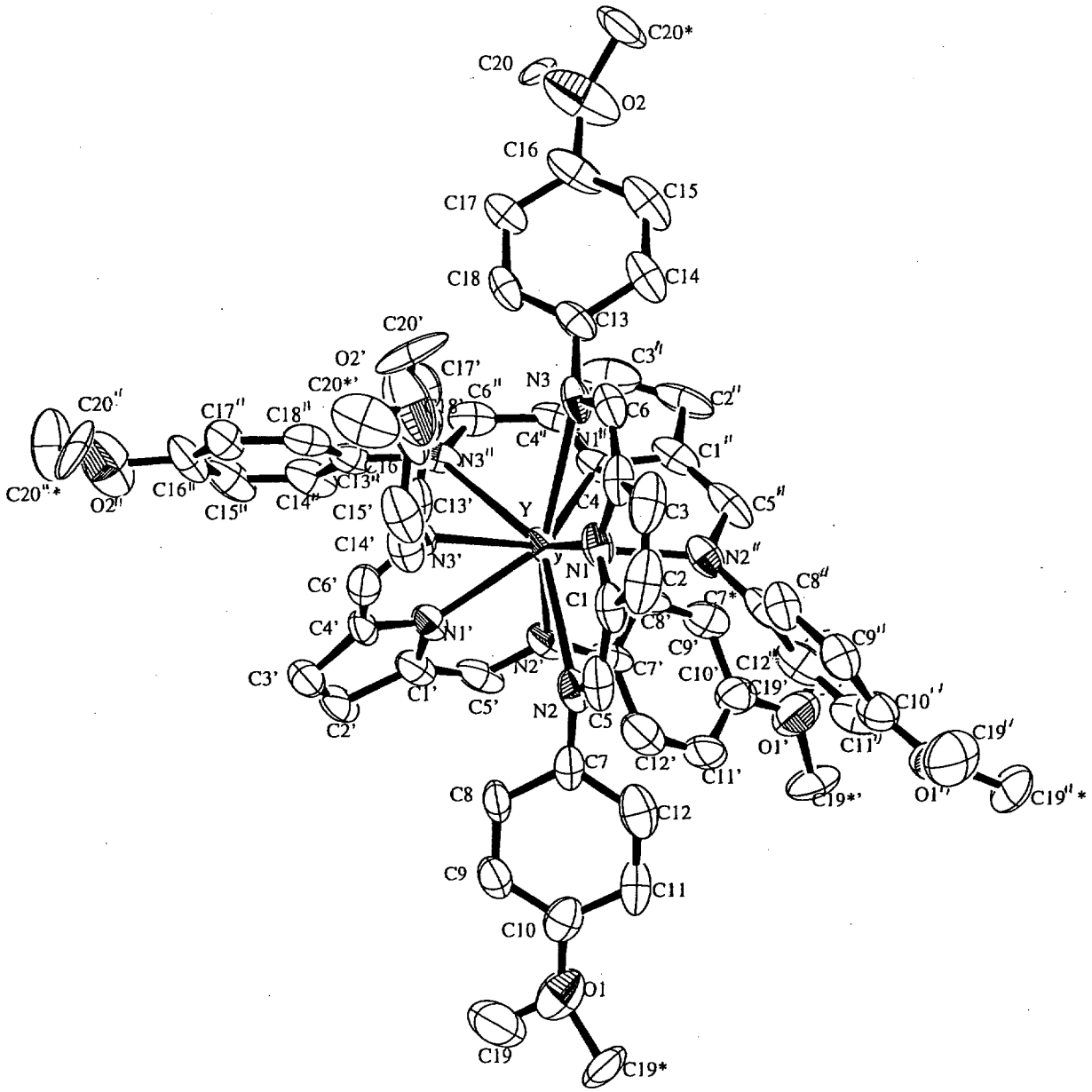

Figure S3. Molecular Structure of $Y(An_2\text{-}pyr)_3$ (**5a**) with a labeling scheme. Hydrogen atoms are omitted for clarity.

Table S9. Positional Parameters and B(eq) for 5a.

atom	x	y	z	B(eq)
Y	0.13988(1)	0.1399	0.1399	4.697(2)
O(1)	-0.0562(2)	-0.0567(1)	0.1446(1)	9.4(1)
O(2)	0.2807(2)	0.3698(2)	0.0814(2)	14.3(2)
N(1)	0.20512(9)	0.08673(10)	0.13055(8)	5.24(7)
N(2)	0.1192(1)	0.04303(8)	0.14136(9)	5.51(7)
N(3)	0.22906(8)	0.1817(1)	0.12397(8)	5.25(7)
C(1)	0.2046(1)	0.0382(1)	0.1341(1)	6.0(1)
C(2)	0.2518(2)	0.0194(1)	0.1269(1)	8.2(1)
C(3)	0.2809(1)	0.0574(2)	0.1195(1)	8.6(1)
C(4)	0.2518(1)	0.0992(1)	0.12189(10)	5.63(9)
C(5)	0.1582(2)	0.01683(10)	0.1395(1)	6.66(9)
C(6)	0.2615(1)	0.1495(1)	0.11609(10)	6.06(10)
C(7)	0.0744(1)	0.0182(1)	0.1429(1)	5.45(9)
C(8)	0.0438(1)	0.0204(1)	0.1828(1)	6.23(9)
C(9)	0.0002(1)	-0.0050(1)	0.1829(1)	6.38(9)
C(10)	-0.0133(2)	-0.0322(1)	0.1439(2)	6.5(1)
C(11)	0.0160(2)	-0.0346(1)	0.1040(1)	7.7(1)
C(12)	0.0594(2)	-0.0096(2)	0.1036(1)	7.6(1)
C(13)	0.24230(10)	0.2314(1)	0.1134(1)	5.41(9)
C(14)	0.2636(1)	0.2431(1)	0.0695(1)	7.0(1)
C(15)	0.2765(1)	0.2893(2)	0.0599(1)	8.4(1)
C(16)	0.2688(1)	0.3242(2)	0.0946(2)	7.9(1)
C(17)	0.2472(1)	0.3139(1)	0.1377(1)	5.99(8)
C(18)	0.23414(10)	0.2671(1)	0.1469(1)	5.50(9)
C(19)	-0.0827(3)	-0.0545(3)	0.1799(3)	12.8(3)
C(19*)	-0.0707(3)	-0.1050(3)	0.1267(3)	8.6(3)
C(20)	0.2779(5)	0.3944(4)	0.1024(3)	10.8(3)
C(20*)	0.3183(3)	0.3905(2)	0.0571(2)	11.0(3)
H(1)	0.2606	-0.0140	0.1274	9.6410
H(2)	0.3148	0.0564	0.1137	9.9748
H(3)	0.1558	-0.0171	0.1418	8.1698
H(4)	0.2933	0.1593	0.1063	7.2239
H(5)	0.0523	0.0389	0.2101	7.3168
H(6)	-0.0203	-0.0033	0.2106	7.6438
H(7)	0.0066	-0.0533	0.0768	9.0775
H(8)	0.0797	-0.0107	0.0760	9.0190
H(9)	0.2690	0.2189	0.0455	8.4967
H(10)	0.2911	0.2974	0.0296	9.9856
H(11)	0.2424	0.3387	0.1610	7.2394
H(12)	0.2191	0.2588	0.1769	6.6311
H(13)	-0.0769	-0.0244	0.1938	19.8850
H(14)	-0.1129	-0.0583	0.1672	19.8850
H(15)	-0.0721	-0.0801	0.1991	19.8850
H(16)	-0.1044	-0.1049	0.1189	23.4242
H(17)	-0.0529	-0.1151	0.0989	23.4242
H(18)	-0.0657	-0.1287	0.1518	23.4242
H(19)	0.3022	0.4047	0.1215	14.6759
H(20)	0.2657	0.4240	0.0835	14.6759
H(21)	0.2484	0.3890	0.1239	14.6759
H(22)	0.3440	0.3989	0.0790	18.1063
H(23)	0.3302	0.3671	0.0348	18.1063
H(24)	0.3077	0.4182	0.0407	18.1063

Table S10. Anisotropic Displacement Parameters for 5a.

atom	U11	U22	U33	U12	U13	U23
Y	0.0595(1)	0.0595	0.0595	0.0192(2)	0.0192	0.0192
O(1)	0.132(3)	0.114(2)	0.110(3)	0.004(2)	-0.040(3)	-0.019(2)
O(2)	0.110(3)	0.168(5)	0.267(6)	0.024(3)	0.068(4)	0.106(5)
N(1)	0.072(2)	0.083(2)	0.045(2)	0.032(2)	0.005(1)	0.010(2)
N(2)	0.093(2)	0.065(2)	0.051(1)	0.022(2)	0.016(2)	0.012(2)
N(3)	0.048(2)	0.109(2)	0.043(2)	0.029(2)	0.009(1)	0.006(2)
C(1)	0.095(3)	0.088(3)	0.046(2)	0.045(3)	0.005(2)	0.008(2)
C(2)	0.121(3)	0.118(3)	0.071(3)	0.091(3)	-0.029(3)	-0.019(3)
C(3)	0.088(3)	0.160(4)	0.078(3)	0.062(3)	-0.016(2)	-0.038(3)
C(4)	0.063(2)	0.105(3)	0.046(2)	0.045(3)	-0.009(2)	-0.004(2)
C(5)	0.137(3)	0.071(2)	0.045(2)	0.060(2)	0.012(3)	0.010(2)
C(6)	0.055(2)	0.126(3)	0.050(2)	0.007(2)	0.005(2)	0.007(2)
C(7)	0.116(3)	0.047(2)	0.045(2)	0.033(2)	0.007(3)	0.004(2)
C(8)	0.135(3)	0.060(2)	0.042(2)	0.007(2)	0.027(2)	-0.001(2)
C(9)	0.106(3)	0.078(2)	0.059(2)	0.009(2)	0.021(2)	0.009(2)
C(10)	0.099(3)	0.072(3)	0.076(3)	0.017(2)	-0.014(3)	-0.008(2)
C(11)	0.109(3)	0.138(4)	0.046(2)	0.041(3)	-0.002(3)	-0.018(2)
C(12)	0.105(3)	0.114(3)	0.071(3)	0.046(3)	0.013(3)	0.012(3)
C(13)	0.035(2)	0.104(3)	0.067(2)	0.004(2)	0.004(2)	0.034(2)
C(14)	0.066(2)	0.137(3)	0.064(2)	0.026(2)	0.018(2)	0.035(2)
C(15)	0.082(3)	0.142(4)	0.094(3)	0.038(3)	0.034(2)	0.064(3)
C(16)	0.061(2)	0.096(4)	0.143(4)	0.029(2)	0.035(3)	0.074(3)
C(17)	0.056(2)	0.091(2)	0.080(2)	0.004(2)	0.019(2)	0.027(2)
C(18)	0.042(2)	0.118(3)	0.049(2)	0.011(2)	0.008(2)	0.020(2)
C(19)	0.147(7)	0.199(7)	0.139(7)	-0.059(6)	0.017(5)	0.038(6)
C(19*)	0.149(7)	0.073(6)	0.104(7)	-0.026(5)	-0.024(5)	-0.041(5)
C(20)	0.23(1)	0.126(8)	0.055(4)	-0.139(8)	-0.009(5)	-0.018(4)
C(20*)	0.173(9)	0.106(6)	0.138(7)	-0.035(5)	0.099(6)	0.027(5)

Table S11. Intramolecular Distances Involving the Nonhydrogen Atoms for 5a.

atom	atom	distance	atom	atom	distance
Y	N(1)	2.340(2)	N(3)	C(13)	1.449(3)
Y	N(1)'	2.340(2)	C(1)	C(2)	1.417(4)
Y	N(1)"	2.340(2)	C(1)	C(5)	1.418(4)
Y	N(2)	2.737(2)	C(2)	C(3)	1.341(4)
Y	N(2)'	2.737(2)	C(3)	C(4)	1.410(4)
Y	N(2)"	2.737(2)	C(4)	C(6)	1.424(4)
Y	N(3)	2.758(3)	C(7)	C(8)	1.391(4)
Y	N(3)'	2.758(3)	C(7)	C(12)	1.393(4)
Y	N(3)"	2.758(3)	C(8)	C(9)	1.394(4)
O(1)	C(10)	1.365(4)	C(9)	C(10)	1.365(4)
O(1)	C(19)	1.221(6)	C(10)	C(11)	1.370(4)
O(1)	C(19*)	1.481(7)	C(11)	C(12)	1.384(4)
O(2)	C(16)	1.353(5)	C(13)	C(14)	1.388(4)
O(2)	C(20)	0.897(8)	C(13)	C(18)	1.372(3)
O(2)	C(20*)	1.364(7)	C(14)	C(15)	1.353(4)
N(1)	C(1)	1.346(3)	C(15)	C(16)	1.375(5)
N(1)	C(4)	1.357(4)	C(16)	C(17)	1.362(4)
N(2)	C(5)	1.299(3)	C(17)	C(18)	1.369(4)
N(2)	C(7)	1.419(3)	C(20)	C(20*)	1.68(1)
N(3)	C(6)	1.283(3)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S12. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for 5a.

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Y	N(1)'	119.965(4)	N(2)'	Y	N(2)"	79.27(9)
N(1)	Y	N(1)"	119.965(4)	N(2)'	Y	N(3)	85.30(7)
N(1)	Y	N(2)	63.15(8)	N(2)'	Y	N(3)'	126.78(8)
N(1)	Y	N(2)'	75.51(8)	N(2)'	Y	N(3)"	146.56(7)
N(1)	Y	N(2)"	137.72(9)	N(2)"	Y	N(3)	146.56(7)
N(1)	Y	N(3)	63.71(8)	N(2)"	Y	N(3)'	85.30(7)
N(1)	Y	N(3)'	136.91(8)	N(2)"	Y	N(3)'	126.78(8)
N(1)	Y	N(3)"	71.05(8)	N(3)	Y	N(3)'	80.49(7)
N(1)'	Y	N(1)"	119.965(4)	N(3)	Y	N(3)"	80.49(7)
N(1)'	Y	N(2)	137.72(9)	N(3)'	Y	N(3)"	80.49(7)
N(1)'	Y	N(2)'	63.15(8)	C(10)	O(1)	C(19)	120.5(5)
N(1)'	Y	N(2)"	75.51(8)	C(10)	O(1)	C(19*)	132.8(5)
N(1)'	Y	N(3)	71.05(8)	C(19)	O(1)	C(19*)	98.5(6)
N(1)'	Y	N(3)'	63.71(8)	C(16)	O(2)	C(20)	121(1)
N(1)'	Y	N(3)"	136.91(8)	C(16)	O(2)	C(20*)	135.2(5)
N(1)"	Y	N(2)	75.51(8)	C(20)	O(2)	C(20*)	94(1)
N(1)"	Y	N(2)'	137.72(9)	Y	N(1)	C(1)	127.6(2)
N(1)"	Y	N(2)"	63.15(8)	Y	N(1)	C(4)	126.3(2)
N(1)"	Y	N(3)	136.91(8)	C(1)	N(1)	C(4)	106.1(3)
N(1)"	Y	N(3)'	71.05(8)	Y	N(2)	C(5)	111.8(2)
N(1)"	Y	N(3)"	63.71(8)	Y	N(2)	C(7)	131.0(2)
N(2)	Y	N(2)'	79.27(9)	C(5)	N(2)	C(7)	117.2(3)
N(2)	Y	N(2)"	79.27(9)	Y	N(3)	C(6)	111.2(2)
N(2)	Y	N(3)	126.78(8)	Y	N(3)	C(13)	130.9(2)
N(2)	Y	N(3)'	146.56(7)	C(6)	N(3)	C(13)	116.5(3)
N(2)	Y	N(3)"	85.30(7)	N(1)	C(1)	C(2)	110.2(3)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont.

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	C(5)	115.6(3)	C(15)	C(16)	C(17)	122.2(4)
C(2)	C(1)	C(5)	133.9(4)	C(16)	C(17)	C(18)	118.3(3)
C(1)	C(2)	C(3)	106.7(3)	C(13)	C(18)	C(17)	120.8(3)
C(2)	C(3)	C(4)	107.0(3)	O(2)	C(20)	C(20*)	54.1(8)
N(1)	C(4)	C(3)	110.0(3)	O(2)	C(20*)	C(20)	32.2(3)
N(1)	C(4)	C(6)	116.6(3)				
C(3)	C(4)	C(6)	133.3(4)				
N(2)	C(5)	C(1)	121.4(3)				
N(3)	C(6)	C(4)	121.7(3)				
N(2)	C(7)	C(8)	122.2(4)				
N(2)	C(7)	C(12)	120.2(3)				
C(8)	C(7)	C(12)	117.6(3)				
C(7)	C(8)	C(9)	120.2(3)				
C(8)	C(9)	C(10)	120.8(3)				
O(1)	C(10)	C(9)	120.0(4)				
O(1)	C(10)	C(11)	120.0(4)				
C(9)	C(10)	C(11)	120.0(4)				
C(10)	C(11)	C(12)	119.7(4)				
C(7)	C(12)	C(11)	121.7(4)				
N(3)	C(13)	C(14)	120.2(4)				
N(3)	C(13)	C(18)	120.3(3)				
C(14)	C(13)	C(18)	119.5(3)				
C(13)	C(14)	C(15)	120.2(4)				
C(14)	C(15)	C(16)	119.0(4)				
O(2)	C(16)	C(15)	115.3(5)				
O(2)	C(16)	C(17)	122.3(5)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

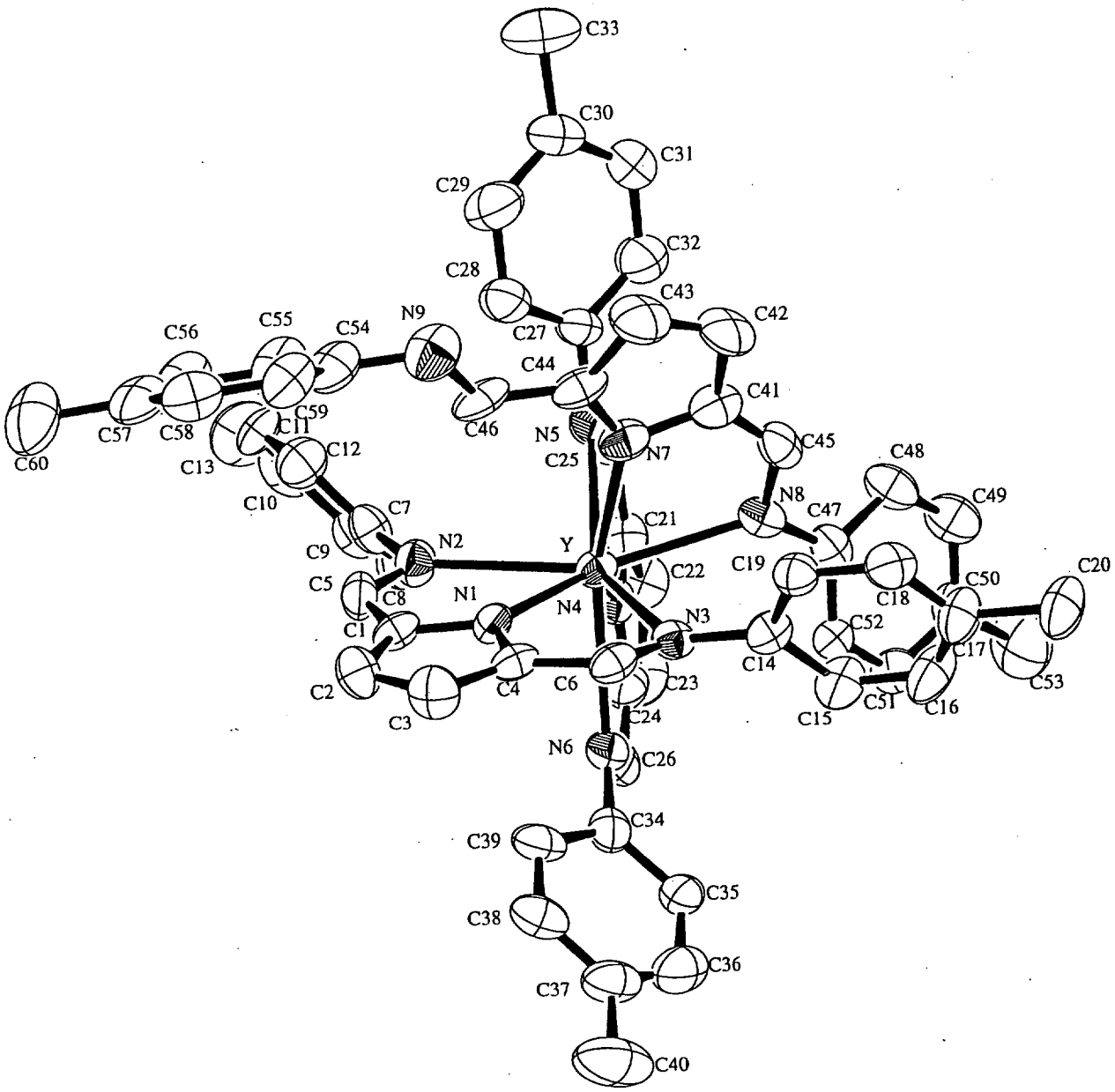

Figure S4. Molecular Structure of Y(*p*-Tol$_2$-pyr)$_3$ (**5b**) with a labeling scheme. Hydrogen atoms are omitted for clarity.

Table S13. Positional Parameters and B(eq) for 5b.

atom	x	y	z	B(eq)
Y	-0.24315(5)	-0.27188(5)	-0.21711(5)	2.64(2)
N(1)	-0.3589(4)	-0.2112(4)	-0.0891(4)	2.9(1)
N(2)	-0.3314(4)	-0.3749(4)	-0.1903(4)	3.4(2)
N(3)	-0.2618(4)	-0.1154(4)	-0.1084(4)	2.8(1)
N(4)	-0.1096(4)	-0.4168(4)	-0.2596(4)	3.0(1)
N(5)	-0.2398(4)	-0.3557(4)	-0.3984(4)	3.1(1)
N(6)	-0.1177(4)	-0.3431(4)	-0.0725(4)	3.2(1)
N(7)	-0.3554(4)	-0.1446(4)	-0.2994(4)	3.6(1)
N(8)	-0.1510(4)	-0.2216(4)	-0.3191(4)	3.2(1)
N(9)	-0.6147(5)	-0.0619(4)	-0.2633(5)	5.0(2)
C(1)	-0.4118(5)	-0.2517(5)	-0.0575(5)	2.8(2)
C(2)	-0.4698(5)	-0.1972(5)	0.0254(5)	3.9(2)
C(3)	-0.4505(5)	-0.1208(5)	0.0468(5)	4.4(2)
C(4)	-0.3825(5)	-0.1313(5)	-0.0235(5)	3.0(2)
C(5)	-0.3954(5)	-0.3380(5)	-0.1162(5)	3.5(2)
C(6)	-0.3328(5)	-0.0786(5)	-0.0420(5)	3.2(2)
C(7)	-0.3215(5)	-0.4618(5)	-0.2442(5)	3.4(2)
C(8)	-0.2287(5)	-0.5387(5)	-0.2555(5)	3.6(2)
C(9)	-0.2151(5)	-0.6253(5)	-0.3079(5)	3.7(2)
C(10)	-0.2925(7)	-0.6342(6)	-0.3481(5)	5.1(2)
C(11)	-0.3862(6)	-0.5568(7)	-0.3371(6)	4.9(3)
C(12)	-0.3998(6)	-0.4695(6)	-0.2845(5)	4.6(2)
C(13)	-0.2768(7)	-0.7275(6)	-0.4061(6)	6.9(3)
C(14)	-0.2224(5)	-0.0551(5)	-0.1307(5)	3.0(2)
C(15)	-0.1239(5)	-0.0818(5)	-0.1238(5)	3.9(2)
C(16)	-0.0872(6)	-0.0256(6)	-0.1469(6)	5.0(2)
C(17)	-0.1450(6)	0.0610(5)	-0.1775(6)	4.2(2)
C(18)	-0.2427(6)	0.0875(5)	-0.1845(5)	4.1(2)
C(19)	-0.2815(5)	0.0312(5)	-0.1607(5)	3.3(2)
C(20)	-0.1045(6)	0.1247(6)	-0.2007(6)	5.4(2)
C(21)	-0.0858(5)	-0.4683(5)	-0.3513(5)	3.2(2)
C(22)	0.0014(5)	-0.5492(5)	-0.3513(5)	3.8(2)
C(23)	0.0363(5)	-0.5488(5)	-0.2580(6)	4.1(2)
C(24)	-0.0339(5)	-0.4661(5)	-0.2023(5)	3.3(2)
C(25)	-0.1591(5)	-0.4318(5)	-0.4236(5)	3.3(2)
C(26)	-0.0427(5)	-0.4229(6)	-0.1024(6)	3.8(2)
C(27)	-0.3077(5)	-0.3229(5)	-0.4729(5)	3.3(2)
C(28)	-0.4044(6)	-0.2920(6)	-0.4521(5)	4.5(2)
C(29)	-0.4714(6)	-0.2582(6)	-0.5240(6)	5.3(2)
C(30)	-0.4453(6)	-0.2532(5)	-0.6177(5)	4.3(2)
C(31)	-0.3472(6)	-0.2825(6)	-0.6362(6)	5.1(2)
C(32)	-0.2800(5)	-0.3177(6)	-0.5651(6)	4.9(2)
C(33)	-0.5186(7)	-0.2185(7)	-0.6940(6)	7.3(3)
C(34)	-0.1168(5)	-0.3018(5)	0.0244(5)	3.5(2)
C(35)	-0.0371(6)	-0.2921(6)	0.0619(6)	4.4(2)
C(36)	-0.0432(7)	-0.2482(6)	0.1585(7)	5.8(3)
C(37)	-0.1251(8)	-0.2121(6)	0.2173(6)	5.1(3)
C(38)	-0.2060(6)	-0.2201(5)	0.1806(5)	4.5(2)
C(39)	-0.2012(6)	-0.2648(5)	0.0858(5)	4.0(2)
C(40)	-0.1322(8)	-0.1599(7)	0.3213(6)	8.4(3)
C(41)	-0.3102(6)	-0.1119(5)	-0.3586(5)	3.8(2)
C(42)	-0.3799(6)	-0.0374(5)	-0.4027(6)	4.9(2)
C(43)	-0.4709(7)	-0.0229(6)	-0.3698(6)	5.4(2)
C(44)	-0.4524(5)	-0.0901(5)	-0.3068(5)	3.8(2)

C(45)	-0.2095(6)	-0.1537(5)	-0.3673(5)	3.6(2)
C(46)	-0.5223(5)	-0.1093(5)	-0.2601(5)	4.1(2)
C(47)	-0.0472(5)	-0.2679(5)	-0.3402(5)	3.1(2)
C(48)	-0.0064(5)	-0.2817(5)	-0.4336(5)	3.8(2)
C(49)	0.0931(6)	-0.3291(6)	-0.4505(5)	4.7(2)
C(50)	0.1571(6)	-0.3686(6)	-0.3774(6)	4.5(2)
C(51)	0.1155(5)	-0.3562(5)	-0.2853(5)	4.1(2)
C(52)	0.0153(5)	-0.3069(5)	-0.2677(5)	3.0(2)
C(53)	0.2657(6)	-0.4249(7)	-0.3989(6)	6.8(3)
C(54)	-0.6733(6)	-0.0956(6)	-0.2206(6)	4.5(2)
C(55)	-0.6526(6)	-0.1891(6)	-0.2388(7)	5.6(2)
C(56)	-0.7088(7)	-0.2212(6)	-0.1958(8)	6.2(3)
C(57)	-0.7866(6)	-0.1598(6)	-0.1331(7)	5.0(2)
C(58)	-0.8077(6)	-0.0658(6)	-0.1170(6)	5.0(2)
C(59)	-0.7512(6)	-0.0350(5)	-0.1609(6)	4.3(2)
C(60)	-0.8472(6)	-0.1945(7)	-0.0844(8)	7.7(3)
C(61)	-0.6532(7)	-0.4143(7)	-0.0093(7)	5.9(3)
C(62)	-0.6077(7)	-0.4642(7)	-0.0991(8)	6.5(3)
C(63)	-0.6362(9)	-0.5276(8)	-0.1524(7)	7.9(3)
C(64)	-0.7083(9)	-0.5395(8)	-0.114(1)	8.4(4)
C(65)	-0.7553(8)	-0.4892(9)	-0.024(1)	8.5(4)
C(66)	-0.7261(8)	-0.4284(7)	0.0243(8)	6.9(3)
C(67)	-0.6242(7)	-0.3480(7)	0.0454(8)	9.0(3)
C(68)	-0.0262	0.0496	0.4276	13.7279
C(69)	0.0562	0.0166	0.4587	11.2507
C(70)	0.1300	-0.0300	0.5065	22.2384
C(71)	-0.1070	0.0831	0.3931	16.3500
H(1)	-0.5153	-0.2089	0.0618	4.8645
H(2)	-0.4809	-0.0670	0.1000	5.5846
H(3)	-0.4298	-0.3716	-0.1018	3.8034
H(4)	-0.3518	-0.0139	-0.0044	3.8910
H(5)	-0.1733	-0.5300	-0.2278	4.4082
H(6)	-0.1480	-0.6823	-0.3142	4.6340
H(7)	-0.4415	-0.5635	-0.3649	5.1985
H(8)	-0.4674	-0.4145	-0.2762	5.3525
H(9)	-0.3345	-0.7270	-0.4323	8.1973
H(10)	-0.2492	-0.7785	-0.3653	8.1973
H(11)	-0.2292	-0.7485	-0.4613	8.1973
H(12)	-0.0816	-0.1422	-0.1019	4.6340
H(13)	-0.0166	-0.0461	-0.1436	5.8578
H(14)	-0.2843	0.1459	-0.2089	4.8503
H(15)	-0.3510	0.0505	-0.1668	3.9092
H(16)	-0.0353	0.0990	-0.1900	6.2644
H(17)	-0.1352	0.1856	-0.1587	6.2644
H(18)	-0.1146	0.1367	-0.2671	6.2644
H(19)	0.0304	-0.5991	-0.4096	4.5834
H(20)	0.0979	-0.5976	-0.2367	5.2870
H(21)	-0.1488	-0.4647	-0.4908	4.5140
H(22)	0.0093	-0.4554	-0.0595	4.9182
H(23)	-0.4252	-0.2928	-0.3859	5.4441
H(24)	-0.5426	-0.2313	-0.5047	6.7548
H(25)	-0.3261	-0.2786	-0.7017	6.5282
H(26)	-0.2107	-0.3361	-0.5821	6.5589
H(27)	-0.4915	-0.2166	-0.7546	8.4784
H(28)	-0.5686	-0.1513	-0.6719	8.4784
H(29)	-0.5544	-0.2524	-0.7056	8.4784
H(30)	0.0257	-0.3133	0.0218	6.6734
H(31)	0.0154	-0.2436	0.1913	6.7698
H(32)	-0.2630	-0.1922	0.2252	5.7654

H(33)	-0.2590	-0.2657	0.0618	5.1669
H(34)	-0.0778	-0.1537	0.3450	9.8759
H(35)	-0.1523	-0.1865	0.3724	9.8759
H(36)	-0.1881	-0.0927	0.3299	9.8759
H(37)	-0.3685	0.0009	-0.4485	6.1081
H(38)	-0.5357	0.0264	-0.3878	7.0887
H(39)	-0.1811	-0.1309	-0.4154	4.3624
H(40)	-0.4966	-0.1603	-0.2190	5.0896
H(41)	-0.5975	-0.2320	-0.2807	7.5467
H(42)	-0.6987	-0.2863	-0.2120	7.6178
H(43)	-0.8642	-0.0198	-0.0721	6.1515
H(44)	-0.7678	0.0334	-0.1459	5.5649
H(45)	-0.9002	-0.1481	-0.0400	9.0137
H(46)	-0.8080	-0.2450	-0.0444	9.0137
H(47)	-0.8776	-0.2239	-0.1316	9.0137
H(48)	-0.0492	-0.2601	-0.4888	4.6482
H(49)	0.1226	-0.3347	-0.5149	5.4780
H(50)	0.1565	-0.3832	-0.2316	4.7824
H(51)	-0.0099	-0.3008	-0.2021	3.5602
H(52)	0.2822	-0.4768	-0.4457	7.8175
H(53)	0.2995	-0.4447	-0.3383	7.8175
H(54)	0.2915	-0.3850	-0.4205	7.8175
H(55)	-0.5585	-0.4575	-0.1348	7.2419
H(56)	-0.6029	-0.5670	-0.2154	9.6312
H(57)	-0.7326	-0.5833	-0.1465	11.7180
H(58)	-0.8066	-0.4940	0.0125	11.6801
H(59)	-0.7604	-0.3839	0.0922	11.0705
H(60)	-0.5738	-0.3413	0.0197	9.3817
H(61)	-0.6060	-0.3618	0.1157	9.3817
H(62)	-0.6807	-0.2822	0.0608	9.3817
H(63)	-0.1253	0.1506	0.3935	16.7572
H(64)	-0.0974	0.0575	0.3233	16.7572
H(65)	-0.1554	0.0778	0.4216	16.7572
H(66)	0.0934	0.0359	0.4161	12.4951
H(67)	0.1516	0.0034	0.5568	25.0467

Table S14. Anisotropic Displacement Parameters for 5b.

atom	U11	U22	U33	U12	U13	U23
Y	0.0308(4)	0.0298(4)	0.0368(4)	-0.0115(3)	-0.0046(3)	0.0058(3)
N(1)	0.035(3)	0.042(4)	0.041(3)	-0.023(3)	-0.008(3)	0.008(3)
N(2)	0.047(4)	0.044(4)	0.045(4)	-0.028(3)	0.002(3)	0.002(3)
N(3)	0.039(4)	0.029(3)	0.037(3)	-0.015(3)	-0.006(3)	0.008(3)
N(4)	0.030(3)	0.036(4)	0.049(4)	-0.016(3)	-0.001(3)	0.012(3)
N(5)	0.041(4)	0.036(4)	0.041(3)	-0.016(3)	-0.002(3)	0.007(3)
N(6)	0.040(4)	0.043(4)	0.038(4)	-0.019(3)	-0.006(3)	0.014(3)
N(7)	0.048(4)	0.041(4)	0.043(4)	-0.019(3)	-0.010(3)	0.000(3)
N(8)	0.046(4)	0.034(4)	0.034(3)	-0.014(3)	0.000(3)	0.004(3)
N(9)	0.044(4)	0.049(4)	0.086(5)	-0.013(4)	-0.010(4)	0.013(4)
C(1)	0.032(4)	0.028(4)	0.039(4)	-0.010(3)	-0.007(3)	-0.006(3)
C(2)	0.047(5)	0.046(5)	0.051(5)	-0.019(4)	0.011(4)	0.006(4)
C(3)	0.056(5)	0.053(5)	0.052(5)	-0.022(5)	0.010(4)	-0.004(4)
C(4)	0.038(4)	0.030(4)	0.040(4)	-0.013(4)	-0.013(3)	0.001(3)
C(5)	0.036(4)	0.046(5)	0.058(5)	-0.024(4)	-0.003(4)	0.018(4)
C(6)	0.036(4)	0.034(4)	0.047(5)	-0.013(4)	-0.012(4)	0.005(4)
C(7)	0.052(5)	0.031(4)	0.043(4)	-0.018(4)	0.010(4)	0.004(4)
C(8)	0.061(5)	0.039(5)	0.045(5)	-0.029(4)	-0.001(4)	0.007(4)
C(9)	0.055(5)	0.041(5)	0.045(5)	-0.021(4)	0.003(4)	0.009(4)
C(10)	0.096(8)	0.055(6)	0.044(5)	-0.038(6)	0.011(5)	-0.006(4)
C(11)	0.077(7)	0.084(7)	0.061(5)	-0.068(6)	-0.025(5)	0.013(5)
C(12)	0.070(6)	0.059(6)	0.056(5)	-0.040(5)	-0.005(4)	0.001(4)
C(13)	0.125(9)	0.064(6)	0.085(7)	-0.061(6)	-0.011(6)	-0.012(5)
C(14)	0.041(5)	0.028(4)	0.041(4)	-0.015(4)	-0.003(3)	-0.005(3)
C(15)	0.033(5)	0.028(4)	0.079(6)	-0.005(4)	-0.010(4)	0.016(4)
C(16)	0.052(5)	0.051(6)	0.098(7)	-0.033(5)	-0.017(5)	0.010(5)
C(17)	0.049(5)	0.042(5)	0.077(6)	-0.028(4)	-0.002(4)	0.006(4)
C(18)	0.064(6)	0.034(5)	0.059(5)	-0.023(4)	-0.015(4)	0.014(4)
C(19)	0.039(4)	0.041(5)	0.044(4)	-0.017(4)	-0.004(3)	0.008(4)
C(20)	0.070(6)	0.065(6)	0.093(7)	-0.049(5)	-0.007(5)	0.010(5)
C(21)	0.030(4)	0.031(4)	0.058(5)	-0.009(4)	0.005(4)	0.008(4)
C(22)	0.041(5)	0.027(4)	0.060(5)	-0.006(4)	0.008(4)	-0.006(4)
C(23)	0.021(4)	0.037(5)	0.086(6)	0.000(4)	-0.003(4)	0.021(4)
C(24)	0.037(5)	0.038(5)	0.057(5)	-0.020(4)	-0.014(4)	0.018(4)
C(25)	0.050(5)	0.038(5)	0.042(4)	-0.026(4)	-0.006(4)	0.000(4)
C(26)	0.044(5)	0.057(6)	0.063(5)	-0.032(5)	-0.019(4)	0.039(5)
C(27)	0.048(5)	0.046(5)	0.031(4)	-0.022(4)	-0.008(4)	0.008(4)
C(28)	0.052(5)	0.081(7)	0.039(5)	-0.030(5)	-0.003(4)	0.011(4)
C(29)	0.053(6)	0.083(7)	0.061(6)	-0.028(5)	-0.015(5)	0.010(5)
C(30)	0.064(6)	0.056(6)	0.041(5)	-0.024(5)	-0.016(4)	0.014(4)
C(31)	0.068(6)	0.086(7)	0.056(5)	-0.044(6)	-0.010(5)	0.027(5)
C(32)	0.049(5)	0.083(7)	0.056(5)	-0.029(5)	-0.007(4)	0.019(5)
C(33)	0.087(7)	0.098(8)	0.075(6)	-0.026(6)	-0.043(5)	0.026(6)
C(34)	0.035(4)	0.043(5)	0.057(5)	-0.015(4)	-0.009(4)	0.025(4)
C(35)	0.069(6)	0.068(6)	0.057(5)	-0.048(5)	-0.029(4)	0.035(5)
C(36)	0.105(8)	0.070(7)	0.080(7)	-0.065(7)	-0.046(6)	0.036(6)
C(37)	0.105(8)	0.050(6)	0.051(6)	-0.047(6)	-0.030(5)	0.014(4)
C(38)	0.072(6)	0.047(5)	0.044(5)	-0.019(5)	-0.007(4)	0.016(4)
C(39)	0.073(6)	0.044(5)	0.037(4)	-0.028(5)	-0.018(4)	0.016(4)
C(40)	0.19(1)	0.088(8)	0.064(6)	-0.082(8)	-0.049(7)	0.020(6)
C(41)	0.050(5)	0.030(4)	0.057(5)	-0.013(4)	-0.016(4)	0.009(4)
C(42)	0.071(6)	0.048(5)	0.064(6)	-0.019(5)	-0.017(5)	0.035(4)
C(43)	0.079(7)	0.053(6)	0.071(6)	-0.025(5)	-0.022(5)	0.029(5)
C(44)	0.033(5)	0.042(5)	0.057(5)	-0.007(4)	-0.019(4)	0.006(4)

C(45)	0.067(6)	0.039(5)	0.040(4)	-0.033(5)	0.001(4)	0.005(4)
C(46)	0.035(5)	0.039(5)	0.071(5)	-0.011(4)	-0.030(4)	0.012(4)
C(47)	0.056(5)	0.033(4)	0.033(4)	-0.025(4)	0.006(4)	0.000(3)
C(48)	0.057(5)	0.038(5)	0.036(4)	-0.011(4)	0.006(4)	0.005(4)
C(49)	0.069(6)	0.068(6)	0.035(4)	-0.029(5)	0.012(4)	-0.005(4)
C(50)	0.060(6)	0.055(6)	0.052(5)	-0.027(5)	0.020(4)	-0.004(4)
C(51)	0.046(5)	0.058(6)	0.055(5)	-0.025(5)	-0.011(4)	0.017(4)
C(52)	0.037(4)	0.048(5)	0.036(4)	-0.024(4)	-0.005(3)	0.008(4)
C(53)	0.068(7)	0.096(8)	0.082(7)	-0.031(6)	0.027(5)	-0.003(6)
C(54)	0.040(5)	0.047(6)	0.079(6)	-0.015(5)	-0.018(4)	0.014(5)
C(55)	0.047(5)	0.050(6)	0.103(7)	-0.013(5)	-0.008(5)	0.014(5)
C(56)	0.071(7)	0.041(6)	0.133(9)	-0.031(5)	-0.031(6)	0.028(6)
C(57)	0.043(5)	0.058(6)	0.087(7)	-0.018(5)	-0.032(5)	0.030(5)
C(58)	0.062(6)	0.059(6)	0.061(6)	-0.023(5)	-0.011(4)	0.007(5)
C(59)	0.047(5)	0.028(5)	0.079(6)	-0.013(4)	-0.011(4)	0.002(4)
C(60)	0.057(6)	0.088(8)	0.164(10)	-0.037(6)	-0.032(6)	0.063(7)
C(61)	0.070(7)	0.081(7)	0.081(7)	-0.034(6)	-0.013(5)	0.043(6)
C(62)	0.083(7)	0.069(7)	0.095(8)	-0.028(6)	0.020(6)	0.027(6)
C(63)	0.104(10)	0.080(9)	0.067(7)	-0.003(7)	0.012(6)	0.006(6)
C(64)	0.085(9)	0.084(9)	0.16(1)	-0.037(8)	-0.046(8)	0.047(9)
C(65)	0.079(8)	0.09(1)	0.14(1)	-0.014(8)	0.019(8)	0.069(9)
C(66)	0.077(8)	0.060(7)	0.114(9)	-0.013(6)	-0.001(6)	0.047(6)
C(67)	0.094(8)	0.074(8)	0.15(1)	-0.025(7)	-0.050(7)	-0.003(7)

Table S15. Intramolecular Distances Involving the Nonhydrogen Atoms for 5b.

atom	atom	distance	atom	atom	distance
Y	N(1)	2.309(5)	C(1)	C(2)	1.387(8)
Y	N(2)	2.667(5)	C(1)	C(5)	1.427(9)
Y	N(3)	2.652(5)	C(2)	C(3)	1.395(9)
Y	N(4)	2.306(5)	C(3)	C(4)	1.383(9)
Y	N(5)	2.652(5)	C(4)	C(6)	1.439(9)
Y	N(6)	2.716(5)	C(7)	C(8)	1.393(9)
Y	N(7)	2.401(6)	C(7)	C(12)	1.369(9)
Y	N(8)	2.484(5)	C(8)	C(9)	1.409(9)
N(1)	C(1)	1.375(7)	C(9)	C(10)	1.37(1)
N(1)	C(4)	1.370(7)	C(10)	C(11)	1.40(1)
N(2)	C(5)	1.308(8)	C(10)	C(13)	1.52(1)
N(2)	C(7)	1.439(8)	C(11)	C(12)	1.42(1)
N(3)	C(6)	1.300(7)	C(14)	C(15)	1.383(9)
N(3)	C(14)	1.440(8)	C(14)	C(19)	1.384(9)
N(4)	C(21)	1.365(8)	C(15)	C(16)	1.352(9)
N(4)	C(24)	1.373(8)	C(16)	C(17)	1.39(1)
N(5)	C(25)	1.296(8)	C(17)	C(18)	1.373(9)
N(5)	C(27)	1.416(8)	C(17)	C(20)	1.505(9)
N(6)	C(26)	1.295(8)	C(18)	C(19)	1.379(9)
N(6)	C(34)	1.405(8)	C(21)	C(22)	1.378(9)
N(7)	C(41)	1.389(8)	C(21)	C(25)	1.448(9)
N(7)	C(44)	1.354(8)	C(22)	C(23)	1.375(9)
N(8)	C(45)	1.309(8)	C(23)	C(24)	1.405(9)
N(8)	C(47)	1.443(8)	C(24)	C(26)	1.429(9)
N(9)	C(46)	1.275(8)	C(27)	C(28)	1.365(9)
N(9)	C(54)	1.431(9)	C(27)	C(32)	1.374(9)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms cont.

atom	atom	distance	atom	atom	distance
C(28)	C(29)	1.38(1)	C(55)	C(56)	1.38(1)
C(29)	C(30)	1.38(1)	C(56)	C(57)	1.38(1)
C(30)	C(31)	1.38(1)	C(57)	C(58)	1.39(1)
C(30)	C(33)	1.48(1)	C(57)	C(60)	1.51(1)
C(31)	C(32)	1.38(1)	C(58)	C(59)	1.38(1)
C(34)	C(35)	1.390(9)	C(61)	C(62)	1.38(1)
C(34)	C(39)	1.405(9)	C(61)	C(66)	1.36(1)
C(35)	C(36)	1.40(1)	C(61)	C(67)	1.46(1)
C(36)	C(37)	1.36(1)	C(62)	C(63)	1.41(1)
C(37)	C(38)	1.39(1)	C(63)	C(64)	1.35(1)
C(37)	C(40)	1.53(1)	C(64)	C(65)	1.39(1)
C(38)	C(39)	1.384(9)	C(65)	C(66)	1.35(1)
C(41)	C(42)	1.395(9)	C(68)	C(69)	1.223
C(41)	C(45)	1.383(9)	C(68)	C(71)	1.220
C(42)	C(43)	1.40(1)	C(69)	C(70)	1.266
C(43)	C(44)	1.40(1)	C(70)	C(71)	1.846
C(44)	C(46)	1.44(1)			
C(47)	C(48)	1.389(8)			
C(47)	C(52)	1.369(9)			
C(48)	C(49)	1.374(9)			
C(49)	C(50)	1.39(1)			
C(50)	C(51)	1.382(9)			
C(50)	C(53)	1.51(1)			
C(51)	C(52)	1.386(9)			
C(54)	C(55)	1.38(1)			
C(54)	C(59)	1.35(1)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table S16. Intramolecular Bond Angles Involving the Nonhydrogen Atoms for 5b.

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Y	N(2)	64.3(2)	N(6)	Y	N(8)	102.2(2)
N(1)	Y	N(3)	64.2(2)	N(7)	Y	N(8)	70.5(2)
N(1)	Y	N(4)	132.9(2)	Y	N(1)	C(1)	127.3(4)
N(1)	Y	N(5)	132.0(2)	Y	N(1)	C(4)	126.8(4)
N(1)	Y	N(6)	83.4(2)	C(1)	N(1)	C(4)	105.7(5)
N(1)	Y	N(7)	86.5(2)	Y	N(2)	C(5)	113.2(4)
N(1)	Y	N(8)	140.0(2)	Y	N(2)	C(7)	130.9(4)
N(2)	Y	N(3)	128.4(2)	C(5)	N(2)	C(7)	115.9(5)
N(2)	Y	N(4)	83.4(2)	Y	N(3)	C(6)	114.4(4)
N(2)	Y	N(5)	77.8(2)	Y	N(3)	C(14)	127.2(4)
N(2)	Y	N(6)	91.5(2)	C(6)	N(3)	C(14)	116.1(6)
N(2)	Y	N(7)	106.7(2)	Y	N(4)	C(21)	126.2(4)
N(2)	Y	N(8)	152.7(2)	Y	N(4)	C(24)	128.3(5)
N(3)	Y	N(4)	131.9(2)	C(21)	N(4)	C(24)	105.3(6)
N(3)	Y	N(5)	145.4(2)	Y	N(5)	C(25)	113.7(4)
N(3)	Y	N(6)	79.0(2)	Y	N(5)	C(27)	128.8(4)
N(3)	Y	N(7)	73.9(2)	C(25)	N(5)	C(27)	117.0(6)
N(3)	Y	N(8)	77.8(2)	Y	N(6)	C(26)	113.4(4)
N(4)	Y	N(5)	64.7(2)	Y	N(6)	C(34)	129.7(4)
N(4)	Y	N(6)	63.3(2)	C(26)	N(6)	C(34)	116.5(6)
N(4)	Y	N(7)	137.4(2)	Y	N(7)	C(41)	113.6(4)
N(4)	Y	N(8)	82.0(2)	Y	N(7)	C(44)	140.7(5)
N(5)	Y	N(6)	127.7(2)	C(41)	N(7)	C(44)	105.7(6)
N(5)	Y	N(7)	77.0(2)	Y	N(8)	C(45)	111.6(5)
N(5)	Y	N(8)	75.2(2)	Y	N(8)	C(47)	127.2(4)
N(6)	Y	N(7)	152.8(2)	C(45)	N(8)	C(47)	120.4(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont.

atom	atom	atom	angle	atom	atom	atom	angle
C(46)	N(9)	C(54)	117.8(7)	C(16)	C(17)	C(18)	116.7(7)
N(1)	C(1)	C(2)	110.8(6)	C(16)	C(17)	C(20)	122.6(7)
N(1)	C(1)	C(5)	114.1(6)	C(18)	C(17)	C(20)	120.7(7)
C(2)	C(1)	C(5)	135.1(7)	C(17)	C(18)	C(19)	121.5(7)
C(1)	C(2)	C(3)	106.0(6)	C(14)	C(19)	C(18)	120.8(7)
C(2)	C(3)	C(4)	107.3(6)	N(4)	C(21)	C(22)	110.8(6)
N(1)	C(4)	C(3)	110.3(6)	N(4)	C(21)	C(25)	114.9(6)
N(1)	C(4)	C(6)	114.9(6)	C(22)	C(21)	C(25)	134.1(7)
C(3)	C(4)	C(6)	134.9(7)	C(21)	C(22)	C(23)	107.8(6)
N(2)	C(5)	C(1)	121.0(6)	C(22)	C(23)	C(24)	105.6(6)
N(3)	C(6)	C(4)	119.0(6)	N(4)	C(24)	C(23)	110.5(6)
N(2)	C(7)	C(8)	117.8(7)	N(4)	C(24)	C(26)	114.8(7)
N(2)	C(7)	C(12)	121.8(7)	C(23)	C(24)	C(26)	134.7(7)
C(8)	C(7)	C(12)	120.5(7)	N(5)	C(25)	C(21)	119.8(6)
C(7)	C(8)	C(9)	120.0(7)	N(6)	C(26)	C(24)	120.1(6)
C(8)	C(9)	C(10)	120.3(7)	N(5)	C(27)	C(28)	119.4(6)
C(9)	C(10)	C(11)	119.8(7)	N(5)	C(27)	C(32)	122.0(7)
C(9)	C(10)	C(13)	119.9(8)	C(28)	C(27)	C(32)	118.5(7)
C(11)	C(10)	C(13)	120.3(8)	C(27)	C(28)	C(29)	119.8(7)
C(10)	C(11)	C(12)	119.9(7)	C(28)	C(29)	C(30)	122.8(7)
C(7)	C(12)	C(11)	119.6(7)	C(29)	C(30)	C(31)	116.3(7)
N(3)	C(14)	C(15)	121.1(6)	C(29)	C(30)	C(33)	121.6(8)
N(3)	C(14)	C(19)	121.2(6)	C(31)	C(30)	C(33)	122.1(8)
C(15)	C(14)	C(19)	117.7(6)	C(30)	C(31)	C(32)	120.9(7)
C(14)	C(15)	C(16)	120.7(7)	C(27)	C(32)	C(31)	121.6(7)
C(15)	C(16)	C(17)	122.6(7)	N(6)	C(34)	C(35)	123.0(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms cont.

atom	atom	atom	angle	atom	atom	atom	angle
N(6)	C(34)	C(39)	119.2(6)	C(51)	C(50)	C(53)	122.1(8)
C(35)	C(34)	C(39)	117.8(7)	C(50)	C(51)	C(52)	121.4(7)
C(34)	C(35)	C(36)	119.2(8)	C(47)	C(52)	C(51)	121.9(6)
C(35)	C(36)	C(37)	122.7(8)	N(9)	C(54)	C(55)	121.8(8)
C(36)	C(37)	C(38)	118.8(8)	N(9)	C(54)	C(59)	119.6(8)
C(36)	C(37)	C(40)	122.0(9)	C(55)	C(54)	C(59)	118.6(8)
C(38)	C(37)	C(40)	119.2(9)	C(54)	C(55)	C(56)	121.3(8)
C(37)	C(38)	C(39)	119.6(8)	C(55)	C(56)	C(57)	119.9(8)
C(34)	C(39)	C(38)	121.8(7)	C(56)	C(57)	C(58)	118.2(8)
N(7)	C(41)	C(42)	110.2(7)	C(56)	C(57)	C(60)	120.3(8)
N(7)	C(41)	C(45)	120.1(6)	C(58)	C(57)	C(60)	121.4(9)
C(42)	C(41)	C(45)	129.6(8)	C(57)	C(58)	C(59)	121.0(8)
C(41)	C(42)	C(43)	106.7(7)	C(54)	C(59)	C(58)	120.9(7)
C(42)	C(43)	C(44)	106.1(7)	C(62)	C(61)	C(66)	118(1)
N(7)	C(44)	C(43)	111.2(7)	C(62)	C(61)	C(67)	121(1)
N(7)	C(44)	C(46)	120.7(7)	C(66)	C(61)	C(67)	122(1)
C(43)	C(44)	C(46)	127.8(7)	C(61)	C(62)	C(63)	120.6(9)
N(8)	C(45)	C(41)	124.1(7)	C(62)	C(63)	C(64)	119(1)
N(9)	C(46)	C(44)	125.0(7)	C(63)	C(64)	C(65)	121(1)
N(8)	C(47)	C(48)	123.0(6)	C(64)	C(65)	C(66)	118(1)
N(8)	C(47)	C(52)	119.6(6)	C(61)	C(66)	C(65)	124(1)
C(48)	C(47)	C(52)	117.3(7)	C(69)	C(68)	C(71)	177.36
C(47)	C(48)	C(49)	120.7(7)	C(68)	C(69)	C(70)	161.4954(1)
C(48)	C(49)	C(50)	122.4(7)	C(69)	C(70)	C(71)	115.3077(6)
C(49)	C(50)	C(51)	116.3(7)	C(68)	C(71)	C(70)	80.3573(6)
C(49)	C(50)	C(53)	121.6(7)				

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.