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

	x	y	z	U(eq)
Ti(1)	8579(1)	1223(1)	3951(1)	29(1)
Ti(2)	6387(1)	-1297(1)	843(1)	32(1)
Cl(1)	7844(1)	1749(1)	2619(1)	52(1)
Cl(2)	10237(1)	838(1)	3942(1)	47(1)
Cl(3)	7215(1)	-1926(1)	2002(1)	59(1)
Cl(4)	4733(1)	-988(1)	1000(1)	55(1)
N(1)	8553(2)	1651(1)	5084(1)	30(1)
N(2)	7594(2)	648(1)	4015(1)	30(1)
N(3)	6433(2)	-1621(1)	-376(1)	30(1)
N(4)	7322(2)	-678(1)	896(2)	33(1)
Si(1)	9209(1)	2355(1)	5247(1)	40(1)
Si(2)	6223(1)	437(1)	3454(1)	38(1)
Si(3)	5826(1)	-2330(1)	-681(1)	38(1)
Si(4)	8678(1)	-461(1)	1509(1)	40(1)
C(1)	8024(2)	1426(1)	5776(2)	31(1)
C(2)	7736(2)	1782(1)	6459(2)	42(1)
C(3)	7220(2)	1542(2)	7117(2)	53(1)
C(4)	6981(2)	954(2)	7101(2)	56(1)
C(5)	7265(2)	594(1)	6423(2)	46(1)
C(6)	7789(2)	823(1)	5767(2)	32(1)
C(7)	8129(2)	448(1)	5033(2)	34(1)
C(8)	6066(3)	-341(2)	3800(3)	70(1)
C(9)	5283(3)	928(2)	3890(2)	69(1)
C(10)	5971(2)	506(1)	2122(2)	53(1)
C(11)	10064(3)	2398(2)	4372(3)	66(1)
C(12)	10114(3)	2405(2)	6496(2)	66(1)
C(13)	8187(3)	2960(1)	4968(2)	56(1)
C(14)	6983(2)	-1323(1)	-982(2)	31(1)
C(15)	7368(2)	-1611(1)	-1687(2)	40(1)
C(16)	7910(2)	-1300(2)	-2258(2)	50(1)
C(17)	8067(2)	-703(2)	-2143(2)	51(1)
C(18)	7689(2)	-412(1)	-1443(2)	45(1)
C(19)	7151(2)	-715(1)	-866(2)	34(1)
C(20)	6768(2)	-423(1)	-75(2)	36(1)
C(21)	8869(3)	-583(1)	2827(2)	58(1)
C(22)	8820(3)	328(1)	1226(2)	58(1)
C(23)	9665(3)	-916(2)	1073(3)	74(1)
C(24)	4852(3)	-2438(2)	70(2)	59(1)
C(25)	6875(3)	-2921(1)	-390(2)	58(1)
C(26)	5043(2)	-2340(1)	-1982(2)	52(1)

Table S2. Bond lengths [Å] and angles [°] for 2.

Ti(1)-N(2)	1.825(2)	Ti(1)-N(1)	1.895(2)
Ti(1)-Cl(1)	2.2316(11)	Ti(1)-Cl(2)	2.2714(12)
Ti(1)-C(7)	2.506(3)	Ti(2)-N(4)	1.827(2)
Ti(2)-N(3)	1.904(2)	Ti(2)-Cl(3)	2.2272(11)
Ti(2)-Cl(4)	2.2697(13)	Ti(2)-C(20)	2.500(3)
N(1)-C(1)	1.426(3)	N(1)-Si(1)	1.792(2)
N(2)-C(7)	1.500(3)	N(2)-Si(2)	1.770(2)
N(3)-C(14)	1.417(3)	N(3)-Si(3)	1.792(2)
N(4)-C(20)	1.494(3)	N(4)-Si(4)	1.773(2)
Si(1)-C(12)	1.849(3)	Si(1)-C(13)	1.856(3)
Si(1)-C(11)	1.857(3)	Si(2)-C(10)	1.848(3)
Si(2)-C(9)	1.854(3)	Si(2)-C(8)	1.865(3)
Si(3)-C(24)	1.849(3)	Si(3)-C(25)	1.856(3)
Si(3)-C(26)	1.858(3)	Si(4)-C(23)	1.852(3)
Si(4)-C(21)	1.852(3)	Si(4)-C(22)	1.862(3)
C(1)-C(2)	1.389(4)	C(1)-C(6)	1.405(4)
C(2)-C(3)	1.388(4)	C(3)-C(4)	1.372(5)
C(4)-C(5)	1.387(4)	C(5)-C(6)	1.383(4)
C(6)-C(7)	1.499(4)	C(14)-C(15)	1.392(4)
C(14)-C(19)	1.406(4)	C(15)-C(16)	1.389(4)
C(16)-C(17)	1.379(4)	C(17)-C(18)	1.385(4)
C(18)-C(19)	1.382(4)	C(19)-C(20)	1.497(4)

N(2)-Ti(1)-N(1)	99.25(9)	N(2)-Ti(1)-Cl(1)	107.07(7)
N(1)-Ti(1)-Cl(1)	110.66(7)	N(2)-Ti(1)-Cl(2)	111.38(8)
N(1)-Ti(1)-Cl(2)	115.33(7)	Cl(1)-Ti(1)-Cl(2)	112.17(4)
N(2)-Ti(1)-C(7)	36.42(8)	N(1)-Ti(1)-C(7)	77.24(9)
Cl(1)-Ti(1)-C(7)	142.38(7)	Cl(2)-Ti(1)-C(7)	95.29(7)
N(4)-Ti(2)-N(3)	99.25(9)	N(4)-Ti(2)-Cl(3)	107.18(8)
N(3)-Ti(2)-Cl(3)	107.89(7)	N(4)-Ti(2)-Cl(4)	110.92(8)
N(3)-Ti(2)-Cl(4)	117.48(7)	Cl(3)-Ti(2)-Cl(4)	112.91(4)
N(4)-Ti(2)-C(20)	36.37(9)	N(3)-Ti(2)-C(20)	76.91(9)
Cl(3)-Ti(2)-C(20)	141.63(7)	Cl(4)-Ti(2)-C(20)	96.53(7)
C(1)-N(1)-Si(1)	121.07(16)	C(1)-N(1)-Ti(1)	121.54(16)
Si(1)-N(1)-Ti(1)	117.39(11)	C(7)-N(2)-Si(2)	119.39(16)
C(7)-N(2)-Ti(1)	97.36(15)	Si(2)-N(2)-Ti(1)	140.34(12)
C(14)-N(3)-Si(3)	122.00(17)	C(14)-N(3)-Ti(2)	120.73(16)
Si(3)-N(3)-Ti(2)	117.18(11)	C(20)-N(4)-Si(4)	120.11(17)
C(20)-N(4)-Ti(2)	97.16(15)	Si(4)-N(4)-Ti(2)	139.79(13)
N(1)-Si(1)-C(12)	109.08(14)	N(1)-Si(1)-C(13)	111.51(13)
C(12)-Si(1)-C(13)	112.17(16)	N(1)-Si(1)-C(11)	106.89(12)
C(12)-Si(1)-C(11)	108.92(17)	C(13)-Si(1)-C(11)	108.10(16)
N(2)-Si(2)-C(10)	108.83(13)	N(2)-Si(2)-C(9)	108.66(14)
C(10)-Si(2)-C(9)	110.02(15)	N(2)-Si(2)-C(8)	107.33(13)
C(10)-Si(2)-C(8)	110.64(16)	C(9)-Si(2)-C(8)	111.27(18)
N(3)-Si(3)-C(24)	106.65(12)	N(3)-Si(3)-C(25)	111.46(13)
C(24)-Si(3)-C(25)	108.52(16)	N(3)-Si(3)-C(26)	109.50(13)
C(24)-Si(3)-C(26)	108.57(15)	C(25)-Si(3)-C(26)	111.96(15)
N(4)-Si(4)-C(23)	108.94(14)	N(4)-Si(4)-C(21)	107.95(13)
C(23)-Si(4)-C(21)	109.78(17)	N(4)-Si(4)-C(22)	107.37(13)
C(23)-Si(4)-C(22)	110.88(17)	C(21)-Si(4)-C(22)	111.80(15)
C(2)-C(1)-C(6)	118.9(2)	C(2)-C(1)-N(1)	122.3(2)
C(6)-C(1)-N(1)	118.8(2)	C(3)-C(2)-C(1)	120.1(3)
C(4)-C(3)-C(2)	120.9(3)	C(3)-C(4)-C(5)	119.5(3)
C(6)-C(5)-C(4)	120.5(3)	C(5)-C(6)-C(1)	120.1(3)

C(5)-C(6)-C(7)	122.3(3)	C(1)-C(6)-C(7)	117.6(2)
C(6)-C(7)-N(2)	111.5(2)	C(6)-C(7)-Ti(1)	100.59(16)
N(2)-C(7)-Ti(1)	46.22(11)	C(15)-C(14)-C(19)	118.7(2)
C(15)-C(14)-N(3)	122.5(2)	C(19)-C(14)-N(3)	118.9(2)
C(16)-C(15)-C(14)	120.3(3)	C(17)-C(16)-C(15)	120.7(3)
C(16)-C(17)-C(18)	119.5(3)	C(19)-C(18)-C(17)	120.5(3)
C(18)-C(19)-C(14)	120.3(3)	C(18)-C(19)-C(20)	122.3(3)
C(14)-C(19)-C(20)	117.3(2)	N(4)-C(20)-C(19)	111.1(2)
N(4)-C(20)-Ti(2)	46.47(11)	C(19)-C(20)-Ti(2)	100.72(16)

Symmetry transformations used to generate equivalent atoms:

Table S3. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ti(1)	31(1)	28(1)	28(1)	1(1)	9(1)	1(1)
Ti(2)	33(1)	35(1)	29(1)	1(1)	9(1)	-3(1)
Cl(1)	55(1)	54(1)	45(1)	21(1)	11(1)	3(1)
Cl(2)	39(1)	51(1)	55(1)	-2(1)	19(1)	10(1)
Cl(3)	61(1)	59(1)	48(1)	23(1)	-1(1)	-11(1)
Cl(4)	45(1)	65(1)	63(1)	-10(1)	27(1)	1(1)
N(1)	28(1)	28(1)	32(1)	-2(1)	8(1)	-1(1)
N(2)	35(1)	25(1)	28(1)	0(1)	5(1)	0(1)
N(3)	29(1)	30(1)	32(1)	-1(1)	10(1)	-2(1)
N(4)	34(1)	32(1)	32(1)	-2(1)	6(1)	-1(1)
Si(1)	37(1)	31(1)	50(1)	-6(1)	11(1)	-6(1)
Si(2)	32(1)	40(1)	41(1)	-3(1)	5(1)	-2(1)
Si(3)	37(1)	32(1)	43(1)	-4(1)	8(1)	-5(1)
Si(4)	33(1)	38(1)	47(1)	-10(1)	5(1)	0(1)
C(1)	26(1)	39(2)	26(1)	0(1)	4(1)	2(1)
C(2)	40(2)	49(2)	36(2)	-3(1)	8(1)	10(1)
C(3)	49(2)	78(2)	34(2)	3(2)	15(1)	20(2)
C(4)	44(2)	87(3)	39(2)	20(2)	18(1)	8(2)
C(5)	40(2)	54(2)	41(2)	20(2)	8(1)	0(1)
C(6)	27(1)	39(2)	27(1)	6(1)	1(1)	2(1)
C(7)	36(2)	27(1)	36(1)	7(1)	4(1)	0(1)
C(8)	57(2)	58(2)	86(3)	7(2)	5(2)	-26(2)
C(9)	44(2)	101(3)	61(2)	-4(2)	14(2)	21(2)
C(10)	47(2)	60(2)	43(2)	-12(2)	0(1)	0(2)
C(11)	64(2)	50(2)	94(3)	-7(2)	41(2)	-22(2)
C(12)	47(2)	67(2)	74(2)	-16(2)	-4(2)	-13(2)
C(13)	67(2)	36(2)	66(2)	2(2)	20(2)	2(2)
C(14)	26(1)	36(2)	28(1)	4(1)	6(1)	2(1)
C(15)	37(2)	43(2)	41(2)	2(1)	13(1)	6(1)
C(16)	44(2)	72(2)	41(2)	7(2)	21(1)	14(2)
C(17)	41(2)	70(2)	48(2)	24(2)	21(1)	6(2)
C(18)	39(2)	47(2)	47(2)	15(1)	9(1)	0(1)
C(19)	28(1)	38(2)	33(1)	10(1)	5(1)	3(1)
C(20)	36(2)	30(2)	38(2)	3(1)	5(1)	0(1)
C(21)	61(2)	54(2)	47(2)	-8(2)	-6(2)	1(2)
C(22)	52(2)	52(2)	69(2)	-7(2)	12(2)	-18(2)
C(23)	44(2)	79(3)	96(3)	-27(2)	16(2)	12(2)
C(24)	60(2)	57(2)	64(2)	-6(2)	22(2)	-28(2)
C(25)	66(2)	36(2)	69(2)	-3(2)	11(2)	8(2)
C(26)	40(2)	57(2)	54(2)	-13(2)	3(1)	-4(2)

Table S4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 4. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ti(1)	1164(1)	4032(1)	2365(1)	34(1)
Ti(2)	3828(1)	7127(1)	6353(1)	36(1)
Si(1)	1266(1)	1272(1)	2252(1)	37(1)
Si(2)	883(1)	6138(1)	3679(1)	40(1)
Si(3)	3922(1)	9557(1)	7292(1)	38(1)
Si(4)	3072(1)	4961(1)	5913(1)	35(1)
N(1)	1013(1)	2462(3)	2690(2)	32(1)
N(2)	846(1)	4918(3)	3040(2)	33(1)
N(3)	3636(1)	8216(3)	7122(2)	38(1)
N(4)	3456(1)	5870(3)	6500(2)	38(1)
C(1)	704(1)	2265(3)	3250(2)	33(1)
C(2)	679(1)	1198(4)	3651(2)	39(1)
C(3)	366(1)	1024(4)	4179(2)	47(1)
C(4)	75(1)	1907(4)	4324(2)	51(1)
C(5)	98(1)	2968(4)	3938(2)	44(1)
C(6)	406(1)	3167(3)	3403(2)	35(1)
C(7)	402(1)	4290(3)	2937(2)	41(1)
C(8)	823(1)	243(4)	1784(2)	53(1)
C(9)	1687(1)	445(4)	2957(3)	49(1)
C(10)	1556(1)	1885(4)	1428(2)	50(1)
C(11)	766(2)	5690(5)	4689(3)	77(2)
C(12)	1449(1)	6813(4)	3789(3)	63(1)
C(13)	463(2)	7256(4)	3263(3)	73(2)
C(14)	837(2)	4456(4)	1181(2)	56(1)
C(15)	1219(2)	5175(4)	1005(2)	55(1)
C(16)	1530(2)	4773(4)	513(3)	62(1)
C(17)	1917(2)	5382(5)	456(3)	85(2)
C(18)	2014(2)	6397(5)	883(4)	104(2)
C(19)	1711(2)	6845(5)	1350(4)	94(2)
C(20)	1314(2)	6246(4)	1405(3)	68(2)
C(21)	1859(1)	4353(3)	2697(2)	36(1)
C(22)	2122(1)	3545(3)	3279(2)	32(1)
C(23)	2504(1)	2955(3)	3093(2)	37(1)
C(24)	2739(1)	2185(4)	3629(3)	45(1)
C(25)	2607(1)	1977(4)	4370(3)	48(1)
C(26)	2232(1)	2543(4)	4576(2)	45(1)
C(27)	1996(1)	3319(3)	4039(2)	39(1)
C(31)	3287(1)	7886(4)	7599(2)	38(1)
C(32)	3021(1)	8706(4)	7929(2)	47(1)
C(33)	2695(1)	8351(4)	8377(3)	51(1)
C(34)	2616(1)	7191(4)	8505(2)	50(1)
C(35)	2875(1)	6357(4)	8186(2)	43(1)
C(36)	3212(1)	6685(3)	7738(2)	37(1)
C(37)	3508(1)	5809(3)	7405(2)	40(1)
C(38)	4416(1)	9535(3)	6740(2)	41(1)
C(39)	3556(2)	10811(4)	6902(3)	78(2)
C(40)	4135(2)	9726(5)	8375(3)	76(2)
C(41)	2518(2)	5687(4)	5674(3)	73(2)
C(42)	3295(2)	4611(4)	4974(3)	67(1)
C(43)	2996(2)	3625(4)	6492(3)	77(2)
C(44)	3698(1)	7628(4)	5128(2)	50(1)

C(46)	3687(1)	9773(4)	4776(2)	48(1)
C(47)	3887(2)	10765(4)	4515(3)	57(1)
C(48)	4304(2)	10700(4)	4264(3)	60(1)
C(49)	4515(2)	9637(5)	4270(2)	56(1)
C(50)	4317(1)	8637(4)	4529(2)	47(1)
C(51)	4504(1)	6516(3)	6614(3)	45(1)
C(52)	4530(1)	5251(3)	6419(2)	37(1)
C(53)	4566(1)	4880(4)	5640(2)	45(1)
C(54)	4572(1)	3704(4)	5445(3)	52(1)
C(55)	4543(2)	2854(4)	6016(3)	55(1)
C(56)	4513(1)	3205(4)	6799(3)	52(1)
C(57)	4507(1)	4375(4)	6995(2)	46(1)

Table S5. Bond lengths [Å] and angles [°] for 4.

Ti(1)-N(2)	1.873(3)	Ti(1)-N(1)	1.942(3)
Ti(1)-C(21)	2.114(4)	Ti(1)-C(14)	2.138(4)
Ti(1)-C(7)	2.614(4)	Ti(1)-C(15)	2.647(4)
Ti(2)-N(4)	1.854(3)	Ti(2)-N(3)	1.934(3)
Ti(2)-C(44)	2.111(4)	Ti(2)-C(51)	2.129(4)
Ti(2)-C(37)	2.597(4)	Si(1)-N(1)	1.763(3)
Si(1)-C(9)	1.859(4)	Si(1)-C(8)	1.860(4)
Si(1)-C(10)	1.867(4)	Si(2)-N(2)	1.749(3)
Si(2)-C(11)	1.845(4)	Si(2)-C(12)	1.850(4)
Si(2)-C(13)	1.858(4)	Si(3)-N(3)	1.757(3)
Si(3)-C(40)	1.846(4)	Si(3)-C(38)	1.855(4)
Si(3)-C(39)	1.864(5)	Si(4)-N(4)	1.746(3)
Si(4)-C(43)	1.836(4)	Si(4)-C(42)	1.837(4)
Si(4)-C(41)	1.850(4)	N(1)-C(1)	1.425(4)
N(2)-C(7)	1.500(4)	N(3)-C(31)	1.450(4)
N(4)-C(37)	1.501(4)	C(1)-C(2)	1.397(5)
C(1)-C(6)	1.410(5)	C(2)-C(3)	1.390(5)
C(3)-C(4)	1.376(6)	C(4)-C(5)	1.377(6)
C(5)-C(6)	1.392(5)	C(6)-C(7)	1.498(5)
C(14)-C(15)	1.470(6)	C(15)-C(20)	1.402(6)
C(15)-C(16)	1.405(6)	C(16)-C(17)	1.370(7)
C(17)-C(18)	1.369(8)	C(18)-C(19)	1.377(8)
C(19)-C(20)	1.387(7)	C(21)-C(22)	1.485(5)
C(22)-C(27)	1.399(5)	C(22)-C(23)	1.403(5)
C(23)-C(24)	1.376(5)	C(24)-C(25)	1.373(6)
C(25)-C(26)	1.382(5)	C(26)-C(27)	1.383(5)
C(31)-C(32)	1.392(5)	C(31)-C(36)	1.413(5)
C(32)-C(33)	1.375(5)	C(33)-C(34)	1.366(6)
C(34)-C(35)	1.381(6)	C(35)-C(36)	1.393(5)
C(36)-C(37)	1.495(5)	C(44)-C(45)	1.491(5)
C(45)-C(46)	1.387(6)	C(45)-C(50)	1.393(5)
C(46)-C(47)	1.379(6)	C(47)-C(48)	1.376(6)
C(48)-C(49)	1.368(6)	C(49)-C(50)	1.383(6)
C(51)-C(52)	1.482(5)	C(52)-C(53)	1.389(5)
C(52)-C(57)	1.397(5)	C(53)-C(54)	1.382(6)
C(54)-C(55)	1.373(6)	C(55)-C(56)	1.384(6)
C(56)-C(57)	1.374(6)		

N(2)-Ti(1)-N(1)	99.84(13)	N(2)-Ti(1)-C(21)	108.32(14)
N(1)-Ti(1)-C(21)	110.21(13)	N(2)-Ti(1)-C(14)	103.4(2)
N(1)-Ti(1)-C(14)	112.0(2)	C(21)-Ti(1)-C(14)	120.7(2)
N(2)-Ti(1)-C(7)	34.29(12)	N(1)-Ti(1)-C(7)	75.65(12)
C(21)-Ti(1)-C(7)	139.88(14)	C(14)-Ti(1)-C(7)	90.3(2)
N(2)-Ti(1)-C(15)	110.52(14)	N(1)-Ti(1)-C(15)	137.72(14)
C(21)-Ti(1)-C(15)	87.8(2)	C(14)-Ti(1)-C(15)	33.7(2)
C(7)-Ti(1)-C(15)	114.98(13)	N(4)-Ti(2)-N(3)	99.61(13)
N(4)-Ti(2)-C(44)	107.8(2)	N(3)-Ti(2)-C(44)	116.1(2)
N(4)-Ti(2)-C(51)	107.0(2)	N(3)-Ti(2)-C(51)	116.03(14)
C(44)-Ti(2)-C(51)	109.2(2)	N(4)-Ti(2)-C(37)	34.57(12)
N(3)-Ti(2)-C(37)	75.39(13)	C(44)-Ti(2)-C(37)	141.13(14)
C(51)-Ti(2)-C(37)	95.96(14)	N(1)-Si(1)-C(9)	114.8(2)
N(1)-Si(1)-C(8)	109.7(2)	C(9)-Si(1)-C(8)	109.2(2)
N(1)-Si(1)-C(10)	106.9(2)	C(9)-Si(1)-C(10)	108.2(2)
C(8)-Si(1)-C(10)	107.8(2)	N(2)-Si(2)-C(11)	109.6(2)
N(2)-Si(2)-C(12)	111.8(2)	C(11)-Si(2)-C(12)	108.4(2)
N(2)-Si(2)-C(13)	109.6(2)	C(11)-Si(2)-C(13)	109.0(2)
C(12)-Si(2)-C(13)	108.4(2)	N(3)-Si(3)-C(40)	110.1(2)
N(3)-Si(3)-C(38)	108.3(2)	C(40)-Si(3)-C(38)	107.4(2)

C(38)-Si(3)-C(39)	108.0(2)	N(4)-Si(4)-C(43)	108.5(2)
N(4)-Si(4)-C(42)	108.6(2)	C(43)-Si(4)-C(42)	111.0(2)
N(4)-Si(4)-C(41)	111.0(2)	C(43)-Si(4)-C(41)	108.1(3)
C(42)-Si(4)-C(41)	109.7(2)	C(1)-N(1)-Si(1)	120.6(2)
C(1)-N(1)-Ti(1)	121.8(2)	Si(1)-N(1)-Ti(1)	117.6(2)
C(7)-N(2)-Si(2)	115.5(2)	C(7)-N(2)-Ti(1)	101.0(2)
Si(2)-N(2)-Ti(1)	143.5(2)	C(31)-N(3)-Si(3)	120.7(2)
C(31)-N(3)-Ti(2)	120.3(2)	Si(3)-N(3)-Ti(2)	118.8(2)
C(37)-N(4)-Si(4)	120.4(2)	C(37)-N(4)-Ti(2)	100.9(2)
Si(4)-N(4)-Ti(2)	138.3(2)	C(2)-C(1)-C(6)	118.0(3)
C(2)-C(1)-N(1)	122.5(3)	C(6)-C(1)-N(1)	119.5(3)
C(3)-C(2)-C(1)	121.1(4)	C(4)-C(3)-C(2)	120.6(4)
C(3)-C(4)-C(5)	119.0(4)	C(4)-C(5)-C(6)	121.8(4)
C(5)-C(6)-C(1)	119.5(4)	C(5)-C(6)-C(7)	121.2(3)
C(1)-C(6)-C(7)	119.2(3)	C(6)-C(7)-N(2)	114.0(3)
C(6)-C(7)-Ti(1)	98.7(2)	N(2)-C(7)-Ti(1)	44.7(2)
C(15)-C(14)-Ti(1)	92.5(3)	C(20)-C(15)-C(16)	117.1(5)
C(20)-C(15)-C(14)	120.2(4)	C(16)-C(15)-C(14)	122.3(5)
C(20)-C(15)-Ti(1)	93.0(3)	C(16)-C(15)-Ti(1)	118.0(3)
C(14)-C(15)-Ti(1)	53.8(2)	C(17)-C(16)-C(15)	121.0(5)
C(18)-C(17)-C(16)	120.8(5)	C(17)-C(18)-C(19)	120.1(6)
C(18)-C(19)-C(20)	119.7(6)	C(19)-C(20)-C(15)	121.2(5)
C(22)-C(21)-Ti(1)	118.5(2)	C(27)-C(22)-C(23)	116.6(4)
C(27)-C(22)-C(21)	121.6(3)	C(23)-C(22)-C(21)	121.8(3)
C(24)-C(23)-C(22)	121.4(4)	C(25)-C(24)-C(23)	120.8(4)
C(24)-C(25)-C(26)	119.5(4)	C(25)-C(26)-C(27)	119.8(4)
C(26)-C(27)-C(22)	121.9(4)	C(32)-C(31)-C(36)	118.2(4)
C(32)-C(31)-N(3)	122.8(4)	C(36)-C(31)-N(3)	119.1(3)
C(33)-C(32)-C(31)	120.6(4)	C(34)-C(33)-C(32)	121.6(4)
C(33)-C(34)-C(35)	119.1(4)	C(34)-C(35)-C(36)	120.8(4)
C(35)-C(36)-C(31)	119.6(4)	C(35)-C(36)-C(37)	122.4(4)
C(31)-C(36)-C(37)	118.0(3)	C(36)-C(37)-N(4)	111.2(3)
C(36)-C(37)-Ti(2)	99.3(2)	N(4)-C(37)-Ti(2)	44.5(2)
C(45)-C(44)-Ti(2)	123.6(3)	C(46)-C(45)-C(50)	117.3(4)
C(46)-C(45)-C(44)	121.8(4)	C(50)-C(45)-C(44)	120.8(4)
C(47)-C(46)-C(45)	121.5(4)	C(48)-C(47)-C(46)	120.4(4)
C(49)-C(48)-C(47)	119.0(4)	C(48)-C(49)-C(50)	120.9(4)
C(49)-C(50)-C(45)	120.8(4)	C(52)-C(51)-Ti(2)	110.6(3)
C(53)-C(52)-C(57)	116.6(4)	C(53)-C(52)-C(51)	121.0(4)
C(57)-C(52)-C(51)	122.4(4)	C(54)-C(53)-C(52)	121.5(4)
C(55)-C(54)-C(53)	121.1(4)	C(54)-C(55)-C(56)	118.3(4)
C(57)-C(56)-C(55)	120.8(4)	C(56)-C(57)-C(52)	121.7(4)

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 4.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ti(1)	28(1)	41(1)	32(1)	0(1)	5(1)	3(1)
Ti(2)	36(1)	36(1)	39(1)	-5(1)	12(1)	-7(1)
Si(1)	30(1)	41(1)	42(1)	-10(1)	6(1)	-5(1)
Si(2)	37(1)	45(1)	37(1)	-1(1)	7(1)	9(1)
Si(3)	43(1)	32(1)	41(1)	-3(1)	13(1)	-2(1)
Si(4)	34(1)	33(1)	37(1)	3(1)	5(1)	-3(1)
N(1)	26(2)	41(2)	30(2)	-7(1)	4(1)	-1(1)
N(2)	23(2)	40(2)	36(2)	1(2)	3(1)	4(1)
N(3)	29(2)	42(2)	46(2)	-3(2)	9(2)	-1(2)
N(4)	41(2)	42(2)	33(2)	0(2)	6(2)	-7(2)
C(1)	23(2)	44(2)	31(2)	-4(2)	-1(2)	-4(2)
C(2)	37(2)	45(3)	33(2)	-4(2)	4(2)	-1(2)
C(3)	49(3)	57(3)	34(2)	5(2)	4(2)	-8(2)
C(4)	41(3)	71(3)	43(3)	-2(2)	14(2)	-9(2)
C(5)	30(2)	55(3)	48(2)	-2(2)	10(2)	1(2)
C(6)	24(2)	45(2)	36(2)	-1(2)	2(2)	1(2)
C(7)	26(2)	48(3)	48(2)	-1(2)	6(2)	7(2)
C(8)	45(3)	68(3)	48(3)	-17(2)	10(2)	-16(2)
C(9)	38(2)	39(3)	68(3)	-5(2)	4(2)	0(2)
C(10)	45(3)	51(3)	57(3)	-10(2)	20(2)	-3(2)
C(11)	112(5)	76(4)	46(3)	-6(3)	26(3)	-4(3)
C(12)	55(3)	63(3)	73(3)	-23(3)	11(3)	-3(2)
C(13)	71(4)	54(3)	90(4)	-2(3)	-4(3)	21(3)
C(14)	60(3)	67(3)	38(2)	3(2)	2(2)	18(3)
C(15)	78(4)	55(3)	33(2)	15(2)	13(2)	18(3)
C(16)	92(4)	50(3)	49(3)	13(2)	24(3)	10(3)
C(17)	116(5)	60(4)	92(4)	12(3)	60(4)	4(3)
C(18)	138(6)	64(4)	127(6)	4(4)	75(5)	-21(4)
C(19)	148(6)	41(3)	104(5)	3(3)	54(4)	-10(4)
C(20)	102(4)	48(3)	58(3)	14(3)	30(3)	18(3)
C(21)	31(2)	32(2)	47(2)	-5(2)	12(2)	-2(2)
C(22)	24(2)	31(2)	39(2)	-8(2)	4(2)	-5(2)
C(23)	27(2)	41(2)	44(2)	-10(2)	6(2)	-4(2)
C(24)	28(2)	46(3)	60(3)	-14(2)	-1(2)	4(2)
C(25)	40(3)	47(3)	53(3)	-1(2)	-8(2)	1(2)
C(26)	42(3)	54(3)	40(2)	-3(2)	6(2)	-7(2)
C(27)	30(2)	42(2)	46(2)	-10(2)	9(2)	-4(2)
C(31)	31(2)	45(3)	39(2)	0(2)	8(2)	2(2)
C(32)	44(3)	43(3)	57(3)	3(2)	12(2)	7(2)
C(33)	31(2)	63(3)	61(3)	0(2)	8(2)	11(2)
C(34)	31(2)	74(3)	45(2)	11(2)	11(2)	0(2)
C(35)	37(2)	45(3)	45(2)	10(2)	0(2)	-6(2)
C(36)	30(2)	44(3)	37(2)	-1(2)	3(2)	-1(2)
C(37)	43(2)	40(2)	38(2)	3(2)	2(2)	3(2)
C(38)	40(2)	44(3)	39(2)	1(2)	4(2)	-1(2)
C(39)	79(4)	44(3)	118(5)	21(3)	42(3)	11(3)
C(40)	68(3)	111(5)	51(3)	-20(3)	19(3)	-35(3)
C(41)	55(3)	73(4)	85(4)	-21(3)	-6(3)	13(3)
C(42)	67(3)	80(4)	58(3)	-23(3)	21(3)	-26(3)
C(43)	112(4)	45(3)	67(3)	7(3)	-10(3)	-22(3)
C(44)	50(3)	53(3)	49(3)	-5(2)	12(2)	-11(2)

C(46)	38(3)	60(3)	43(2)	2(2)	-4(2)	1(2)
C(47)	66(3)	49(3)	51(3)	1(2)	-13(3)	4(2)
C(48)	77(4)	61(3)	41(3)	5(2)	2(2)	-20(3)
C(49)	52(3)	75(4)	42(3)	1(3)	14(2)	-9(3)
C(50)	55(3)	53(3)	33(2)	-2(2)	11(2)	2(2)
C(51)	42(2)	45(3)	52(3)	-10(2)	15(2)	-6(2)
C(52)	27(2)	39(2)	46(2)	-4(2)	7(2)	-1(2)
C(53)	48(3)	46(3)	43(2)	5(2)	15(2)	7(2)
C(54)	58(3)	53(3)	45(3)	-8(2)	7(2)	14(2)
C(55)	61(3)	37(3)	65(3)	-4(2)	3(2)	9(2)
C(56)	55(3)	44(3)	56(3)	11(2)	5(2)	3(2)
C(57)	41(3)	60(3)	35(2)	-1(2)	0(2)	8(2)

Table S7. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr(1)	2550(1)	3377(1)	2464(1)	21(1)
Si(1)	1187(1)	3141(1)	1026(1)	34(1)
Si(2)	3012(1)	1915(1)	3903(1)	32(1)
Si(3)	-582(1)	4265(1)	3259(1)	30(1)
Si(4)	5026(1)	4413(1)	1455(1)	31(1)
N(1)	2136(2)	2862(1)	1655(1)	28(1)
N(2)	3250(2)	2329(1)	3029(1)	28(1)
N(3)	1076(2)	4189(1)	2974(1)	27(1)
N(4)	3959(2)	4112(1)	2210(1)	27(1)
C(1)	2789(2)	2005(1)	1669(1)	33(1)
C(2)	4126(2)	1904(1)	1824(1)	31(1)
C(3)	5196(2)	1681(1)	1285(1)	43(1)
C(4)	6429(2)	1553(2)	1401(2)	52(1)
C(5)	6623(2)	1644(2)	2062(2)	51(1)
C(6)	5586(2)	1886(1)	2607(1)	41(1)
C(7)	4321(2)	2025(1)	2496(1)	30(1)
C(8)	2154(3)	2983(2)	105(1)	57(1)
C(9)	-114(2)	2522(2)	1188(2)	53(1)
C(10)	496(3)	4227(2)	1079(1)	51(1)
C(11)	4118(3)	2162(2)	4430(1)	60(1)
C(12)	1355(2)	2346(2)	4342(1)	47(1)
C(13)	3221(3)	803(1)	3901(1)	52(1)
C(14)	1636(2)	4880(1)	3118(1)	29(1)
C(15)	2892(2)	4611(1)	3370(1)	27(1)
C(16)	2942(2)	4709(1)	4067(1)	36(1)
C(17)	4074(3)	4514(1)	4309(1)	43(1)
C(18)	5189(2)	4206(1)	3852(1)	44(1)
C(19)	5165(2)	4078(1)	3165(1)	36(1)
C(20)	4022(2)	4277(1)	2906(1)	27(1)
C(21)	-1053(2)	4438(2)	4228(1)	44(1)
C(22)	-1031(2)	3299(1)	3104(1)	41(1)
C(23)	-1479(2)	5134(2)	2798(1)	50(1)
C(24)	6692(2)	3834(2)	1343(2)	61(1)
C(25)	4362(3)	4240(2)	691(1)	51(1)
C(26)	5120(3)	5487(1)	1495(1)	51(1)
Zr(2)	2279(1)	8379(1)	2545(1)	19(1)
Si(5)	3732(1)	7536(1)	3969(1)	30(1)
Si(6)	1648(1)	7402(1)	1153(1)	32(1)
Si(7)	5363(1)	8720(1)	1651(1)	30(1)
Si(8)	-228(1)	9722(1)	3560(1)	30(1)
N(5)	2795(2)	7573(1)	3342(1)	24(1)
N(6)	1554(2)	7613(1)	2024(1)	26(1)
N(7)	3728(2)	8973(1)	1992(1)	24(1)
N(8)	865(2)	9378(1)	2808(1)	24(1)
C(27)	3168(2)	9836(1)	1872(1)	28(1)
C(28)	1898(2)	9937(1)	1639(1)	24(1)
C(29)	1820(2)	10227(1)	946(1)	34(1)
C(30)	678(2)	10349(1)	713(1)	40(1)

C(31)	-422(2)	10175(1)	1183(1)	39(1)
C(32)	-373(2)	9870(1)	1869(1)	31(1)
C(33)	781(2)	9740(1)	2113(1)	24(1)
C(34)	6334(2)	9268(2)	2054(2)	51(1)
C(35)	5746(2)	9016(2)	676(1)	52(1)
C(36)	5821(2)	7614(1)	1817(1)	43(1)
C(37)	-1860(2)	9443(2)	3689(2)	62(1)
C(38)	-418(3)	10840(1)	3510(1)	52(1)
C(39)	477(2)	9237(1)	4325(1)	44(1)
C(40)	2210(2)	6839(1)	3351(1)	28(1)
C(41)	835(2)	7045(1)	3242(1)	25(1)
C(42)	-166(2)	6880(1)	3804(1)	34(1)
C(43)	-1432(2)	7034(2)	3732(1)	43(1)
C(44)	-1716(2)	7371(2)	3091(1)	45(1)
C(45)	-751(2)	7553(1)	2533(1)	37(1)
C(46)	547(2)	7393(1)	2589(1)	26(1)
C(47)	5046(2)	6651(2)	3869(1)	47(1)
C(48)	2760(3)	7423(2)	4893(1)	49(1)
C(49)	4391(2)	8492(1)	3841(1)	44(1)
C(50)	457(3)	8084(2)	702(1)	63(1)
C(51)	3270(3)	7554(2)	641(1)	55(1)
C(52)	1405(3)	6349(1)	1138(1)	49(1)

Table S8. Bond lengths [Å] and angles [°] for 6.

Zr(1)-N(1)	2.0543(16)	Zr(1)-N(3)	2.0554(16)
Zr(1)-N(4)	2.0884(16)	Zr(1)-N(2)	2.0949(16)
Zr(1)-C(7)	2.715(2)	Zr(1)-C(20)	2.7306(19)
Si(1)-N(1)	1.7408(18)	Si(1)-C(9)	1.865(3)
Si(1)-C(10)	1.867(2)	Si(1)-C(8)	1.878(2)
Si(2)-N(2)	1.7429(17)	Si(2)-C(12)	1.858(2)
Si(2)-C(13)	1.866(2)	Si(2)-C(11)	1.870(3)
Si(3)-N(3)	1.7396(17)	Si(3)-C(23)	1.869(2)
Si(3)-C(22)	1.873(2)	Si(3)-C(21)	1.877(2)
Si(4)-N(4)	1.7404(16)	Si(4)-C(25)	1.863(3)
Si(4)-C(26)	1.863(2)	Si(4)-C(24)	1.868(3)
N(1)-C(1)	1.498(3)	N(2)-C(7)	1.428(3)
N(3)-C(14)	1.499(2)	N(4)-C(20)	1.431(3)
C(1)-C(2)	1.520(3)	C(2)-C(3)	1.400(3)
C(2)-C(7)	1.413(3)	C(3)-C(4)	1.378(4)
C(4)-C(5)	1.377(4)	C(5)-C(6)	1.394(3)
C(6)-C(7)	1.407(3)	C(14)-C(15)	1.522(3)
C(15)-C(16)	1.396(3)	C(15)-C(20)	1.413(3)
C(16)-C(17)	1.382(3)	C(17)-C(18)	1.382(4)
C(18)-C(19)	1.382(3)	C(19)-C(20)	1.409(3)
Zr(2)-N(5)	2.0532(16)	Zr(2)-N(7)	2.0536(15)
Zr(2)-N(8)	2.0926(16)	Zr(2)-N(6)	2.0950(16)
Zr(2)-C(46)	2.7217(19)	Zr(2)-C(33)	2.7344(19)
Si(5)-N(5)	1.7420(16)	Si(5)-C(47)	1.865(3)
Si(5)-C(49)	1.866(2)	Si(5)-C(48)	1.873(2)
Si(6)-N(6)	1.7455(16)	Si(6)-C(51)	1.860(3)
Si(6)-C(52)	1.865(2)	Si(6)-C(50)	1.870(3)
Si(7)-N(7)	1.7352(16)	Si(7)-C(36)	1.867(2)
Si(7)-C(34)	1.868(2)	Si(7)-C(35)	1.874(2)
Si(8)-N(8)	1.7424(16)	Si(8)-C(39)	1.863(2)
Si(8)-C(37)	1.870(3)	Si(8)-C(38)	1.869(2)
N(5)-C(40)	1.498(2)	N(6)-C(46)	1.432(3)
N(7)-C(27)	1.496(2)	N(8)-C(33)	1.433(2)
C(27)-C(28)	1.518(3)	C(28)-C(29)	1.394(3)
C(28)-C(33)	1.415(3)	C(29)-C(30)	1.384(3)
C(30)-C(31)	1.384(3)	C(31)-C(32)	1.382(3)
C(32)-C(33)	1.406(3)	C(40)-C(41)	1.522(3)
C(41)-C(42)	1.397(3)	C(41)-C(46)	1.413(3)
C(42)-C(43)	1.383(3)	C(43)-C(44)	1.385(3)
C(44)-C(45)	1.377(3)	C(45)-C(46)	1.408(3)

N(1)-Zr(1)-N(3)	115.08(6)	N(1)-Zr(1)-N(4)	118.22(6)
N(3)-Zr(1)-N(4)	97.92(6)	N(1)-Zr(1)-N(2)	98.52(6)
N(3)-Zr(1)-N(2)	119.59(6)	N(4)-Zr(1)-N(2)	108.58(6)
N(1)-Zr(1)-C(7)	83.16(7)	N(3)-Zr(1)-C(7)	150.53(6)
N(4)-Zr(1)-C(7)	92.47(6)	N(2)-Zr(1)-C(7)	31.31(6)
N(1)-Zr(1)-C(20)	149.10(6)	N(3)-Zr(1)-C(20)	82.47(6)
N(4)-Zr(1)-C(20)	31.06(6)	N(2)-Zr(1)-C(20)	93.42(6)
C(7)-Zr(1)-C(20)	92.91(6)	N(1)-Si(1)-C(9)	110.13(11)
N(1)-Si(1)-C(10)	108.54(10)	C(9)-Si(1)-C(10)	110.75(12)
N(1)-Si(1)-C(8)	111.39(11)	C(9)-Si(1)-C(8)	107.28(12)
C(10)-Si(1)-C(8)	108.75(13)	N(2)-Si(2)-C(12)	106.63(10)
N(2)-Si(2)-C(13)	108.84(10)	C(12)-Si(2)-C(13)	111.62(12)
N(2)-Si(2)-C(11)	114.54(11)	C(12)-Si(2)-C(11)	106.78(13)
C(13)-Si(2)-C(11)	108.46(13)	N(3)-Si(3)-C(23)	112.53(10)

N(3)-Si(3)-C(22)	107.57(9)	C(23)-Si(3)-C(22)	110.82(12)
N(3)-Si(3)-C(21)	109.77(10)	C(23)-Si(3)-C(21)	105.99(12)
C(22)-Si(3)-C(21)	110.19(11)	N(4)-Si(4)-C(25)	105.63(10)
N(4)-Si(4)-C(26)	108.54(10)	C(25)-Si(4)-C(26)	112.66(12)
N(4)-Si(4)-C(24)	114.68(11)	C(25)-Si(4)-C(24)	107.50(14)
C(26)-Si(4)-C(24)	107.94(13)	C(1)-N(1)-Si(1)	115.16(13)
C(1)-N(1)-Zr(1)	107.67(12)	Si(1)-N(1)-Zr(1)	137.04(9)
C(7)-N(2)-Si(2)	122.20(14)	C(7)-N(2)-Zr(1)	99.05(12)
Si(2)-N(2)-Zr(1)	137.70(9)	C(14)-N(3)-Si(3)	115.43(13)
C(14)-N(3)-Zr(1)	108.04(12)	Si(3)-N(3)-Zr(1)	136.54(9)
C(20)-N(4)-Si(4)	122.20(13)	C(20)-N(4)-Zr(1)	100.09(11)
Si(4)-N(4)-Zr(1)	137.23(9)	N(1)-C(1)-C(2)	112.62(16)
C(3)-C(2)-C(7)	119.0(2)	C(3)-C(2)-C(1)	119.1(2)
C(7)-C(2)-C(1)	121.87(18)	C(4)-C(3)-C(2)	121.7(2)
C(5)-C(4)-C(3)	119.5(2)	C(4)-C(5)-C(6)	120.5(2)
C(5)-C(6)-C(7)	120.7(2)	C(6)-C(7)-C(2)	118.50(19)
C(6)-C(7)-N(2)	121.8(2)	C(2)-C(7)-N(2)	119.59(18)
C(6)-C(7)-Zr(1)	132.29(15)	C(2)-C(7)-Zr(1)	86.72(12)
N(2)-C(7)-Zr(1)	49.64(9)	N(3)-C(14)-C(15)	112.54(16)
C(16)-C(15)-C(20)	119.06(19)	C(16)-C(15)-C(14)	119.83(19)
C(20)-C(15)-C(14)	121.09(18)	C(17)-C(16)-C(15)	121.9(2)
C(18)-C(17)-C(16)	119.2(2)	C(17)-C(18)-C(19)	120.4(2)
C(18)-C(19)-C(20)	121.4(2)	C(19)-C(20)-C(15)	118.08(19)
C(19)-C(20)-N(4)	122.32(19)	C(15)-C(20)-N(4)	119.50(18)
C(19)-C(20)-Zr(1)	132.74(14)	C(15)-C(20)-Zr(1)	87.26(12)
N(4)-C(20)-Zr(1)	48.85(9)	N(5)-Zr(2)-N(7)	113.84(6)
N(5)-Zr(2)-N(8)	119.03(6)	N(7)-Zr(2)-N(8)	98.32(6)
N(5)-Zr(2)-N(6)	98.31(6)	N(7)-Zr(2)-N(6)	119.53(6)
N(8)-Zr(2)-N(6)	109.03(6)	N(5)-Zr(2)-C(46)	82.40(6)
N(7)-Zr(2)-C(46)	150.70(6)	N(8)-Zr(2)-C(46)	93.88(6)
N(6)-Zr(2)-C(46)	31.28(6)	N(5)-Zr(2)-C(33)	150.05(6)
N(7)-Zr(2)-C(33)	82.05(6)	N(8)-Zr(2)-C(33)	31.06(6)
N(6)-Zr(2)-C(33)	94.72(6)	C(46)-Zr(2)-C(33)	95.50(6)
N(5)-Si(5)-C(47)	110.55(10)	N(5)-Si(5)-C(49)	107.66(9)
C(47)-Si(5)-C(49)	111.30(12)	N(5)-Si(5)-C(48)	111.30(10)
C(47)-Si(5)-C(48)	106.58(12)	C(49)-Si(5)-C(48)	109.48(12)
N(6)-Si(6)-C(51)	107.01(10)	N(6)-Si(6)-C(52)	109.71(10)
C(51)-Si(6)-C(52)	110.97(13)	N(6)-Si(6)-C(50)	113.93(10)
C(51)-Si(6)-C(50)	106.64(14)	C(52)-Si(6)-C(50)	108.54(13)
N(7)-Si(7)-C(36)	107.94(9)	N(7)-Si(7)-C(34)	111.93(10)
C(36)-Si(7)-C(34)	110.76(12)	N(7)-Si(7)-C(35)	110.54(10)
C(36)-Si(7)-C(35)	110.13(12)	C(34)-Si(7)-C(35)	105.55(12)
N(8)-Si(8)-C(39)	105.38(10)	N(8)-Si(8)-C(37)	115.02(10)
C(39)-Si(8)-C(37)	107.31(13)	N(8)-Si(8)-C(38)	108.72(10)
C(39)-Si(8)-C(38)	112.41(11)	C(37)-Si(8)-C(38)	108.09(14)
C(40)-N(5)-Si(5)	115.33(12)	C(40)-N(5)-Zr(2)	108.51(11)
Si(5)-N(5)-Zr(2)	136.15(9)	C(46)-N(6)-Si(6)	121.34(12)
C(46)-N(6)-Zr(2)	99.29(11)	Si(6)-N(6)-Zr(2)	137.57(9)
C(27)-N(7)-Si(7)	115.62(12)	C(27)-N(7)-Zr(2)	108.11(11)
Si(7)-N(7)-Zr(2)	136.28(9)	C(33)-N(8)-Si(8)	121.48(13)
C(33)-N(8)-Zr(2)	100.04(11)	Si(8)-N(8)-Zr(2)	137.63(9)
N(7)-C(27)-C(28)	112.09(15)	C(29)-C(28)-C(33)	118.95(18)
C(29)-C(28)-C(27)	119.88(18)	C(33)-C(28)-C(27)	121.17(17)
C(30)-C(29)-C(28)	122.1(2)	C(29)-C(30)-C(31)	118.9(2)
C(32)-C(31)-C(30)	120.5(2)	C(31)-C(32)-C(33)	121.3(2)
C(32)-C(33)-C(28)	118.21(18)	C(32)-C(33)-N(8)	122.02(17)
C(28)-C(33)-N(8)	119.69(17)	C(32)-C(33)-Zr(2)	132.52(14)
C(28)-C(33)-Zr(2)	87.60(11)	N(8)-C(33)-Zr(2)	48.90(9)
N(5)-C(40)-C(41)	112.21(16)	C(42)-C(41)-C(46)	119.28(19)

C(42)-C(41)-C(40)	118.92(18)	C(46)-C(41)-C(40)	121.80(17)
C(43)-C(42)-C(41)	121.6(2)	C(42)-C(43)-C(44)	119.2(2)
C(45)-C(44)-C(43)	120.4(2)	C(44)-C(45)-C(46)	121.6(2)
C(45)-C(46)-C(41)	117.94(18)	C(45)-C(46)-N(6)	122.07(18)
C(41)-C(46)-N(6)	119.90(17)	C(45)-C(46)-Zr(2)	131.83(14)
C(41)-C(46)-Zr(2)	87.74(11)	N(6)-C(46)-Zr(2)	49.43(8)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters [$Å^2$ x 10^3] for 6.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Zr(1)	21(1)	21(1)	21(1)	-3(1)	-2(1)	-4(1)
Si(1)	35(1)	36(1)	33(1)	-14(1)	-11(1)	1(1)
Si(2)	40(1)	28(1)	29(1)	3(1)	-9(1)	-9(1)
Si(3)	25(1)	34(1)	30(1)	-8(1)	0(1)	-2(1)
Si(4)	29(1)	30(1)	32(1)	1(1)	2(1)	-8(1)
N(1)	28(1)	25(1)	30(1)	-7(1)	-4(1)	-3(1)
N(2)	27(1)	27(1)	28(1)	0(1)	-5(1)	-3(1)
N(3)	26(1)	26(1)	28(1)	-4(1)	-4(1)	-5(1)
N(4)	26(1)	28(1)	26(1)	-2(1)	-4(1)	-6(1)
C(1)	39(1)	26(1)	35(1)	-10(1)	-6(1)	-3(1)
C(2)	32(1)	20(1)	35(1)	-1(1)	-2(1)	0(1)
C(3)	46(2)	32(1)	38(1)	-1(1)	2(1)	7(1)
C(4)	40(2)	44(2)	54(2)	4(1)	8(1)	10(1)
C(5)	25(1)	46(2)	72(2)	11(1)	-4(1)	4(1)
C(6)	32(1)	40(1)	47(1)	6(1)	-10(1)	-1(1)
C(7)	29(1)	21(1)	36(1)	3(1)	-2(1)	-2(1)
C(8)	65(2)	71(2)	36(1)	-18(1)	-12(1)	-1(2)
C(9)	40(1)	60(2)	66(2)	-29(1)	-18(1)	-4(1)
C(10)	63(2)	43(2)	48(2)	-10(1)	-22(1)	6(1)
C(11)	73(2)	72(2)	45(2)	5(1)	-28(1)	-23(2)
C(12)	55(2)	49(2)	31(1)	-2(1)	1(1)	-8(1)
C(13)	69(2)	35(1)	49(2)	6(1)	-6(1)	-12(1)
C(14)	32(1)	24(1)	31(1)	-8(1)	-2(1)	-3(1)
C(15)	33(1)	20(1)	29(1)	-2(1)	-6(1)	-9(1)
C(16)	47(1)	32(1)	30(1)	-5(1)	-4(1)	-12(1)
C(17)	63(2)	40(1)	33(1)	1(1)	-20(1)	-18(1)
C(18)	49(2)	44(1)	49(2)	4(1)	-27(1)	-16(1)
C(19)	30(1)	39(1)	41(1)	-1(1)	-9(1)	-9(1)
C(20)	31(1)	25(1)	28(1)	0(1)	-6(1)	-12(1)
C(21)	40(1)	53(2)	37(1)	-14(1)	5(1)	-11(1)
C(22)	34(1)	46(1)	46(1)	-11(1)	-4(1)	-10(1)
C(23)	40(1)	49(2)	55(2)	-8(1)	-8(1)	8(1)
C(24)	38(2)	61(2)	68(2)	3(1)	13(1)	2(1)
C(25)	67(2)	59(2)	30(1)	-2(1)	1(1)	-32(1)
C(26)	62(2)	38(1)	54(2)	4(1)	-8(1)	-20(1)
Zr(2)	20(1)	20(1)	19(1)	1(1)	-5(1)	-6(1)
Si(5)	32(1)	33(1)	30(1)	10(1)	-15(1)	-15(1)
Si(6)	48(1)	25(1)	27(1)	-3(1)	-16(1)	-7(1)
Si(7)	23(1)	33(1)	32(1)	4(1)	-2(1)	-7(1)
Si(8)	30(1)	32(1)	28(1)	-9(1)	0(1)	-5(1)
N(5)	25(1)	24(1)	26(1)	3(1)	-7(1)	-9(1)
N(6)	30(1)	25(1)	25(1)	0(1)	-10(1)	-9(1)
N(7)	23(1)	24(1)	25(1)	2(1)	-6(1)	-6(1)
N(8)	24(1)	26(1)	24(1)	0(1)	-5(1)	-6(1)
C(27)	27(1)	24(1)	31(1)	2(1)	-4(1)	-9(1)
C(28)	28(1)	18(1)	27(1)	-1(1)	-6(1)	-2(1)
C(29)	42(1)	28(1)	29(1)	1(1)	-3(1)	-5(1)
C(30)	57(2)	30(1)	32(1)	2(1)	-21(1)	2(1)

C(31)	40(1)	34(1)	46(1)	-7(1)	-25(1)	6(1)
C(32)	25(1)	31(1)	37(1)	-6(1)	-9(1)	0(1)
C(33)	28(1)	19(1)	27(1)	-5(1)	-7(1)	-1(1)
C(34)	33(1)	56(2)	68(2)	9(1)	-16(1)	-21(1)
C(35)	47(2)	55(2)	41(1)	6(1)	10(1)	-5(1)
C(36)	39(1)	39(1)	45(1)	2(1)	-5(1)	-1(1)
C(37)	39(2)	91(2)	54(2)	-27(2)	13(1)	-21(2)
C(38)	68(2)	36(1)	51(2)	-15(1)	-18(1)	5(1)
C(39)	58(2)	42(1)	28(1)	-5(1)	-1(1)	-5(1)
C(40)	30(1)	24(1)	31(1)	5(1)	-11(1)	-9(1)
C(41)	28(1)	20(1)	31(1)	-4(1)	-7(1)	-7(1)
C(42)	38(1)	36(1)	30(1)	-4(1)	-4(1)	-14(1)
C(43)	31(1)	49(2)	48(2)	-9(1)	4(1)	-16(1)
C(44)	26(1)	49(2)	64(2)	-8(1)	-12(1)	-11(1)
C(45)	33(1)	40(1)	45(1)	1(1)	-18(1)	-13(1)
C(46)	29(1)	22(1)	32(1)	-5(1)	-8(1)	-8(1)
C(47)	36(1)	45(1)	62(2)	19(1)	-22(1)	-12(1)
C(48)	56(2)	65(2)	31(1)	12(1)	-18(1)	-21(1)
C(49)	56(2)	44(1)	43(1)	10(1)	-25(1)	-26(1)
C(50)	101(2)	49(2)	47(2)	-11(1)	-47(2)	12(2)
C(51)	75(2)	62(2)	29(1)	-3(1)	-3(1)	-26(2)
C(52)	69(2)	34(1)	49(2)	-10(1)	-16(1)	-13(1)

Figure Captions

Figure S1. X-ray crystal structure of **2** with atom numbering scheme.

Figure S2. X-ray crystal structure of **4** with atom numbering scheme.

Figure S3. X-ray crystal structure of **6** with atom numbering scheme.

Figure S1

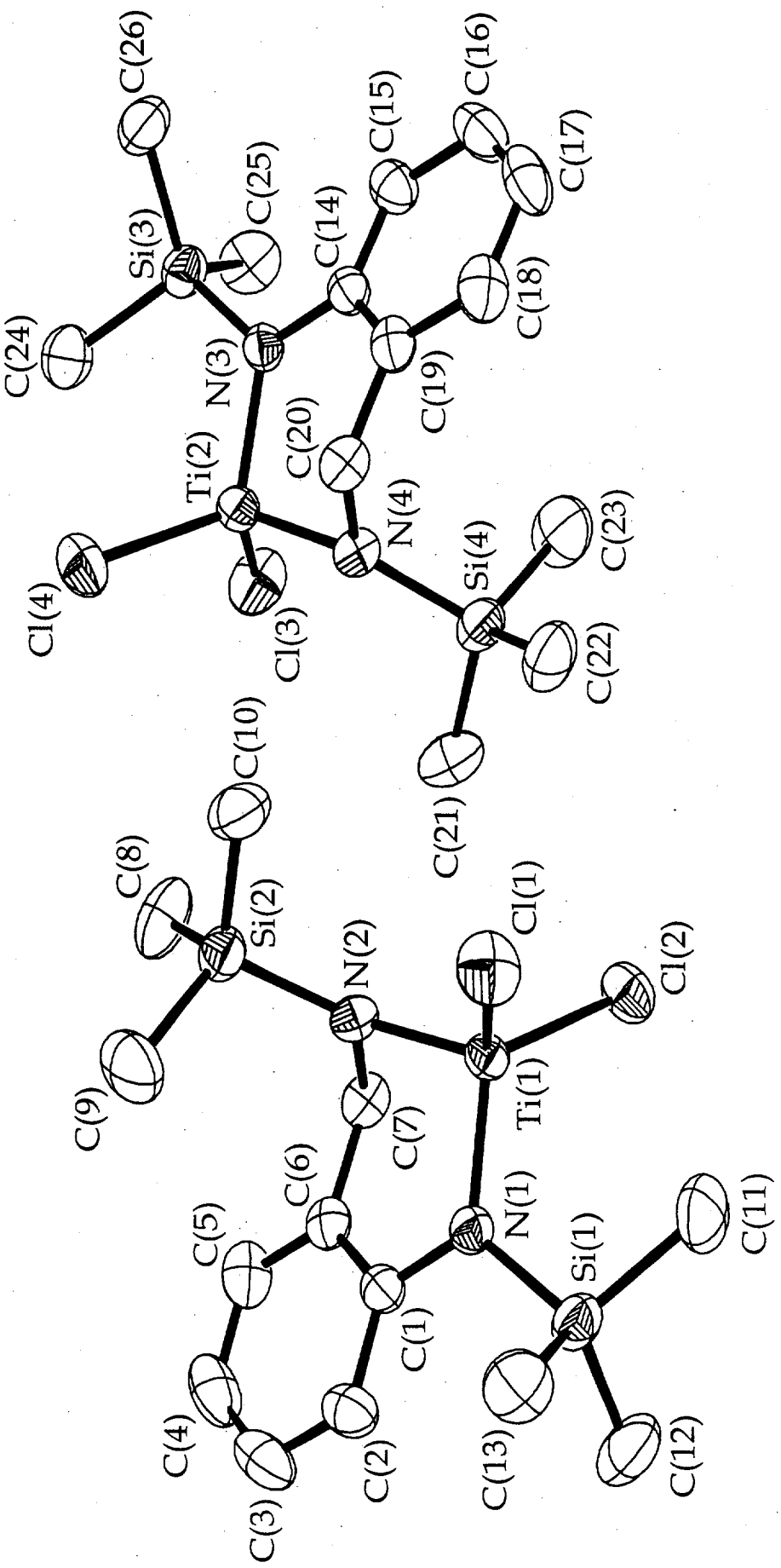

Figure S2

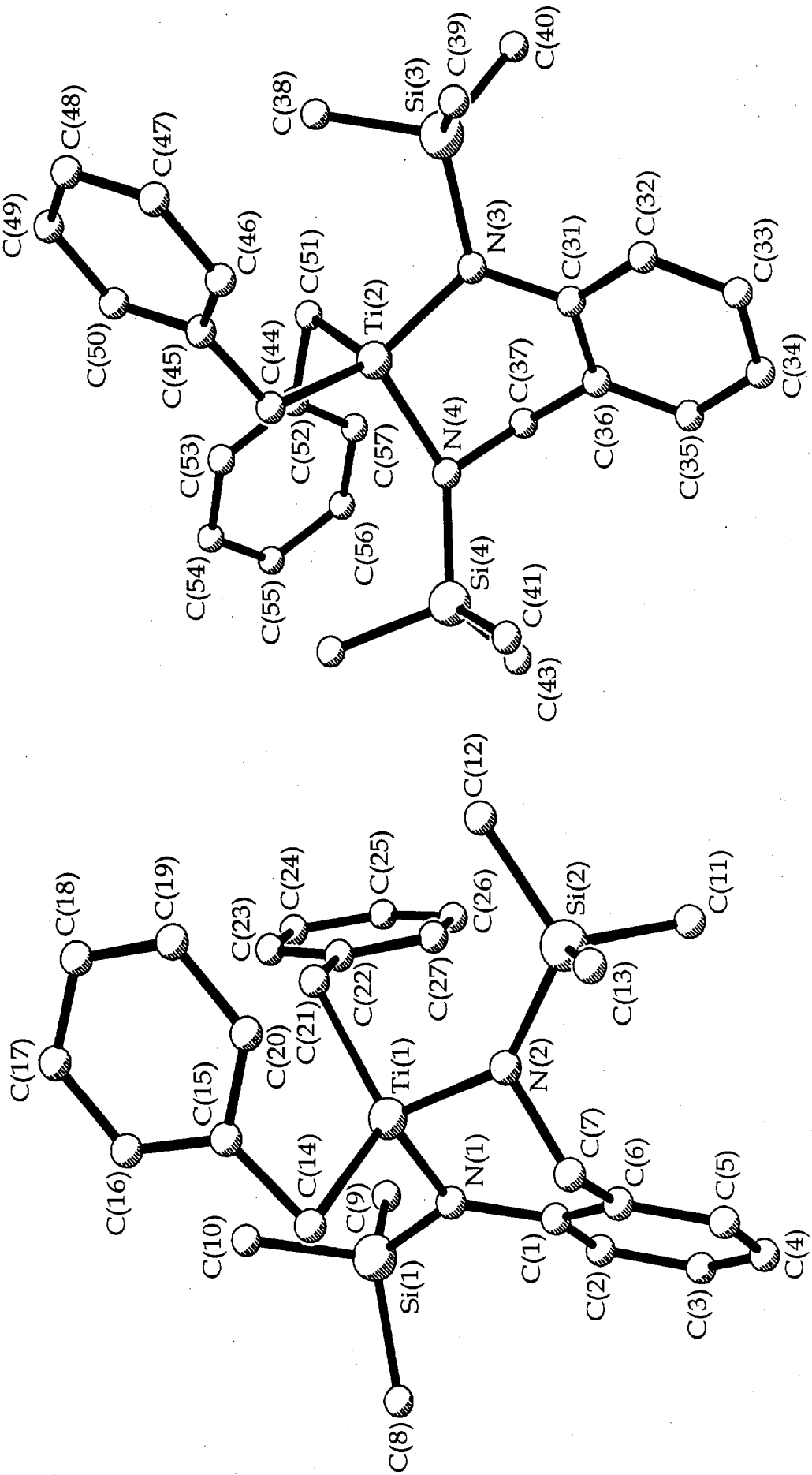

Figure S3