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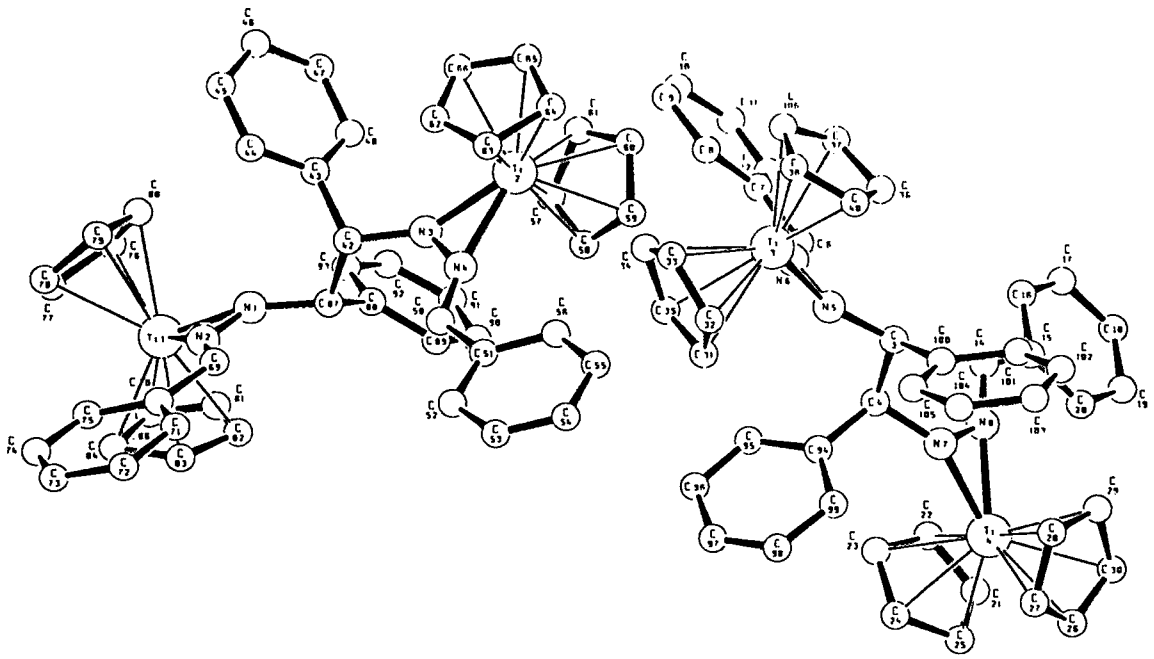


SCHAKAL

Table 1. Crystal data and structure refinement for 3.

Identification code	737
Empirical formula	C48 H44 N4 Ti2
Formula weight	772.67
Crystal system	Monoclinic
Space group	Pn
Unit cell dimensions	a= 12.007(2) A alpha= 90 deg. b= 15.337(2) A beta= 103.99(2) deg. c= 22.660(4) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	2000
Theta for cell determination	4 to 18 deg
Volume	4049.1(11) A^3
Z	4
Density (calculated)	1.267 Mg/m^3
Absorption coefficient	0.432 mm^-1
F(000)	1616
Crystal colour	brown-black
Crystal description	prism
Crystal size	0.5 x 0.3 x 0.2 mm
Temperature	293(2) K
Wavelength	0.71069 A
Radiation type	MoK\a
Radiation source	fine-focus sealed tube
Monochromator	graphite
Measurment device	STOE-IPDS
Scan method	laser scanned imaging plate
Standards (intensity + orient.)	50-200
Intensity after	360 sec
Theta range for data collection	1.85 to 24.34 deg.
Index ranges	-13<=h<=13, -16<=k<=16, 0<=l<=26
Reflections collected	10793
Independent reflections	5982 [R(int) = 0.0592]

Reflections unique	5982
Reflections observed	3181
Criterion	>2sigma(I)
Absorption correction	No
Structure solution primary	direct
Structure solution secondary	difmap
Hydrogen positions	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5982 / 2 / 973
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.0983
R indices (all data)	R1 = 0.1171, wR2 = 0.1261
Goodness-of-fit on F^2(all)	0.922
Goodness-of-fit on F^2(obs)	1.076
Shift/esd(mean)	0.138
Absolute structure parameter	0.06(4)
Weighting scheme	
calc w=1/[\s^2^(Fo^2^)+(0.0620P)^2^+0.0855P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	0.190 and -0.265 e.A^-3
Diff. density rms	0.043
Data collection	STOE-EXPOSE
Cell refinement	STOE-CELL
Data reduction	STOE-INTEGRATE
Structure solution	SHELXS-86 (Sheldrick, 1990)
Structure refinement	SHELXL-93 (Sheldrick, 1993)
Molecular graphics	SCHAKAL-92
Publication material	SHELXL-93

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

	x	y	z	U(eq)
C(3)	751(8)	3175(5)	7312(4)	38(2)
C(4)	814(8)	4184(5)	7329(4)	39(2)
C(6)	2971(10)	3011(7)	8184(5)	55(3)
C(7)	4074(9)	2816(6)	8597(5)	48(3)
C(8)	4210(10)	2320(7)	9116(5)	65(3)
C(9)	5263(15)	2138(9)	9502(7)	91(5)
C(10)	6210(16)	2515(9)	9369(7)	104(6)
C(11)	6166(12)	2989(9)	8849(8)	93(5)
C(12)	5074(12)	3159(7)	8482(6)	75(4)
C(14)	2182(11)	4351(7)	6413(6)	65(4)
C(15)	2870(13)	4572(7)	5996(6)	68(4)
C(16)	3997(14)	4288(8)	6139(7)	97(5)
C(17)	4733(18)	4487(12)	5786(11)	133(8)
C(18)	4380(20)	4978(13)	5274(10)	134(9)
C(19)	3281(21)	5303(10)	5129(7)	124(8)
C(20)	2539(12)	5123(7)	5492(5)	79(4)
C(21)	647(22)	6971(10)	6086(7)	127(8)
C(22)	1348(12)	6561(7)	6554(7)	76(4)
C(23)	737(17)	6473(7)	6992(6)	88(5)
C(24)	-341(18)	6842(14)	6753(13)	151(11)
C(25)	-416(29)	7136(14)	6173(15)	191(18)
C(26)	-1849(18)	5937(14)	5345(8)	136(8)
C(27)	-2201(14)	5461(11)	5730(9)	127(7)
C(28)	-1724(15)	4615(10)	5719(9)	100(6)
C(29)	-1025(15)	4646(10)	5340(8)	103(5)
C(30)	-1061(18)	5524(12)	5096(7)	119(7)
C(31)	-199(13)	2939(8)	8965(6)	74(4)
C(32)	-662(14)	2106(9)	9024(8)	101(6)
C(33)	167(20)	1635(11)	9433(7)	121(7)
C(34)	1151(16)	2133(10)	9601(6)	93(5)
C(35)	930(13)	2943(8)	9313(5)	73(4)
C(36)	852(18)	897(8)	7739(6)	87(5)
C(37)	1880(13)	769(8)	8157(9)	91(5)
C(38)	433(32)	334(11)	8552(12)	156(13)
C(40)	16(15)	608(12)	7983(13)	143(10)
C(42)	-1250(8)	755(6)	12273(4)	46(3)
C(43)	-147(10)	326(5)	12626(5)	53(3)
C(44)	-68(11)	55(7)	13211(6)	81(4)
C(45)	927(20)	-337(9)	13531(10)	141(9)
C(46)	1823(23)	-499(14)	13280(14)	185(15)
C(47)	1751(14)	-176(11)	12713(11)	144(8)
C(48)	765(11)	238(8)	12369(7)	91(4)
C(50)	-3563(11)	624(7)	11466(6)	61(3)
C(51)	-4697(11)	417(6)	11096(6)	54(3)
C(52)	-5644(11)	666(7)	11304(6)	63(3)
C(53)	-6739(13)	486(9)	10946(8)	85(4)
C(54)	-6845(13)	92(9)	10395(7)	88(5)
C(55)	-5936(13)	-183(8)	10203(6)	75(4)
C(56)	-4852(11)	-10(7)	10541(6)	76(4)
C(57)	-400(14)	452(11)	10601(6)	81(5)
C(58)	-1510(15)	538(8)	10293(6)	81(4)
C(59)	-1887(16)	-194(12)	9990(6)	103(6)
C(60)	-966(24)	-784(11)	10106(9)	129(8)
C(61)	-10(16)	-377(14)	10495(10)	117(7)
C(62)	-1694(18)	-1463(8)	11827(7)	84(4)
C(63)	-2614(13)	-1610(9)	11383(11)	103(6)
C(64)	-2161(24)	-1976(9)	10908(8)	120(8)

C(65)	-1005(24)	-2040(10)	11148(13)	130(8)
C(66)	-721(14)	-1697(8)	11694(9)	96(5)
C(69)	-2562(10)	1961(6)	13195(5)	50(3)
C(70)	-3265(11)	2193(6)	13612(5)	51(3)
C(71)	-4398(12)	1919(7)	13491(6)	68(3)
C(72)	-5123(12)	2148(8)	13873(8)	84(5)
C(73)	-4668(15)	2625(9)	14390(7)	88(5)
C(74)	-3567(13)	2886(9)	14521(7)	80(4)
C(75)	-2851(11)	2686(7)	14147(5)	67(3)
C(76)	1876(12)	2762(10)	14032(8)	100(5)
C(77)	1384(18)	3175(9)	14450(8)	116(7)
C(78)	562(15)	2607(15)	14582(7)	118(7)
C(79)	597(13)	1896(8)	14237(6)	80(4)
C(80)	1399(12)	1986(9)	13909(7)	84(4)
C(81)	182(17)	4251(9)	12938(11)	108(6)
C(82)	-883(18)	4022(8)	12742(7)	89(5)
C(83)	-1414(13)	4155(9)	13184(12)	105(6)
C(84)	-689(30)	4486(10)	13715(8)	156(12)
C(86)	372(20)	4529(8)	13470(14)	147(11)
C(87)	-1190(8)	1788(5)	12292(4)	45(3)
C(88)	-466(11)	2146(6)	11893(6)	61(3)
C(89)	-1044(14)	2406(7)	11295(6)	90(5)
C(90)	-315(26)	2748(9)	10926(10)	146(10)
C(91)	839(30)	2823(14)	11148(14)	177(14)
C(92)	1359(20)	2610(14)	11739(12)	171(11)
C(93)	672(13)	2289(8)	12109(7)	104(5)
C(94)	160(11)	4594(6)	7748(5)	54(3)
C(95)	731(13)	4828(6)	8329(6)	81(4)
C(96)	209(18)	5228(8)	8726(8)	102(6)
C(97)	-919(24)	5353(10)	8547(12)	133(9)
C(98)	-1546(17)	5143(13)	7994(10)	138(7)
C(99)	-997(14)	4747(8)	7569(7)	99(4)
C(100)	-385(9)	2807(5)	6935(5)	52(3)
C(101)	-466(11)	2582(6)	6324(5)	64(3)
C(102)	-1446(16)	2235(9)	5982(8)	107(6)
C(103)	-2402(17)	2144(10)	6198(10)	119(7)
C(104)	-2349(13)	2364(9)	6807(10)	115(6)
C(105)	-1328(11)	2700(9)	7172(6)	87(4)
C(106)	1662(23)	458(9)	8660(8)	113(7)
N(1)	-797(7)	2119(5)	12910(4)	55(2)
N(2)	-1516(9)	2240(5)	13274(4)	50(2)
N(3)	-1522(7)	424(5)	11652(4)	47(2)
N(4)	-2622(8)	317(5)	11348(4)	44(2)
N(5)	945(7)	2809(4)	7921(4)	46(2)
N(6)	1998(9)	2709(5)	8266(4)	46(2)
N(7)	406(7)	4567(5)	6713(4)	49(2)
N(8)	1154(9)	4683(5)	6361(4)	52(3)
Ti(4)	-215(2)	5604(1)	6148(1)	59(1)
Ti(3)	844(2)	1853(1)	8544(1)	50(1)
Ti(2)	-1507(2)	-544(1)	11027(1)	49(1)
Ti(1)	-75(2)	3048(1)	13541(1)	57(1)

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

C(3)-N(5)	1.456(11)
C(3)-C(100)	1.531(12)
C(3)-C(4)	1.550(11)
C(4)-N(7)	1.485(11)
C(4)-C(94)	1.506(13)
C(6)-N(6)	1.311(13)
C(6)-C(7)	1.457(14)
C(7)-C(8)	1.376(14)
C(7)-C(12)	1.39(2)
C(8)-C(9)	1.38(2)
C(9)-C(10)	1.37(2)
C(10)-C(11)	1.37(2)
C(11)-C(12)	1.40(2)
C(14)-N(8)	1.314(13)
C(14)-C(15)	1.44(2)
C(15)-C(16)	1.38(2)
C(15)-C(20)	1.40(2)
C(16)-C(17)	1.36(2)
C(17)-C(18)	1.36(3)
C(18)-C(19)	1.37(2)
C(19)-C(20)	1.38(2)
C(21)-C(25)	1.36(3)
C(21)-C(22)	1.34(2)
C(21)-Ti(4)	2.357(14)
C(22)-C(23)	1.38(2)
C(22)-Ti(4)	2.385(11)
C(23)-C(24)	1.40(2)
C(23)-Ti(4)	2.384(11)
C(24)-C(25)	1.37(3)
C(24)-Ti(4)	2.368(14)
C(25)-Ti(4)	2.36(2)
C(26)-C(27)	1.29(2)
C(26)-C(30)	1.37(2)
C(26)-Ti(4)	2.39(2)
C(27)-C(28)	1.42(2)
C(27)-Ti(4)	2.35(2)
C(28)-C(29)	1.34(2)
C(28)-Ti(4)	2.382(14)
C(29)-C(30)	1.45(2)
C(29)-Ti(4)	2.365(13)
C(30)-Ti(4)	2.36(2)
C(31)-C(32)	1.41(2)
C(31)-C(35)	1.39(2)
C(31)-Ti(3)	2.414(13)
C(32)-C(33)	1.39(2)
C(32)-Ti(3)	2.357(12)
C(33)-C(34)	1.38(2)
C(33)-Ti(3)	2.371(13)
C(34)-C(35)	1.40(2)
C(34)-Ti(3)	2.373(13)
C(35)-Ti(3)	2.399(11)
C(36)-C(40)	1.33(2)
C(36)-C(37)	1.38(2)
C(36)-Ti(3)	2.343(11)
C(37)-C(106)	1.32(2)
C(37)-Ti(3)	2.369(11)
C(38)-C(40)	1.33(3)
C(38)-C(106)	1.45(3)
C(38)-Ti(3)	2.38(2)
C(40)-Ti(3)	2.375(14)
C(42)-N(3)	1.458(12)
C(42)-C(43)	1.522(13)

C(42)-C(87)	1.586(12)
C(43)-C(44)	1.37(2)
C(43)-C(48)	1.37(2)
C(44)-C(45)	1.38(2)
C(45)-C(46)	1.36(3)
C(46)-C(47)	1.36(3)
C(47)-C(48)	1.40(2)
C(50)-N(4)	1.309(12)
C(50)-C(51)	1.45(2)
C(51)-C(52)	1.386(14)
C(51)-C(56)	1.39(2)
C(52)-C(53)	1.40(2)
C(53)-C(54)	1.37(2)
C(54)-C(55)	1.34(2)
C(55)-C(56)	1.37(2)
C(57)-C(58)	1.35(2)
C(57)-C(61)	1.39(2)
C(57)-Ti(2)	2.377(12)
C(58)-C(59)	1.34(2)
C(58)-Ti(2)	2.350(11)
C(59)-C(60)	1.40(2)
C(59)-Ti(2)	2.345(13)
C(60)-C(61)	1.41(2)
C(60)-Ti(2)	2.360(14)
C(61)-Ti(2)	2.41(2)
C(62)-C(66)	1.32(2)
C(62)-C(63)	1.32(2)
C(62)-Ti(2)	2.350(12)
C(63)-C(64)	1.43(2)
C(63)-Ti(2)	2.368(13)
C(64)-C(65)	1.37(2)
C(64)-Ti(2)	2.326(12)
C(65)-C(66)	1.31(2)
C(65)-Ti(2)	2.371(14)
C(66)-Ti(2)	2.369(12)
C(69)-N(2)	1.298(12)
C(69)-C(70)	1.46(2)
C(70)-C(71)	1.39(2)
C(70)-C(75)	1.412(14)
C(71)-C(72)	1.41(2)
C(72)-C(73)	1.38(2)
C(73)-C(74)	1.34(2)
C(74)-C(75)	1.38(2)
C(76)-C(80)	1.32(2)
C(76)-C(77)	1.38(2)
C(76)-Ti(1)	2.378(12)
C(77)-C(78)	1.40(2)
C(77)-Ti(1)	2.367(14)
C(78)-C(79)	1.35(2)
C(78)-Ti(1)	2.39(2)
C(79)-C(80)	1.36(2)
C(79)-Ti(1)	2.376(11)
C(80)-Ti(1)	2.402(12)
C(81)-C(86)	1.25(2)
C(81)-C(82)	1.30(2)
C(81)-Ti(1)	2.361(14)
C(82)-C(83)	1.33(2)
C(82)-Ti(1)	2.367(13)
C(83)-C(84)	1.40(2)
C(83)-Ti(1)	2.343(11)
C(84)-C(86)	1.51(3)
C(84)-Ti(1)	2.387(12)
C(86)-Ti(1)	2.348(14)
C(87)-N(1)	1.456(12)
C(87)-C(88)	1.502(13)
C(88)-C(93)	1.35(2)

C(88)-C(89)	1.42(2)
C(89)-C(90)	1.45(2)
C(90)-C(91)	1.36(3)
C(91)-C(92)	1.37(3)
C(92)-C(93)	1.40(2)
C(94)-C(99)	1.37(2)
C(94)-C(95)	1.38(2)
C(95)-C(96)	1.36(2)
C(96)-C(97)	1.33(2)
C(97)-C(98)	1.34(2)
C(98)-C(99)	1.43(2)
C(100)-C(105)	1.375(14)
C(100)-C(101)	1.408(14)
C(101)-C(102)	1.35(2)
C(102)-C(103)	1.36(2)
C(103)-C(104)	1.41(2)
C(104)-C(105)	1.40(2)
C(106)-Ti(3)	2.342(14)
N(1)-N(2)	1.343(11)
N(1)-Ti(1)	2.057(8)
N(2)-Ti(1)	2.096(10)
N(3)-N(4)	1.344(10)
N(3)-Ti(2)	2.054(8)
N(4)-Ti(2)	2.129(9)
N(5)-N(6)	1.325(10)
N(5)-Ti(3)	2.059(8)
N(6)-Ti(3)	2.112(9)
N(7)-N(8)	1.349(11)
N(7)-Ti(4)	2.065(8)
N(8)-Ti(4)	2.133(10)

N(5)-C(3)-C(100)	107.7(7)
N(5)-C(3)-C(4)	111.4(7)
C(100)-C(3)-C(4)	114.4(7)
N(7)-C(4)-C(94)	108.8(7)
N(7)-C(4)-C(3)	111.6(7)
C(94)-C(4)-C(3)	113.7(7)
N(6)-C(6)-C(7)	122.6(11)
C(8)-C(7)-C(12)	116.0(11)
C(8)-C(7)-C(6)	124.4(11)
C(12)-C(7)-C(6)	119.6(12)
C(7)-C(8)-C(9)	123.7(13)
C(10)-C(9)-C(8)	117(2)
C(9)-C(10)-C(11)	123(2)
C(10)-C(11)-C(12)	116(2)
C(7)-C(12)-C(11)	123.2(14)
N(8)-C(14)-C(15)	121.8(12)
C(16)-C(15)-C(20)	116.7(13)
C(16)-C(15)-C(14)	117.2(13)
C(20)-C(15)-C(14)	125.8(13)
C(17)-C(16)-C(15)	122(2)
C(16)-C(17)-C(18)	121(2)
C(19)-C(18)-C(17)	119(2)
C(18)-C(19)-C(20)	120(2)
C(19)-C(20)-C(15)	121(2)
C(25)-C(21)-C(22)	114(2)
C(25)-C(21)-Ti(4)	73.5(13)
C(22)-C(21)-Ti(4)	74.7(7)
C(21)-C(22)-C(23)	106(2)
C(21)-C(22)-Ti(4)	72.4(8)
C(23)-C(22)-Ti(4)	73.2(7)
C(22)-C(23)-C(24)	107(2)
C(22)-C(23)-Ti(4)	73.3(7)
C(24)-C(23)-Ti(4)	72.3(8)
C(25)-C(24)-C(23)	110(2)
C(25)-C(24)-Ti(4)	73.0(13)

C(23)-C(24)-Ti(4)	73.5(8)
C(21)-C(25)-C(24)	103(2)
C(21)-C(25)-Ti(4)	72.9(12)
C(24)-C(25)-Ti(4)	73.3(13)
C(27)-C(26)-C(30)	113(2)
C(27)-C(26)-Ti(4)	72.8(10)
C(30)-C(26)-Ti(4)	72.1(10)
C(26)-C(27)-C(28)	108(2)
C(26)-C(27)-Ti(4)	75.7(12)
C(28)-C(27)-Ti(4)	73.7(8)
C(29)-C(28)-C(27)	107(2)
C(29)-C(28)-Ti(4)	72.9(9)
C(27)-C(28)-Ti(4)	71.4(8)
C(28)-C(29)-C(30)	108(2)
C(28)-C(29)-Ti(4)	74.3(10)
C(30)-C(29)-Ti(4)	71.8(8)
C(26)-C(30)-C(29)	103(2)
C(26)-C(30)-Ti(4)	74.4(10)
C(29)-C(30)-Ti(4)	72.4(9)
C(32)-C(31)-C(35)	107.6(14)
C(32)-C(31)-Ti(3)	70.6(7)
C(35)-C(31)-Ti(3)	72.6(7)
C(33)-C(32)-C(31)	107(2)
C(33)-C(32)-Ti(3)	73.5(8)
C(31)-C(32)-Ti(3)	75.0(7)
C(34)-C(33)-C(32)	109(2)
C(34)-C(33)-Ti(3)	73.1(8)
C(32)-C(33)-Ti(3)	72.4(8)
C(33)-C(34)-C(35)	108(2)
C(33)-C(34)-Ti(3)	73.0(8)
C(35)-C(34)-Ti(3)	74.0(7)
C(31)-C(35)-C(34)	108.0(14)
C(31)-C(35)-Ti(3)	73.8(7)
C(34)-C(35)-Ti(3)	71.9(7)
C(40)-C(36)-C(37)	108(2)
C(40)-C(36)-Ti(3)	74.9(9)
C(37)-C(36)-Ti(3)	74.1(7)
C(106)-C(37)-C(36)	108(2)
C(106)-C(37)-Ti(3)	72.6(9)
C(36)-C(37)-Ti(3)	72.0(7)
C(40)-C(38)-C(106)	105(2)
C(40)-C(38)-Ti(3)	73.4(11)
C(106)-C(38)-Ti(3)	70.7(10)
C(36)-C(40)-C(38)	111(2)
C(36)-C(40)-Ti(3)	72.3(7)
C(38)-C(40)-Ti(3)	74.0(12)
N(3)-C(42)-C(43)	108.7(8)
N(3)-C(42)-C(87)	111.8(7)
C(43)-C(42)-C(87)	112.9(8)
C(44)-C(43)-C(48)	120.5(12)
C(44)-C(43)-C(42)	119.2(11)
C(48)-C(43)-C(42)	120.3(10)
C(43)-C(44)-C(45)	119(2)
C(46)-C(45)-C(44)	122(2)
C(45)-C(46)-C(47)	117(2)
C(46)-C(47)-C(48)	123(2)
C(43)-C(48)-C(47)	118(2)
N(4)-C(50)-C(51)	122.7(12)
C(52)-C(51)-C(56)	119.7(12)
C(52)-C(51)-C(50)	118.5(12)
C(56)-C(51)-C(50)	121.8(12)
C(51)-C(52)-C(53)	118.9(13)
C(54)-C(53)-C(52)	119(2)
C(55)-C(54)-C(53)	122(2)
C(54)-C(55)-C(56)	120(2)
C(55)-C(56)-C(51)	120.0(13)

C(58)-C(57)-C(61)	109(2)
C(58)-C(57)-Ti(2)	72.3(7)
C(61)-C(57)-Ti(2)	74.2(8)
C(59)-C(58)-C(57)	110.5(14)
C(59)-C(58)-Ti(2)	73.2(7)
C(57)-C(58)-Ti(2)	74.5(7)
C(58)-C(59)-C(60)	107(2)
C(58)-C(59)-Ti(2)	73.7(8)
C(60)-C(59)-Ti(2)	73.2(9)
C(61)-C(60)-C(59)	109(2)
C(61)-C(60)-Ti(2)	74.6(10)
C(59)-C(60)-Ti(2)	72.1(8)
C(60)-C(61)-C(57)	105(2)
C(60)-C(61)-Ti(2)	70.9(9)
C(57)-C(61)-Ti(2)	71.9(8)
C(66)-C(62)-C(63)	114(2)
C(66)-C(62)-Ti(2)	74.5(7)
C(63)-C(62)-Ti(2)	74.5(9)
C(62)-C(63)-C(64)	104(2)
C(62)-C(63)-Ti(2)	73.0(7)
C(64)-C(63)-Ti(2)	70.6(8)
C(65)-C(64)-C(63)	105(2)
C(65)-C(64)-Ti(2)	74.9(9)
C(63)-C(64)-Ti(2)	73.9(8)
C(66)-C(65)-C(64)	111(2)
C(66)-C(65)-Ti(2)	73.9(8)
C(64)-C(65)-Ti(2)	71.3(8)
C(62)-C(66)-C(65)	106(2)
C(62)-C(66)-Ti(2)	72.9(7)
C(65)-C(66)-Ti(2)	74.0(9)
N(2)-C(69)-C(70)	121.7(11)
C(71)-C(70)-C(75)	117.2(12)
C(71)-C(70)-C(69)	119.5(11)
C(75)-C(70)-C(69)	123.2(11)
C(70)-C(71)-C(72)	121.6(13)
C(73)-C(72)-C(71)	118.4(14)
C(74)-C(73)-C(72)	120.9(14)
C(73)-C(74)-C(75)	121.6(14)
C(74)-C(75)-C(70)	120.2(12)
C(80)-C(76)-C(77)	109(2)
C(80)-C(76)-Ti(1)	74.9(8)
C(77)-C(76)-Ti(1)	72.6(8)
C(76)-C(77)-C(78)	107.5(14)
C(76)-C(77)-Ti(1)	73.5(8)
C(78)-C(77)-Ti(1)	73.9(9)
C(79)-C(78)-C(77)	105(2)
C(79)-C(78)-Ti(1)	72.8(8)
C(77)-C(78)-Ti(1)	71.8(9)
C(78)-C(79)-C(80)	111(2)
C(78)-C(79)-Ti(1)	74.3(8)
C(80)-C(79)-Ti(1)	74.5(7)
C(76)-C(80)-C(79)	108(2)
C(76)-C(80)-Ti(1)	73.0(8)
C(79)-C(80)-Ti(1)	72.4(7)
C(86)-C(81)-C(82)	111(2)
C(86)-C(81)-Ti(1)	74.1(11)
C(82)-C(81)-Ti(1)	74.3(8)
C(81)-C(82)-C(83)	108(2)
C(81)-C(82)-Ti(1)	73.8(9)
C(83)-C(82)-Ti(1)	72.7(8)
C(82)-C(83)-C(84)	113(2)
C(82)-C(83)-Ti(1)	74.6(7)
C(84)-C(83)-Ti(1)	74.6(8)
C(83)-C(84)-C(86)	96.0(13)
C(83)-C(84)-Ti(1)	71.1(7)
C(86)-C(84)-Ti(1)	70.0(7)

C(81)-C(86)-C(84)	112(2)
C(81)-C(86)-Ti(1)	75.2(9)
C(84)-C(86)-Ti(1)	72.9(10)
N(1)-C(87)-C(88)	110.6(8)
N(1)-C(87)-C(42)	112.1(7)
C(88)-C(87)-C(42)	112.2(8)
C(93)-C(88)-C(89)	121.2(13)
C(93)-C(88)-C(87)	121.4(12)
C(89)-C(88)-C(87)	117.2(11)
C(88)-C(89)-C(90)	115(2)
C(91)-C(90)-C(89)	121(2)
C(92)-C(91)-C(90)	122(3)
C(91)-C(92)-C(93)	118(2)
C(88)-C(93)-C(92)	122(2)
C(99)-C(94)-C(95)	118.2(12)
C(99)-C(94)-C(4)	122.1(11)
C(95)-C(94)-C(4)	119.7(11)
C(96)-C(95)-C(94)	123.2(14)
C(97)-C(96)-C(95)	117(2)
C(96)-C(97)-C(98)	124(2)
C(97)-C(98)-C(99)	119(2)
C(94)-C(99)-C(98)	118(2)
C(105)-C(100)-C(101)	119.2(11)
C(105)-C(100)-C(3)	122.1(11)
C(101)-C(100)-C(3)	118.6(11)
C(102)-C(101)-C(100)	120.2(14)
C(101)-C(102)-C(103)	122(2)
C(102)-C(103)-C(104)	119(2)
C(105)-C(104)-C(103)	120(2)
C(100)-C(105)-C(104)	119.9(14)
C(37)-C(106)-C(38)	108(2)
C(37)-C(106)-Ti(3)	74.8(8)
C(38)-C(106)-Ti(3)	73.7(11)
N(2)-N(1)-C(87)	122.1(8)
N(2)-N(1)-Ti(1)	72.7(6)
C(87)-N(1)-Ti(1)	153.4(7)
C(69)-N(2)-N(1)	127.9(9)
C(69)-N(2)-Ti(1)	159.8(8)
N(1)-N(2)-Ti(1)	69.6(5)
N(4)-N(3)-C(42)	120.0(8)
N(4)-N(3)-Ti(2)	74.3(5)
C(42)-N(3)-Ti(2)	151.6(6)
C(50)-N(4)-N(3)	129.9(9)
C(50)-N(4)-Ti(2)	159.5(8)
N(3)-N(4)-Ti(2)	68.3(5)
N(6)-N(5)-C(3)	121.0(8)
N(6)-N(5)-Ti(3)	73.7(5)
C(3)-N(5)-Ti(3)	154.4(6)
C(6)-N(6)-N(5)	129.1(9)
C(6)-N(6)-Ti(3)	158.9(7)
N(5)-N(6)-Ti(3)	69.3(5)
N(8)-N(7)-C(4)	119.5(8)
N(8)-N(7)-Ti(4)	74.0(6)
C(4)-N(7)-Ti(4)	151.2(6)
C(14)-N(8)-N(7)	129.9(9)
C(14)-N(8)-Ti(4)	158.9(8)
N(7)-N(8)-Ti(4)	68.5(5)
N(7)-Ti(4)-N(8)	37.5(3)
N(7)-Ti(4)-C(27)	110.9(6)
N(8)-Ti(4)-C(27)	132.9(4)
N(7)-Ti(4)-C(21)	128.6(6)
N(8)-Ti(4)-C(21)	106.1(7)
C(27)-Ti(4)-C(21)	118.4(8)
N(7)-Ti(4)-C(30)	126.2(5)
N(8)-Ti(4)-C(30)	108.4(6)
C(27)-Ti(4)-C(30)	56.1(8)

C(21)-Ti(4)-C(30)	94.3(6)
N(7)-Ti(4)-C(24)	108.8(8)
N(8)-Ti(4)-C(24)	123.6(7)
C(27)-Ti(4)-C(24)	96.1(6)
C(21)-Ti(4)-C(24)	54.0(8)
C(30)-Ti(4)-C(24)	123.7(9)
N(7)-Ti(4)-C(29)	91.2(5)
N(8)-Ti(4)-C(29)	85.1(5)
C(27)-Ti(4)-C(29)	56.2(6)
C(21)-Ti(4)-C(29)	127.6(6)
C(30)-Ti(4)-C(29)	35.8(5)
C(24)-Ti(4)-C(29)	150.9(8)
N(7)-Ti(4)-C(25)	140.7(8)
N(8)-Ti(4)-C(25)	136.9(8)
C(27)-Ti(4)-C(25)	90.1(9)
C(21)-Ti(4)-C(25)	33.5(8)
C(30)-Ti(4)-C(25)	93.1(9)
C(24)-Ti(4)-C(25)	33.7(8)
C(29)-Ti(4)-C(25)	127.6(8)
N(7)-Ti(4)-C(28)	83.6(5)
N(8)-Ti(4)-C(28)	98.0(5)
C(27)-Ti(4)-C(28)	34.9(5)
C(21)-Ti(4)-C(28)	147.5(6)
C(30)-Ti(4)-C(28)	57.0(7)
C(24)-Ti(4)-C(28)	126.7(7)
C(29)-Ti(4)-C(28)	32.8(5)
C(25)-Ti(4)-C(28)	124.8(8)
N(7)-Ti(4)-C(26)	138.2(6)
N(8)-Ti(4)-C(26)	139.6(6)
C(27)-Ti(4)-C(26)	31.5(6)
C(21)-Ti(4)-C(26)	93.2(7)
C(30)-Ti(4)-C(26)	33.5(6)
C(24)-Ti(4)-C(26)	96.5(9)
C(29)-Ti(4)-C(26)	55.6(6)
C(25)-Ti(4)-C(26)	74.7(8)
C(28)-Ti(4)-C(26)	54.6(6)
N(7)-Ti(4)-C(22)	95.8(4)
N(8)-Ti(4)-C(22)	80.1(4)
C(27)-Ti(4)-C(22)	147.0(5)
C(21)-Ti(4)-C(22)	32.8(5)
C(30)-Ti(4)-C(22)	121.9(6)
C(24)-Ti(4)-C(22)	55.8(6)
C(29)-Ti(4)-C(22)	145.0(6)
C(25)-Ti(4)-C(22)	56.9(8)
C(28)-Ti(4)-C(22)	177.5(6)
C(26)-Ti(4)-C(22)	126.0(6)
N(7)-Ti(4)-C(23)	84.3(4)
N(8)-Ti(4)-C(23)	89.7(5)
C(27)-Ti(4)-C(23)	128.1(7)
C(21)-Ti(4)-C(23)	54.4(5)
C(30)-Ti(4)-C(23)	147.8(5)
C(24)-Ti(4)-C(23)	34.2(5)
C(29)-Ti(4)-C(23)	174.8(6)
C(25)-Ti(4)-C(23)	57.1(7)
C(28)-Ti(4)-C(23)	148.5(7)
C(26)-Ti(4)-C(23)	129.6(7)
C(22)-Ti(4)-C(23)	33.5(4)
N(5)-Ti(3)-N(6)	37.0(3)
N(5)-Ti(3)-C(106)	129.4(6)
N(6)-Ti(3)-C(106)	108.3(7)
N(5)-Ti(3)-C(36)	84.3(4)
N(6)-Ti(3)-C(36)	91.8(6)
C(106)-Ti(3)-C(36)	55.6(5)
N(5)-Ti(3)-C(32)	112.2(5)
N(6)-Ti(3)-C(32)	131.8(4)
C(106)-Ti(3)-C(32)	116.5(7)

C(32)-Ti(3)-C(32)	127.6(6)
N(5)-Ti(3)-C(37)	97.0(5)
N(6)-Ti(3)-C(37)	83.4(4)
C(106)-Ti(3)-C(37)	32.6(5)
C(36)-Ti(3)-C(37)	33.9(4)
C(32)-Ti(3)-C(37)	144.8(5)
N(5)-Ti(3)-C(33)	140.5(5)
N(6)-Ti(3)-C(33)	136.5(5)
C(106)-Ti(3)-C(33)	89.8(7)
C(36)-Ti(3)-C(33)	129.8(6)
C(32)-Ti(3)-C(33)	34.1(5)
C(37)-Ti(3)-C(33)	122.3(6)
N(5)-Ti(3)-C(34)	122.9(5)
N(6)-Ti(3)-C(34)	103.6(5)
C(106)-Ti(3)-C(34)	95.3(5)
C(36)-Ti(3)-C(34)	150.5(5)
C(32)-Ti(3)-C(34)	56.9(6)
C(37)-Ti(3)-C(34)	122.3(6)
C(33)-Ti(3)-C(34)	33.8(5)
N(5)-Ti(3)-C(40)	106.9(8)
N(6)-Ti(3)-C(40)	124.0(7)
C(106)-Ti(3)-C(40)	55.7(8)
C(36)-Ti(3)-C(40)	32.8(5)
C(32)-Ti(3)-C(40)	96.4(6)
C(37)-Ti(3)-C(40)	55.0(5)
C(33)-Ti(3)-C(40)	99.0(8)
C(34)-Ti(3)-C(40)	129.0(9)
N(5)-Ti(3)-C(38)	138.4(7)
N(6)-Ti(3)-C(38)	139.6(7)
C(106)-Ti(3)-C(38)	35.7(7)
C(36)-Ti(3)-C(38)	55.5(6)
C(32)-Ti(3)-C(38)	88.5(7)
C(37)-Ti(3)-C(38)	56.3(6)
C(33)-Ti(3)-C(38)	75.0(6)
C(34)-Ti(3)-C(38)	98.7(7)
C(40)-Ti(3)-C(38)	32.6(7)
N(5)-Ti(3)-C(31)	84.4(4)
N(6)-Ti(3)-C(31)	97.4(4)
C(106)-Ti(3)-C(31)	146.0(6)
C(36)-Ti(3)-C(31)	147.1(6)
C(32)-Ti(3)-C(31)	34.4(4)
C(37)-Ti(3)-C(31)	178.5(6)
C(33)-Ti(3)-C(31)	56.3(5)
C(34)-Ti(3)-C(31)	56.3(5)
C(40)-Ti(3)-C(31)	125.2(6)
C(38)-Ti(3)-C(31)	122.9(7)
N(5)-Ti(3)-C(35)	90.1(4)
N(6)-Ti(3)-C(35)	82.3(4)
C(106)-Ti(3)-C(35)	127.7(5)
C(36)-Ti(3)-C(35)	173.9(6)
C(32)-Ti(3)-C(35)	56.8(5)
C(37)-Ti(3)-C(35)	145.5(6)
C(33)-Ti(3)-C(35)	56.3(5)
C(34)-Ti(3)-C(35)	34.1(4)
C(40)-Ti(3)-C(35)	152.7(7)
C(38)-Ti(3)-C(35)	130.5(6)
C(31)-Ti(3)-C(35)	33.7(4)
N(3)-Ti(2)-N(4)	37.4(3)
N(3)-Ti(2)-C(64)	134.7(7)
N(4)-Ti(2)-C(64)	113.8(9)
N(3)-Ti(2)-C(58)	88.8(4)
N(4)-Ti(2)-C(58)	84.8(4)
C(64)-Ti(2)-C(58)	130.0(6)
N(3)-Ti(2)-C(59)	119.5(5)
N(4)-Ti(2)-C(59)	102.3(6)
C(64)-Ti(2)-C(59)	97.0(6)

C(58)-Ti(2)-C(59)	33.1(5)
N(3)-Ti(2)-C(62)	83.3(4)
N(4)-Ti(2)-C(62)	85.6(5)
C(64)-Ti(2)-C(62)	55.3(5)
C(58)-Ti(2)-C(62)	170.4(5)
C(59)-Ti(2)-C(62)	151.5(6)
N(3)-Ti(2)-C(60)	140.5(5)
N(4)-Ti(2)-C(60)	136.7(6)
C(64)-Ti(2)-C(60)	84.7(8)
C(58)-Ti(2)-C(60)	55.8(5)
C(59)-Ti(2)-C(60)	34.7(5)
C(62)-Ti(2)-C(60)	133.4(6)
N(3)-Ti(2)-C(66)	99.7(6)
N(4)-Ti(2)-C(66)	115.6(6)
C(64)-Ti(2)-C(66)	55.9(5)
C(58)-Ti(2)-C(66)	155.7(6)
C(59)-Ti(2)-C(66)	139.5(8)
C(62)-Ti(2)-C(66)	32.6(4)
C(60)-Ti(2)-C(66)	107.2(8)
N(3)-Ti(2)-C(57)	85.1(5)
N(4)-Ti(2)-C(57)	101.5(5)
C(64)-Ti(2)-C(57)	140.0(8)
C(58)-Ti(2)-C(57)	33.3(4)
C(59)-Ti(2)-C(57)	55.9(5)
C(62)-Ti(2)-C(57)	150.0(7)
C(60)-Ti(2)-C(57)	56.0(6)
C(66)-Ti(2)-C(57)	124.3(6)
N(3)-Ti(2)-C(63)	99.6(6)
N(4)-Ti(2)-C(63)	82.1(5)
C(64)-Ti(2)-C(63)	35.5(6)
C(58)-Ti(2)-C(63)	145.5(7)
C(59)-Ti(2)-C(63)	120.6(7)
C(62)-Ti(2)-C(63)	32.6(4)
C(60)-Ti(2)-C(63)	119.4(8)
C(66)-Ti(2)-C(63)	55.8(5)
C(57)-Ti(2)-C(63)	175.3(7)
N(3)-Ti(2)-C(65)	131.6(7)
N(4)-Ti(2)-C(65)	136.4(5)
C(64)-Ti(2)-C(65)	33.8(6)
C(58)-Ti(2)-C(65)	136.2(6)
C(59)-Ti(2)-C(65)	108.6(8)
C(62)-Ti(2)-C(65)	53.1(5)
C(60)-Ti(2)-C(65)	80.5(7)
C(66)-Ti(2)-C(65)	32.1(6)
C(57)-Ti(2)-C(65)	121.1(7)
C(63)-Ti(2)-C(65)	56.0(6)
N(3)-Ti(2)-C(61)	113.6(6)
N(4)-Ti(2)-C(61)	135.4(5)
C(64)-Ti(2)-C(61)	108.3(10)
C(58)-Ti(2)-C(61)	56.2(5)
C(59)-Ti(2)-C(61)	57.5(7)
C(62)-Ti(2)-C(61)	132.2(7)
C(60)-Ti(2)-C(61)	34.5(6)
C(66)-Ti(2)-C(61)	99.7(7)
C(57)-Ti(2)-C(61)	33.9(5)
C(63)-Ti(2)-C(61)	142.4(7)
C(65)-Ti(2)-C(61)	87.7(7)
N(1)-Ti(1)-N(2)	37.7(3)
N(1)-Ti(1)-C(83)	97.1(7)
N(2)-Ti(1)-C(83)	83.1(5)
N(1)-Ti(1)-C(81)	103.4(7)
N(2)-Ti(1)-C(81)	120.6(6)
C(83)-Ti(1)-C(81)	53.8(6)
N(1)-Ti(1)-C(86)	133.4(7)
N(2)-Ti(1)-C(86)	137.6(6)
C(83)-Ti(1)-C(86)	54.9(7)

C(81)-Ti(1)-C(86)	30.7(6)
N(1)-Ti(1)-C(79)	87.9(4)
N(2)-Ti(1)-C(79)	82.9(4)
C(83)-Ti(1)-C(79)	149.6(7)
C(81)-Ti(1)-C(79)	153.5(6)
C(86)-Ti(1)-C(79)	136.0(6)
N(1)-Ti(1)-C(82)	83.1(4)
N(2)-Ti(1)-C(82)	89.7(5)
C(83)-Ti(1)-C(82)	32.7(4)
C(81)-Ti(1)-C(82)	31.8(5)
C(86)-Ti(1)-C(82)	52.8(6)
C(79)-Ti(1)-C(82)	171.0(5)
N(1)-Ti(1)-C(77)	139.5(4)
N(2)-Ti(1)-C(77)	133.3(6)
C(83)-Ti(1)-C(77)	122.9(7)
C(81)-Ti(1)-C(77)	105.5(8)
C(86)-Ti(1)-C(77)	81.2(7)
C(79)-Ti(1)-C(77)	54.8(5)
C(82)-Ti(1)-C(77)	134.0(6)
N(1)-Ti(1)-C(84)	131.3(8)
N(2)-Ti(1)-C(84)	109.1(9)
C(83)-Ti(1)-C(84)	34.4(6)
C(81)-Ti(1)-C(84)	57.5(6)
C(86)-Ti(1)-C(84)	37.1(7)
C(79)-Ti(1)-C(84)	130.3(6)
C(82)-Ti(1)-C(84)	57.1(5)
C(77)-Ti(1)-C(84)	88.5(8)
N(1)-Ti(1)-C(76)	113.5(5)
N(2)-Ti(1)-C(76)	132.6(5)
C(83)-Ti(1)-C(76)	144.2(6)
C(81)-Ti(1)-C(76)	99.4(6)
C(86)-Ti(1)-C(76)	89.7(7)
C(79)-Ti(1)-C(76)	54.2(5)
C(82)-Ti(1)-C(76)	130.5(7)
C(77)-Ti(1)-C(76)	33.9(5)
C(84)-Ti(1)-C(76)	113.7(9)
N(1)-Ti(1)-C(78)	118.0(6)
N(2)-Ti(1)-C(78)	99.3(6)
C(83)-Ti(1)-C(78)	125.0(8)
C(81)-Ti(1)-C(78)	137.4(9)
C(86)-Ti(1)-C(78)	108.5(9)
C(79)-Ti(1)-C(78)	32.8(5)
C(82)-Ti(1)-C(78)	155.0(6)
C(77)-Ti(1)-C(78)	34.3(5)
C(84)-Ti(1)-C(78)	97.9(7)
C(76)-Ti(1)-C(78)	56.2(6)
N(1)-Ti(1)-C(80)	85.5(5)
N(2)-Ti(1)-C(80)	100.7(4)
C(83)-Ti(1)-C(80)	176.1(6)
C(81)-Ti(1)-C(80)	122.9(6)
C(86)-Ti(1)-C(80)	121.3(6)
C(79)-Ti(1)-C(80)	33.0(4)
C(82)-Ti(1)-C(80)	145.6(7)
C(77)-Ti(1)-C(80)	55.0(5)
C(84)-Ti(1)-C(80)	143.2(8)
C(76)-Ti(1)-C(80)	32.1(4)
C(78)-Ti(1)-C(80)	55.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 3. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

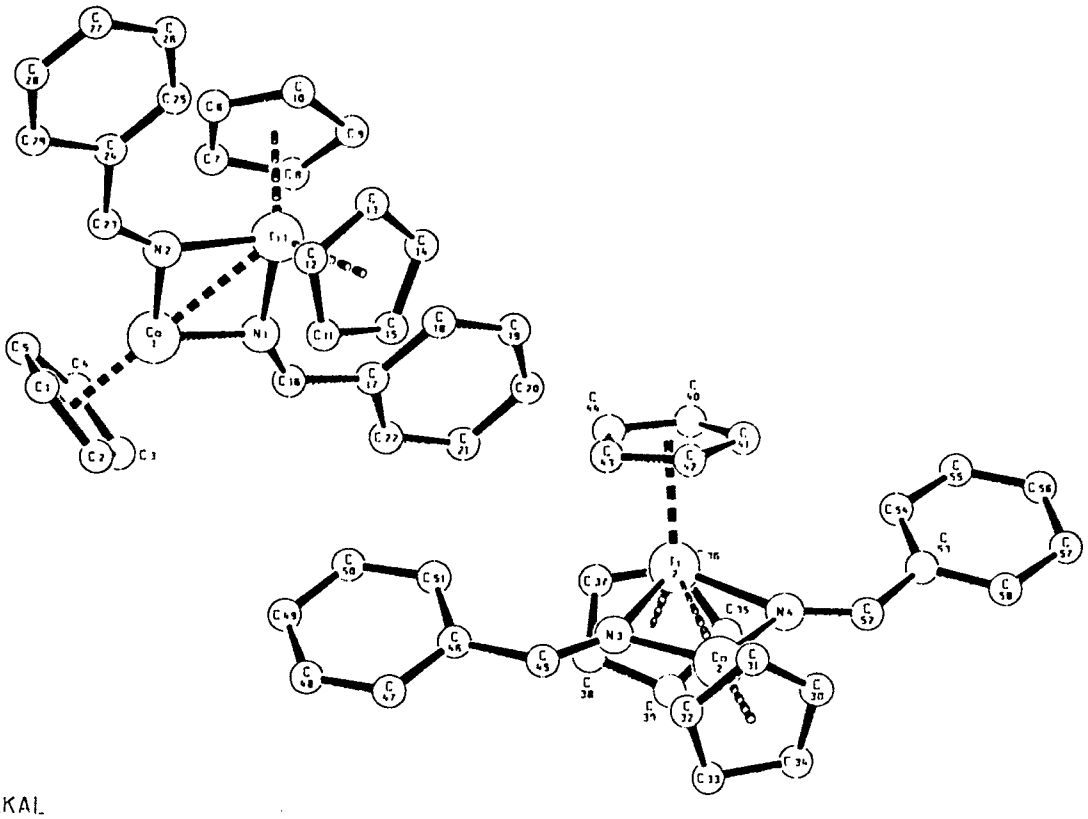
	U11	U22	U33	U23	U13	U12
C(3)	32(6)	42(5)	46(6)	9(4)	17(5)	-2(4)
C(4)	24(6)	56(6)	43(6)	5(4)	15(5)	-4(4)
C(6)	42(8)	68(7)	51(7)	12(6)	4(6)	7(6)
C(7)	22(7)	52(6)	68(8)	-5(5)	9(6)	3(5)
C(8)	64(10)	62(7)	59(8)	4(6)	-6(7)	9(6)
C(9)	96(13)	71(9)	80(10)	-4(7)	-26(9)	-20(9)
C(10)	115(16)	63(9)	100(12)	-25(8)	-39(11)	16(9)
C(11)	34(10)	102(10)	135(16)	-3(10)	4(9)	0(8)
C(12)	50(9)	61(7)	111(11)	9(7)	13(8)	-12(7)
C(14)	58(9)	53(7)	93(9)	18(6)	34(8)	23(7)
C(15)	60(11)	51(7)	110(11)	-18(7)	54(8)	-13(6)
C(16)	82(13)	76(8)	154(14)	-16(8)	70(11)	-32(8)
C(17)	124(18)	121(14)	200(22)	8(13)	133(18)	-6(12)
C(18)	173(22)	111(14)	167(21)	-54(13)	134(19)	-30(14)
C(19)	259(26)	71(10)	81(11)	-5(8)	121(15)	-30(13)
C(20)	117(12)	43(7)	85(9)	7(6)	41(9)	8(6)
C(21)	218(24)	88(12)	57(10)	30(8)	0(14)	-69(14)
C(22)	83(11)	39(6)	102(11)	-7(6)	16(9)	-17(6)
C(23)	131(16)	59(8)	62(9)	-12(6)	2(10)	-48(9)
C(24)	62(14)	136(17)	255(29)	-145(19)	36(18)	-18(13)
C(25)	192(29)	80(12)	230(33)	-38(17)	-87(28)	23(15)
C(26)	147(19)	142(17)	73(13)	30(11)	-63(12)	8(14)
C(27)	86(13)	102(12)	157(18)	-39(11)	-42(12)	51(10)
C(28)	76(13)	78(10)	118(15)	-3(9)	-30(11)	-23(9)
C(29)	96(15)	96(12)	103(13)	-32(10)	-2(11)	-24(10)
C(30)	177(22)	108(13)	64(10)	-12(9)	12(11)	-22(12)
C(31)	81(12)	79(9)	72(10)	1(7)	42(9)	1(8)
C(32)	117(14)	81(10)	143(15)	-30(9)	107(12)	-49(9)
C(33)	234(24)	84(11)	88(13)	4(9)	121(15)	-7(13)
C(34)	146(17)	82(10)	50(9)	13(7)	21(9)	22(10)
C(35)	89(11)	77(8)	60(8)	-15(7)	31(8)	-2(8)
C(36)	130(15)	63(8)	51(8)	-22(6)	-13(10)	34(9)
C(37)	86(13)	58(8)	144(16)	-26(9)	60(12)	17(8)
C(38)	305(39)	50(9)	181(23)	-9(11)	188(27)	-4(14)
C(40)	67(13)	125(15)	263(29)	-116(17)	92(17)	-68(12)
C(42)	30(7)	57(6)	57(7)	9(5)	20(5)	10(5)
C(43)	50(8)	39(5)	62(7)	-5(5)	-3(6)	-2(5)
C(44)	91(11)	47(7)	85(9)	19(6)	-22(8)	-17(6)
C(45)	167(20)	48(8)	151(17)	23(9)	-74(17)	8(11)
C(46)	149(23)	127(16)	219(30)	32(16)	-73(22)	65(15)
C(47)	59(12)	121(13)	232(24)	-50(14)	-6(15)	36(10)
C(48)	31(9)	128(11)	112(11)	-23(8)	13(8)	37(8)
C(50)	45(9)	70(7)	73(8)	5(6)	19(7)	9(7)
C(51)	37(9)	53(6)	71(9)	6(5)	14(7)	3(6)
C(52)	44(9)	61(7)	86(9)	1(6)	19(7)	2(6)
C(53)	46(11)	100(10)	108(12)	8(9)	18(9)	25(8)
C(54)	59(12)	98(11)	94(12)	30(9)	-4(9)	-6(9)
C(55)	59(11)	78(9)	87(10)	5(7)	17(9)	-1(8)
C(56)	44(9)	90(8)	83(10)	16(7)	-7(8)	-1(7)
C(57)	60(11)	120(12)	69(10)	30(8)	27(8)	-30(9)
C(58)	110(14)	57(8)	93(10)	21(7)	61(10)	1(8)
C(59)	149(18)	104(13)	58(9)	19(9)	30(10)	-38(12)
C(60)	244(28)	71(11)	119(16)	-8(10)	134(18)	16(14)
C(61)	101(16)	113(14)	167(20)	56(13)	89(14)	35(12)
C(62)	107(14)	77(8)	95(11)	-11(7)	78(11)	-30(9)
C(63)	47(11)	64(8)	195(20)	-1(10)	23(13)	-27(7)

C(64)	201(22)	43(8)	77(12)	5(7)	-43(13)	-42(11)
C(65)	194(24)	73(10)	162(20)	3(11)	122(19)	62(13)
C(66)	79(13)	72(9)	136(15)	33(9)	24(12)	21(8)
C(69)	39(8)	53(6)	60(8)	-2(5)	19(6)	4(6)
C(70)	48(9)	59(6)	52(7)	7(5)	22(6)	-7(6)
C(71)	59(10)	62(7)	94(9)	-8(7)	42(7)	-6(7)
C(72)	65(11)	64(8)	142(15)	5(9)	61(10)	-5(7)
C(73)	91(14)	86(10)	116(13)	15(9)	80(11)	25(9)
C(74)	55(10)	108(10)	82(10)	-2(8)	27(8)	12(8)
C(75)	50(9)	103(9)	54(8)	-1(6)	22(7)	14(7)
C(76)	40(10)	84(11)	155(15)	6(10)	-13(9)	0(8)
C(77)	135(17)	46(9)	122(15)	-18(8)	-53(12)	21(9)
C(78)	99(16)	193(20)	59(10)	3(11)	12(10)	60(14)
C(79)	77(12)	63(8)	88(10)	16(7)	-6(8)	9(7)
C(80)	45(10)	93(10)	114(13)	0(8)	21(9)	8(8)
C(81)	87(15)	53(9)	193(21)	18(10)	51(14)	-20(8)
C(82)	98(14)	59(8)	98(12)	0(7)	-1(11)	13(9)
C(83)	77(12)	60(9)	199(21)	38(11)	77(14)	55(8)
C(84)	336(35)	66(10)	68(11)	-10(8)	53(16)	106(15)
C(86)	180(24)	24(7)	188(22)	-23(10)	-52(19)	28(9)
C(87)	33(7)	41(5)	65(7)	3(5)	20(5)	6(4)
C(88)	55(9)	54(6)	86(9)	-3(6)	40(7)	-9(6)
C(89)	144(14)	59(7)	92(11)	16(7)	77(10)	10(7)
C(90)	285(31)	38(9)	159(19)	34(9)	141(23)	22(13)
C(91)	262(36)	120(14)	208(30)	-28(16)	170(32)	-85(20)
C(92)	151(21)	207(20)	203(22)	-89(19)	137(21)	-126(17)
C(93)	76(12)	124(12)	139(13)	-40(9)	77(10)	-43(9)
C(94)	41(8)	54(6)	72(8)	11(6)	26(6)	12(6)
C(95)	132(13)	30(6)	90(11)	-9(6)	43(10)	-15(6)
C(96)	139(18)	63(9)	126(14)	-20(8)	75(14)	-20(9)
C(97)	178(25)	80(10)	187(22)	-30(13)	131(21)	0(13)
C(98)	100(16)	160(17)	173(20)	-5(15)	67(16)	38(13)
C(99)	97(13)	108(10)	106(11)	10(8)	50(10)	29(9)
C(100)	37(8)	31(5)	83(9)	2(5)	4(6)	1(5)
C(101)	73(10)	42(6)	67(8)	-7(5)	2(7)	12(6)
C(102)	94(14)	84(9)	114(13)	-36(9)	-29(12)	-1(9)
C(103)	92(15)	107(11)	134(16)	-15(11)	-18(13)	-32(11)
C(104)	48(11)	114(12)	174(17)	33(12)	10(11)	-43(8)
C(105)	40(9)	142(12)	79(9)	7(8)	16(8)	-10(8)
C(106)	212(24)	62(9)	72(11)	5(7)	45(14)	26(12)
N(1)	29(6)	71(6)	67(7)	-11(5)	17(5)	-5(4)
N(2)	42(7)	48(5)	66(7)	-2(4)	23(5)	-2(4)
N(3)	34(6)	54(5)	53(6)	-4(4)	11(5)	-4(4)
N(4)	34(6)	46(4)	54(6)	8(4)	11(5)	4(4)
N(5)	32(6)	54(5)	52(6)	5(4)	9(5)	10(4)
N(6)	36(7)	48(5)	56(6)	9(4)	16(5)	8(4)
N(7)	49(6)	43(5)	57(6)	4(4)	15(5)	19(4)
N(8)	82(9)	28(4)	51(6)	5(4)	26(6)	-1(5)
Ti(4)	65(2)	46(1)	58(1)	4(1)	-5(1)	5(1)
Ti(3)	57(2)	48(1)	51(1)	6(1)	24(1)	-3(1)
Ti(2)	52(2)	51(1)	49(1)	4(1)	20(1)	1(1)
Ti(1)	42(1)	50(1)	74(2)	-2(1)	7(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 3.

	x	y	z	U(eq)
H(3)	1364(8)	2963(5)	7132(4)	46
H(4)	1623(8)	4346(5)	7479(4)	47
H(6)	2955(10)	3363(7)	7848(5)	66
H(8)	3557(10)	2094(7)	9211(5)	78
H(9)	5328(15)	1776(9)	9838(7)	109
H(10)	6917(16)	2447(9)	9644(7)	125
H(11)	6828(12)	3187(9)	8747(8)	112
H(12)	5012(12)	3518(7)	8145(6)	90
H(14)	2472(11)	3962(7)	6727(6)	78
H(16)	4260(14)	3952(8)	6486(7)	116
H(17)	5485(18)	4285(12)	5896(11)	159
H(18)	4877(20)	5091(13)	5026(10)	161
H(19)	3036(21)	5647(10)	4784(7)	148
H(20)	1810(12)	5370(7)	5400(5)	95
H(21)	867(22)	7128(10)	5734(7)	152
H(22)	2095(12)	6374(7)	6578(7)	91
H(23)	992(17)	6217(7)	7372(6)	105
H(24)	-924(18)	6882(14)	6957(13)	182
H(25)	-1042(29)	7388(14)	5904(15)	230
H(26)	-2104(18)	6504(14)	5246(8)	163
H(27)	-2682(14)	5639(11)	5973(9)	152
H(28)	-1871(15)	4130(10)	5934(9)	119
H(29)	-592(15)	4185(10)	5249(8)	123
H(30)	-648(18)	5752(12)	4833(7)	143
H(31)	-578(13)	3400(8)	8735(6)	88
H(32)	-1389(14)	1910(9)	8826(8)	121
H(33)	75(20)	1075(11)	9572(7)	145
H(34)	1839(16)	1960(10)	9861(6)	111
H(35)	1446(13)	3404(8)	9348(5)	88
H(36)	758(18)	1141(8)	7354(6)	104
H(37)	2604(13)	882(8)	8095(9)	109
H(38)	26(32)	113(11)	8820(12)	188
H(40)	-758(15)	600(12)	7782(13)	171
H(42)	-1869(8)	575(6)	12461(4)	56
H(44)	-681(11)	134(7)	13390(6)	98
H(45)	987(20)	-496(9)	13934(10)	169
H(46)	2458(23)	-817(14)	13486(14)	222
H(47)	2383(14)	-232(11)	12546(11)	173
H(48)	733(11)	445(8)	11980(7)	110
H(50)	-3501(11)	988(7)	11800(6)	74
H(52)	-5551(11)	947(7)	11677(6)	76
H(53)	-7388(13)	633(9)	11080(8)	102
H(54)	-7575(13)	11(9)	10144(7)	106
H(55)	-6041(13)	-491(8)	9840(6)	90
H(56)	-4219(11)	-178(7)	10399(6)	92
H(57)	34(14)	877(11)	10845(6)	97
H(58)	-1950(15)	1038(8)	10291(6)	97
H(59)	-2620(16)	-295(12)	9749(6)	123
H(60)	-983(24)	-1347(11)	9952(9)	155
H(61)	718(16)	-610(14)	10647(10)	141
H(62)	-1726(18)	-1219(8)	12199(7)	101
H(63)	-3378(13)	-1502(9)	11379(11)	124
H(64)	-2566(24)	-2136(9)	10520(8)	144
H(65)	-490(24)	-2291(10)	10951(13)	156
H(66)	16(14)	-1631(8)	11939(9)	115
H(69)	-2870(10)	1605(6)	12864(5)	59
H(71)	-4688(12)	1576(7)	13150(6)	81

H(72)	-5890(12)	1980(8)	13778(8)	101
H(73)	-5128(15)	2769(9)	14652(7)	106
H(74)	-3281(13)	3208(9)	14873(7)	96
H(75)	-2093(11)	2877(7)	14246(5)	81
H(76)	2447(12)	2993(10)	13865(8)	120
H(77)	1566(18)	3728(9)	14613(8)	139
H(78)	95(15)	2700(15)	14849(7)	142
H(79)	132(13)	1407(8)	14225(6)	97
H(80)	1579(12)	1575(9)	13645(7)	100
H(81)	731(17)	4213(9)	12711(11)	130
H(82)	-1218(18)	3802(8)	12358(7)	107
H(83)	-2188(13)	4039(9)	13145(12)	125
H(84)	-817(30)	4631(10)	14091(8)	187
H(86)	1079(20)	4737(8)	13688(14)	176
H(87)	-1972(8)	2005(5)	12132(4)	54
H(89)	-1836(14)	2360(7)	11151(6)	108
H(90)	-643(26)	2920(9)	10528(10)	175
H(91)	1287(30)	3024(14)	10894(14)	213
H(92)	2146(20)	2677(14)	11889(12)	205
H(93)	1009(13)	2171(8)	12516(7)	125
H(95)	1512(13)	4707(6)	8457(6)	97
H(96)	625(18)	5407(8)	9108(8)	122
H(97)	-1291(24)	5600(10)	8822(12)	160
H(98)	-2331(17)	5253(13)	7888(10)	166
H(99)	-1414(14)	4597(8)	7181(7)	119
H(101)	157(11)	2672(6)	6154(5)	76
H(102)	-1466(16)	2052(9)	5588(8)	128
H(103)	-3082(17)	1938(10)	5946(10)	142
H(104)	-2988(13)	2288(9)	6965(10)	138
H(105)	-1288(11)	2850(9)	7575(6)	104
H(106)	2201(23)	340(9)	9021(8)	136



SCHAKAL

Identification code	738m
Empirical formula	C29 H27 Co N2 Ti
Formula weight	510.36
Crystal system	Monoclinic
Space group	Pc
Unit cell dimensions	a= 17.962(4) A alpha= 90 deg. b= 15.293(3) A beta= 98.35(3) deg. c= 8.796(2) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	2000
Theta for cell determination	4 to 20 deg
Volume	2390.6(9) A^3
Z	4
Density (calculated)	1.418 Mg/m^3
Absorption coefficient	1.047 mm^-1
F(000)	1056
Crystal colour	red-brown
Crystal description	prism
Crystal size	0.2 x 0.2 x 0.1 mm
Temperature	293(2) K
Wavelength	0.71073 A
Radiation type	MoK\a
Radiation source	fine-focus sealed tube
Monochromator	graphite
Measurment device	STOE-IPDS
Scan method	mean imaging plate
Standards (intensity + orient.)	50-200
Intensity after	360 sec
Theta range for data collection	1.76 to 24.33 deg.
Index ranges	0<=h<=20, -16<=k<=16, -10<=l<=10
Reflections collected	7014
Independent reflections	3759 [R(int) = 0.1084]

Reflections observed	2633
Criterion	>2sigma(I)
Absorption correction	Mean imaging plate intensity method
Structure solution primary	direct
Structure solution secondary	difmap
Hydrogen positions	geom
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3759 / 2 / 596
Final R indices [I>2sigma(I)]	R1 = 0.0619, wR2 = 0.1408
R indices (all data)	R1 = 0.0899, wR2 = 0.1725
Goodness-of-fit on F^2(all)	1.025
Goodness-of-fit on F^2(obs)	1.036
Shift/esd(mean)	0.229
Absolute structure parameter	0.01(4)
Weighting scheme	
calc w=1/[\s^2^(Fo^2^)+(0.0861P)^2^+0.0654P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	0.430 and -0.516 e.A^-3
Diff. density rms	0.094
Data collection	STOE-EXPOSE
Cell refinement	STOE-CELL
Data reduction	STOE-INTEGRATE
Structure solution	SHELXS-86 (Sheldrick, 1990)
Structure refinement	SHELXL-93 (Sheldrick, 1993)
Molecular graphics	SCHAKAL
Publication material	SHELXL-93

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

	x	y	z	U(eq)
Co(1)	-313(1)	3445(1)	1525(2)	50(1)
Ti(1)	7(1)	2105(1)	-16(2)	50(1)
N(1)	421(6)	2599(6)	2034(12)	52(2)
N(2)	-739(6)	3057(6)	-399(12)	49(2)
C(1)	-834(10)	4645(10)	1480(19)	78(4)
C(2)	-73(10)	4824(11)	2058(19)	79(4)
C(3)	72(8)	4297(7)	3344(15)	60(3)
C(4)	-579(12)	3865(13)	3618(18)	88(5)
C(5)	-1170(8)	4115(8)	2462(18)	63(4)
C(6)	-1161(9)	1259(10)	-239(18)	72(4)
C(7)	-882(10)	1369(9)	1304(20)	72(4)
C(8)	-224(12)	915(10)	1665(21)	85(5)
C(9)	-37(10)	497(10)	292(19)	81(5)
C(10)	-642(10)	769(9)	-876(18)	78(4)
C(11)	864(8)	3086(9)	-1113(18)	64(4)
C(12)	354(8)	2755(11)	-2353(17)	69(4)
C(13)	489(10)	1843(10)	-2423(19)	77(4)
C(14)	1073(10)	1631(10)	-1260(22)	86(5)
C(15)	1314(9)	2390(9)	-388(19)	70(4)
C(16)	887(7)	2524(9)	3314(15)	61(3)
C(17)	1469(7)	1856(9)	3742(16)	62(3)
C(18)	1629(9)	1145(9)	2806(18)	72(4)
C(19)	2201(10)	584(12)	3386(23)	92(6)
C(20)	2615(10)	676(12)	4795(22)	87(5)
C(21)	2467(10)	1374(12)	5734(23)	92(5)
C(22)	1894(8)	1929(11)	5235(19)	76(4)
C(23)	-1294(8)	3413(10)	-1297(16)	71(4)
C(24)	-1666(8)	3082(10)	-2865(15)	63(4)
C(25)	-1498(8)	2362(8)	-3587(15)	63(3)
C(26)	-1897(12)	2159(12)	-5038(18)	89(5)
C(27)	-2479(11)	2712(16)	-5733(21)	103(6)
C(28)	-2641(11)	3419(12)	-5007(21)	90(6)
C(29)	-2264(8)	3665(14)	-3573(18)	80(5)
Co(2)	5464(1)	3364(1)	336(2)	56(1)
Ti(2)	4628(1)	2354(1)	1692(3)	53(1)
N(3)	4557(6)	3603(7)	980(13)	59(3)
N(4)	5661(6)	2239(7)	1090(12)	57(3)
C(30)	6294(16)	3422(11)	-1145(33)	101(8)
C(31)	5678(21)	3740(24)	-1906(28)	135(11)
C(32)	5482(15)	4454(15)	-1110(32)	120(8)
C(33)	6005(16)	4616(12)	133(28)	106(7)
C(34)	6539(11)	3887(18)	152(31)	116(8)
C(35)	5376(10)	1987(10)	4168(17)	77(4)
C(36)	4667(12)	1639(11)	4209(19)	86(5)
C(37)	4147(10)	2312(11)	4152(19)	82(5)
C(38)	4512(9)	3115(12)	4047(16)	76(4)
C(39)	5270(8)	2924(11)	4079(15)	72(4)
C(40)	3949(9)	1015(10)	986(22)	83(5)
C(41)	4425(9)	1147(10)	-142(20)	79(4)
C(42)	4149(10)	1938(10)	-949(20)	78(5)
C(43)	3532(8)	2246(10)	-267(19)	77(4)
C(44)	3415(8)	1645(8)	950(21)	73(4)
C(45)	4193(8)	4322(10)	932(17)	72(4)
C(46)	3467(7)	4552(8)	1463(17)	63(3)
C(47)	3278(9)	5407(10)	1566(20)	82(4)
C(48)	2615(11)	5656(11)	2058(22)	96(5)
C(49)	2121(11)	5073(11)	2476(28)	107(6)

C(50)	2369(9)	4196(12)	2423(26)	102(6)
C(51)	2974(9)	3921(9)	1931(20)	79(4)
C(52)	6248(8)	1761(8)	1036(16)	57(3)
C(53)	6393(8)	829(9)	1508(15)	57(3)
C(54)	5896(8)	261(9)	2085(17)	67(4)
C(55)	6111(10)	-590(10)	2394(19)	83(5)
C(56)	6802(9)	-896(9)	2186(18)	77(4)
C(57)	7313(10)	-335(13)	1688(22)	98(5)
C(58)	7105(8)	545(9)	1383(18)	70(4)

Table 3. Bond lengths [A] and angles [deg] for 4.

Co(1)-N(2)	1.851(10)
Co(1)-N(1)	1.856(10)
Co(1)-C(1)	2.06(2)
Co(1)-C(4)	2.07(2)
Co(1)-C(5)	2.114(13)
Co(1)-C(3)	2.101(13)
Co(1)-C(2)	2.19(2)
Co(1)-Ti(1)	2.569(3)
Ti(1)-N(2)	1.975(10)
Ti(1)-N(1)	1.996(10)
Ti(1)-C(7)	2.39(2)
Ti(1)-C(10)	2.419(13)
Ti(1)-C(8)	2.418(14)
Ti(1)-C(13)	2.434(14)
Ti(1)-C(12)	2.444(14)
Ti(1)-C(11)	2.445(12)
Ti(1)-C(14)	2.449(14)
Ti(1)-C(6)	2.449(14)
Ti(1)-C(15)	2.46(2)
Ti(1)-C(9)	2.48(2)
N(1)-C(16)	1.31(2)
N(2)-C(23)	1.30(2)
C(1)-C(2)	1.41(2)
C(1)-C(5)	1.39(2)
C(2)-C(3)	1.38(2)
C(3)-C(4)	1.39(2)
C(4)-C(5)	1.41(2)
C(6)-C(10)	1.38(2)
C(6)-C(7)	1.39(2)
C(7)-C(8)	1.37(2)
C(8)-C(9)	1.45(2)
C(9)-C(10)	1.44(2)
C(11)-C(12)	1.41(2)
C(11)-C(15)	1.43(2)
C(12)-C(13)	1.42(2)
C(13)-C(14)	1.39(3)
C(14)-C(15)	1.42(2)
C(16)-C(17)	1.47(2)
C(17)-C(18)	1.42(2)
C(17)-C(22)	1.42(2)
C(18)-C(19)	1.38(2)
C(19)-C(20)	1.36(3)
C(20)-C(21)	1.40(3)
C(21)-C(22)	1.36(2)
C(23)-C(24)	1.53(2)
C(24)-C(25)	1.33(2)
C(24)-C(29)	1.46(2)
C(25)-C(26)	1.40(2)
C(26)-C(27)	1.41(3)
C(27)-C(28)	1.31(3)
C(28)-C(29)	1.39(2)
Co(2)-N(3)	1.839(12)
Co(2)-N(4)	1.859(11)
Co(2)-C(32)	2.10(2)
Co(2)-C(34)	2.12(2)
Co(2)-C(30)	2.12(2)
Co(2)-C(31)	2.14(2)
Co(2)-C(33)	2.17(2)
Co(2)-Ti(2)	2.566(3)
Ti(2)-N(3)	2.009(11)
Ti(2)-N(4)	2.010(11)
Ti(2)-C(39)	2.408(14)

Ti(2)-C(40)	2.411(14)
Ti(2)-C(43)	2.418(14)
Ti(2)-C(44)	2.426(13)
Ti(2)-C(37)	2.436(13)
Ti(2)-C(41)	2.44(2)
Ti(2)-C(42)	2.444(14)
Ti(2)-C(35)	2.44(2)
Ti(2)-C(36)	2.45(2)
N(3)-C(45)	2.46(2)
N(4)-C(52)	1.28(2)
C(30)-C(31)	1.29(2)
C(30)-C(34)	1.30(4)
C(31)-C(32)	1.36(3)
C(32)-C(33)	1.37(4)
C(33)-C(34)	1.36(3)
C(35)-C(36)	1.47(3)
C(35)-C(39)	1.39(2)
C(36)-C(37)	1.45(2)
C(37)-C(38)	1.39(3)
C(38)-C(39)	1.40(2)
C(40)-C(44)	1.39(2)
C(40)-C(41)	1.36(2)
C(41)-C(42)	1.42(2)
C(42)-C(43)	1.45(2)
C(43)-C(44)	1.42(2)
C(45)-C(46)	1.45(2)
C(46)-C(47)	1.49(2)
C(46)-C(51)	1.36(2)
C(47)-C(48)	1.41(2)
C(48)-C(49)	1.38(2)
C(49)-C(50)	1.35(3)
C(50)-C(51)	1.39(2)
C(52)-C(53)	1.39(2)
C(53)-C(58)	1.50(2)
C(53)-C(54)	1.37(2)
C(54)-C(55)	1.39(2)
C(55)-C(56)	1.37(2)
C(56)-C(57)	1.36(2)
C(57)-C(58)	1.37(3)
	1.41(2)

N(2)-Co(1)-N(1)	100.5(4)
N(2)-Co(1)-C(1)	98.1(6)
N(1)-Co(1)-C(1)	158.7(6)
N(2)-Co(1)-C(4)	142.6(7)
N(1)-Co(1)-C(4)	104.5(6)
C(1)-Co(1)-C(4)	65.0(7)
N(2)-Co(1)-C(5)	106.5(5)
N(1)-Co(1)-C(5)	140.9(5)
C(1)-Co(1)-C(5)	38.8(6)
C(4)-Co(1)-C(5)	39.4(7)
N(2)-Co(1)-C(3)	160.3(4)
N(1)-Co(1)-C(3)	96.0(5)
C(1)-Co(1)-C(3)	63.9(6)
C(4)-Co(1)-C(3)	39.1(7)
C(5)-Co(1)-C(3)	65.2(6)
N(2)-Co(1)-C(2)	123.1(5)
N(1)-Co(1)-C(2)	120.6(5)
C(1)-Co(1)-C(2)	38.7(6)
C(4)-Co(1)-C(2)	64.8(7)
C(5)-Co(1)-C(2)	65.3(6)
C(3)-Co(1)-C(2)	37.5(5)
N(2)-Co(1)-Ti(1)	49.9(3)
N(1)-Co(1)-Ti(1)	50.6(3)
C(1)-Co(1)-Ti(1)	146.9(5)
C(4)-Co(1)-Ti(1)	144.6(5)

C(5)-Co(1)-Ti(1)	145.5(4)
C(3)-Co(1)-Ti(1)	145.3(4)
C(2)-Co(1)-Ti(1)	146.0(5)
N(2)-Ti(1)-N(1)	91.7(4)
N(2)-Ti(1)-C(7)	86.9(5)
N(1)-Ti(1)-C(7)	85.8(5)
N(2)-Ti(1)-C(10)	106.6(5)
N(1)-Ti(1)-C(10)	134.5(5)
C(7)-Ti(1)-C(10)	55.1(5)
N(2)-Ti(1)-C(8)	119.1(6)
N(1)-Ti(1)-C(8)	78.9(5)
C(7)-Ti(1)-C(8)	33.0(6)
C(10)-Ti(1)-C(8)	55.8(6)
N(2)-Ti(1)-C(13)	106.9(5)
N(1)-Ti(1)-C(13)	135.6(5)
C(7)-Ti(1)-C(13)	133.9(5)
C(10)-Ti(1)-C(13)	78.8(6)
C(8)-Ti(1)-C(13)	121.5(6)
N(2)-Ti(1)-C(12)	78.8(5)
N(1)-Ti(1)-C(12)	119.9(5)
C(7)-Ti(1)-C(12)	150.5(6)
C(10)-Ti(1)-C(12)	104.5(5)
C(8)-Ti(1)-C(12)	155.2(6)
C(13)-Ti(1)-C(12)	33.8(5)
N(2)-Ti(1)-C(11)	86.0(4)
N(1)-Ti(1)-C(11)	87.2(5)
C(7)-Ti(1)-C(11)	169.8(5)
C(10)-Ti(1)-C(11)	134.2(6)
C(8)-Ti(1)-C(11)	151.2(6)
C(13)-Ti(1)-C(11)	55.5(5)
C(12)-Ti(1)-C(11)	33.6(5)
N(2)-Ti(1)-C(14)	134.2(5)
N(1)-Ti(1)-C(14)	107.6(6)
C(7)-Ti(1)-C(14)	134.4(5)
C(10)-Ti(1)-C(14)	89.1(6)
C(8)-Ti(1)-C(14)	105.4(6)
C(13)-Ti(1)-C(14)	33.2(6)
C(12)-Ti(1)-C(14)	55.5(5)
C(11)-Ti(1)-C(14)	55.1(5)
N(2)-Ti(1)-C(6)	79.8(5)
N(1)-Ti(1)-C(6)	118.3(5)
C(7)-Ti(1)-C(6)	33.3(5)
C(10)-Ti(1)-C(6)	32.8(5)
C(8)-Ti(1)-C(6)	55.3(6)
C(13)-Ti(1)-C(6)	104.6(6)
C(12)-Ti(1)-C(6)	117.9(5)
C(11)-Ti(1)-C(6)	150.9(6)
C(14)-Ti(1)-C(6)	121.6(6)
N(2)-Ti(1)-C(15)	119.0(4)
N(1)-Ti(1)-C(15)	79.3(5)
C(7)-Ti(1)-C(15)	150.2(6)
C(10)-Ti(1)-C(15)	122.4(5)
C(8)-Ti(1)-C(15)	117.9(6)
C(13)-Ti(1)-C(15)	56.3(6)
C(12)-Ti(1)-C(15)	56.7(5)
C(11)-Ti(1)-C(15)	33.9(5)
C(14)-Ti(1)-C(15)	33.7(5)
C(6)-Ti(1)-C(15)	155.2(5)
N(2)-Ti(1)-C(9)	136.0(5)
N(1)-Ti(1)-C(9)	106.9(5)
C(7)-Ti(1)-C(9)	56.2(5)
C(10)-Ti(1)-C(9)	34.3(5)
C(8)-Ti(1)-C(9)	34.4(5)
C(13)-Ti(1)-C(9)	87.3(5)
C(12)-Ti(1)-C(9)	120.8(5)
C(11)-Ti(1)-C(9)	133.2(5)

C(6)-Ti(1)-C(9)	56.2(6)
C(15)-Ti(1)-C(9)	103.8(5)
C(16)-N(1)-Co(1)	127.7(9)
C(16)-N(1)-Ti(1)	148.6(9)
Co(1)-N(1)-Ti(1)	83.6(4)
C(23)-N(2)-Co(1)	127.0(9)
C(23)-N(2)-Ti(1)	148.8(9)
Co(1)-N(2)-Ti(1)	84.3(4)
C(2)-C(1)-C(5)	112(2)
C(2)-C(1)-Co(1)	75.7(10)
C(5)-C(1)-Co(1)	72.8(9)
C(3)-C(2)-C(1)	104(2)
C(3)-C(2)-Co(1)	67.7(8)
C(1)-C(2)-Co(1)	65.5(9)
C(2)-C(3)-C(4)	110.8(14)
C(2)-C(3)-Co(1)	74.7(8)
C(4)-C(3)-Co(1)	69.3(8)
C(3)-C(4)-C(5)	108.0(14)
C(3)-C(4)-Co(1)	71.7(9)
C(5)-C(4)-Co(1)	72.0(8)
C(4)-C(5)-C(1)	105(2)
C(4)-C(5)-Co(1)	68.6(9)
C(1)-C(5)-Co(1)	68.4(8)
C(10)-C(6)-C(7)	107(2)
C(10)-C(6)-Ti(1)	72.4(8)
C(7)-C(6)-Ti(1)	70.9(9)
C(8)-C(7)-C(6)	110(2)
C(8)-C(7)-Ti(1)	74.7(9)
C(6)-C(7)-Ti(1)	75.8(9)
C(7)-C(8)-C(9)	109(2)
C(7)-C(8)-Ti(1)	72.3(9)
C(9)-C(8)-Ti(1)	75.0(9)
C(10)-C(9)-C(8)	103(2)
C(10)-C(9)-Ti(1)	70.7(8)
C(8)-C(9)-Ti(1)	70.6(8)
C(6)-C(10)-C(9)	110.6(14)
C(6)-C(10)-Ti(1)	74.8(8)
C(9)-C(10)-Ti(1)	75.0(9)
C(12)-C(11)-C(15)	109.9(13)
C(12)-C(11)-Ti(1)	73.2(7)
C(15)-C(11)-Ti(1)	73.5(7)
C(13)-C(12)-C(11)	106.8(14)
C(13)-C(12)-Ti(1)	72.7(8)
C(11)-C(12)-Ti(1)	73.2(8)
C(14)-C(13)-C(12)	108(2)
C(14)-C(13)-Ti(1)	74.0(9)
C(12)-C(13)-Ti(1)	73.5(8)
C(13)-C(14)-C(15)	110.1(14)
C(13)-C(14)-Ti(1)	72.8(8)
C(15)-C(14)-Ti(1)	73.4(8)
C(14)-C(15)-C(11)	105(2)
C(14)-C(15)-Ti(1)	72.8(8)
C(11)-C(15)-Ti(1)	72.6(8)
N(1)-C(16)-C(17)	128.6(12)
C(18)-C(17)-C(22)	118.0(13)
C(18)-C(17)-C(16)	125.5(12)
C(22)-C(17)-C(16)	116.5(13)
C(19)-C(18)-C(17)	118(2)
C(20)-C(19)-C(18)	124(2)
C(19)-C(20)-C(21)	120(2)
C(22)-C(21)-C(20)	119(2)
C(21)-C(22)-C(17)	122(2)
N(2)-C(23)-C(24)	127.4(13)
C(25)-C(24)-C(29)	120.4(14)
C(25)-C(24)-C(23)	127.3(14)

C(24)-C(25)-C(26)	120(2)
C(25)-C(26)-C(27)	121(2)
C(28)-C(27)-C(26)	119(2)
C(27)-C(28)-C(29)	123(2)
C(28)-C(29)-C(24)	117(2)
N(3)-Co(2)-N(4)	101.9(5)
N(3)-Co(2)-C(32)	97.0(7)
N(4)-Co(2)-C(32)	158.7(7)
N(3)-Co(2)-C(34)	143.8(9)
N(4)-Co(2)-C(34)	104.4(8)
C(32)-Co(2)-C(34)	63.8(9)
N(3)-Co(2)-C(30)	156.3(8)
N(4)-Co(2)-C(30)	98.2(6)
C(32)-Co(2)-C(30)	61.3(8)
C(34)-Co(2)-C(30)	37.5(9)
N(3)-Co(2)-C(31)	121.1(12)
N(4)-Co(2)-C(31)	121.7(12)
C(32)-Co(2)-C(31)	37.7(10)
C(34)-Co(2)-C(31)	62.7(10)
C(30)-Co(2)-C(31)	35.5(10)
N(3)-Co(2)-C(33)	106.2(7)
N(4)-Co(2)-C(33)	141.5(9)
C(32)-Co(2)-C(33)	37.1(8)
C(34)-Co(2)-C(33)	40.1(8)
C(30)-Co(2)-C(33)	63.2(8)
C(31)-Co(2)-C(33)	62.9(9)
N(3)-Co(2)-Ti(2)	51.1(3)
N(4)-Co(2)-Ti(2)	51.0(4)
C(32)-Co(2)-Ti(2)	145.2(7)
C(34)-Co(2)-Ti(2)	149.8(6)
C(30)-Co(2)-Ti(2)	145.3(5)
C(31)-Co(2)-Ti(2)	141.7(7)
C(33)-Co(2)-Ti(2)	150.5(5)
N(3)-Ti(2)-N(4)	91.2(5)
N(3)-Ti(2)-C(39)	85.9(5)
N(4)-Ti(2)-C(39)	85.3(5)
N(3)-Ti(2)-C(38)	78.4(5)
N(4)-Ti(2)-C(38)	117.8(5)
C(39)-Ti(2)-C(38)	33.5(5)
N(3)-Ti(2)-C(40)	135.9(5)
N(4)-Ti(2)-C(40)	108.0(5)
C(39)-Ti(2)-C(40)	133.7(6)
C(38)-Ti(2)-C(40)	121.7(6)
N(3)-Ti(2)-C(43)	80.5(5)
N(4)-Ti(2)-C(43)	119.5(5)
C(39)-Ti(2)-C(43)	151.7(5)
C(38)-Ti(2)-C(43)	118.7(6)
C(40)-Ti(2)-C(43)	55.5(6)
N(3)-Ti(2)-C(44)	109.0(5)
N(4)-Ti(2)-C(44)	135.6(5)
C(39)-Ti(2)-C(44)	133.7(6)
C(38)-Ti(2)-C(44)	105.0(6)
C(40)-Ti(2)-C(44)	32.5(5)
C(43)-Ti(2)-C(44)	34.7(6)
N(3)-Ti(2)-C(37)	106.6(5)
N(4)-Ti(2)-C(37)	133.6(6)
C(39)-Ti(2)-C(37)	54.8(5)
C(38)-Ti(2)-C(37)	33.5(5)
C(40)-Ti(2)-C(37)	88.6(6)
C(43)-Ti(2)-C(37)	105.8(6)
C(44)-Ti(2)-C(37)	78.9(6)
N(3)-Ti(2)-C(41)	121.1(6)
N(4)-Ti(2)-C(41)	79.4(5)
C(39)-Ti(2)-C(41)	148.8(6)
C(38)-Ti(2)-C(41)	155.3(6)

C(43)-Ti(2)-C(41)	56.8(6)
C(44)-Ti(2)-C(41)	56.3(5)
C(37)-Ti(2)-C(41)	121.8(6)
N(3)-Ti(2)-C(42)	87.3(5)
N(4)-Ti(2)-C(42)	86.4(5)
C(39)-Ti(2)-C(42)	169.2(5)
C(38)-Ti(2)-C(42)	151.7(6)
C(40)-Ti(2)-C(42)	56.0(6)
C(43)-Ti(2)-C(42)	33.8(5)
C(44)-Ti(2)-C(42)	56.7(6)
C(37)-Ti(2)-C(42)	135.6(6)
C(41)-Ti(2)-C(42)	34.6(5)
N(3)-Ti(2)-C(35)	119.7(5)
N(4)-Ti(2)-C(35)	78.9(5)
C(39)-Ti(2)-C(35)	34.6(5)
C(38)-Ti(2)-C(35)	56.7(6)
C(40)-Ti(2)-C(35)	103.0(6)
C(43)-Ti(2)-C(35)	154.0(6)
C(44)-Ti(2)-C(35)	119.3(6)
C(37)-Ti(2)-C(35)	55.0(6)
C(41)-Ti(2)-C(35)	115.1(6)
C(42)-Ti(2)-C(35)	149.1(6)
N(3)-Ti(2)-C(36)	134.0(6)
N(4)-Ti(2)-C(36)	107.0(6)
C(39)-Ti(2)-C(36)	55.2(6)
C(38)-Ti(2)-C(36)	55.7(6)
C(40)-Ti(2)-C(36)	78.6(6)
C(43)-Ti(2)-C(36)	121.5(6)
C(44)-Ti(2)-C(36)	87.2(6)
C(37)-Ti(2)-C(36)	32.8(6)
C(41)-Ti(2)-C(36)	103.9(6)
C(42)-Ti(2)-C(36)	134.4(6)
C(35)-Ti(2)-C(36)	32.8(6)
C(45)-N(3)-Co(2)	129.3(10)
C(45)-N(3)-Ti(2)	147.0(10)
Co(2)-N(3)-Ti(2)	83.5(4)
C(52)-N(4)-Co(2)	128.8(10)
C(52)-N(4)-Ti(2)	148.2(10)
Co(2)-N(4)-Ti(2)	83.0(5)
C(31)-C(30)-C(34)	113(2)
C(31)-C(30)-Co(2)	73.2(13)
C(34)-C(30)-Co(2)	71.2(11)
C(30)-C(31)-C(32)	107(3)
C(30)-C(31)-Co(2)	71.3(13)
C(32)-C(31)-Co(2)	69.5(11)
C(33)-C(32)-C(31)	111(2)
C(33)-C(32)-Co(2)	74.1(10)
C(31)-C(32)-Co(2)	72.8(12)
C(32)-C(33)-C(34)	104(2)
C(32)-C(33)-Co(2)	68.8(11)
C(34)-C(33)-Co(2)	68.3(9)
C(30)-C(34)-C(33)	105(2)
C(30)-C(34)-Co(2)	71.3(11)
C(33)-C(34)-Co(2)	71.7(10)
C(36)-C(35)-C(39)	106(2)
C(36)-C(35)-Ti(2)	74.0(9)
C(39)-C(35)-Ti(2)	71.0(8)
C(37)-C(36)-C(35)	109.3(14)
C(37)-C(36)-Ti(2)	72.9(9)
C(35)-C(36)-Ti(2)	73.3(9)
C(36)-C(37)-C(38)	110(2)
C(36)-C(37)-Ti(2)	74.3(9)
C(38)-C(37)-Ti(2)	71.9(9)
C(39)-C(38)-C(37)	106(2)
C(39)-C(38)-Ti(2)	73.1(8)

C(38)-C(39)-C(35)	109.3(14)
C(38)-C(39)-Ti(2)	73.4(8)
C(35)-C(39)-Ti(2)	74.4(9)
C(44)-C(40)-C(41)	112(2)
C(44)-C(40)-Ti(2)	74.5(8)
C(41)-C(40)-Ti(2)	74.1(8)
C(40)-C(41)-C(42)	105(2)
C(40)-C(41)-Ti(2)	72.1(8)
C(42)-C(41)-Ti(2)	72.6(8)
C(43)-C(42)-C(41)	108(2)
C(43)-C(42)-Ti(2)	72.5(9)
C(41)-C(42)-Ti(2)	72.8(9)
C(42)-C(43)-C(44)	108.0(14)
C(42)-C(43)-Ti(2)	73.7(8)
C(44)-C(43)-Ti(2)	73.0(8)
C(40)-C(44)-C(43)	107(2)
C(40)-C(44)-Ti(2)	73.0(8)
C(43)-C(44)-Ti(2)	72.3(7)
N(3)-C(45)-C(46)	131.3(12)
C(47)-C(46)-C(51)	117.8(13)
C(47)-C(46)-C(45)	119.1(13)
C(51)-C(46)-C(45)	123.0(12)
C(48)-C(47)-C(46)	122(2)
C(49)-C(48)-C(47)	123(2)
C(48)-C(49)-C(50)	117(2)
C(49)-C(50)-C(51)	122(2)
C(50)-C(51)-C(46)	119.1(14)
N(4)-C(52)-C(53)	129.8(12)
C(58)-C(53)-C(54)	119.1(13)
C(58)-C(53)-C(52)	113.9(12)
C(54)-C(53)-C(52)	126.9(13)
C(55)-C(54)-C(53)	119.2(14)
C(54)-C(55)-C(56)	122.2(14)
C(55)-C(56)-C(57)	119.4(14)
C(56)-C(57)-C(58)	119(2)
C(53)-C(58)-C(57)	120.8(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 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
Co(1)	58(1)	46(1)	43(1)	-4(1)	4(1)	1(1)
Ti(1)	64(1)	41(1)	45(1)	0(1)	11(1)	-3(1)
N(1)	53(6)	49(6)	53(6)	4(4)	2(5)	-3(4)
N(2)	54(6)	34(5)	59(6)	3(4)	7(5)	-3(4)
C(1)	92(12)	76(9)	64(10)	-10(8)	6(9)	9(8)
C(2)	88(12)	73(10)	73(10)	-10(8)	3(9)	-4(8)
C(3)	82(10)	35(7)	60(8)	7(5)	-3(7)	0(6)
C(4)	122(15)	102(13)	42(9)	-2(8)	16(9)	0(12)
C(5)	71(9)	39(7)	85(10)	-8(6)	27(8)	1(6)
C(6)	68(9)	84(10)	68(10)	-9(8)	26(8)	-24(8)
C(7)	83(11)	55(9)	83(11)	-15(8)	29(9)	-16(8)
C(8)	125(15)	63(8)	67(10)	21(8)	12(9)	-28(9)
C(9)	105(12)	47(9)	93(13)	-3(8)	22(10)	6(8)
C(10)	104(12)	58(9)	69(10)	-4(7)	0(9)	-28(8)
C(11)	63(8)	43(7)	89(10)	6(7)	27(8)	-6(6)
C(12)	63(9)	91(11)	54(8)	13(7)	16(7)	-1(8)
C(13)	101(13)	72(10)	66(10)	-3(8)	43(10)	-1(8)
C(14)	91(12)	75(10)	104(13)	14(9)	54(11)	25(8)
C(15)	75(9)	62(8)	78(10)	-4(7)	29(8)	-6(7)
C(16)	64(8)	61(8)	54(8)	0(6)	-6(7)	12(6)
C(17)	62(8)	53(7)	67(9)	15(6)	-4(7)	3(6)
C(18)	84(10)	67(8)	69(9)	15(7)	28(8)	19(7)
C(19)	96(12)	72(11)	111(15)	46(10)	31(12)	30(9)
C(20)	86(11)	75(13)	98(13)	38(11)	7(10)	21(9)
C(21)	89(13)	91(12)	86(12)	36(10)	-20(9)	-3(10)
C(22)	63(9)	82(10)	79(10)	17(8)	-5(8)	4(7)
C(23)	66(9)	87(10)	56(8)	-25(7)	1(7)	5(7)
C(24)	55(8)	82(10)	48(7)	6(7)	-7(6)	-21(7)
C(25)	88(10)	52(7)	49(7)	-7(6)	10(7)	-21(6)
C(26)	115(15)	103(13)	50(9)	-10(8)	14(9)	-44(11)
C(27)	83(12)	156(19)	62(11)	-17(12)	-18(9)	-45(13)
C(28)	87(12)	101(14)	70(12)	20(10)	-27(9)	-20(10)
C(29)	48(8)	124(13)	64(10)	18(9)	-3(7)	-7(8)
Co(2)	58(1)	57(1)	53(1)	-1(1)	11(1)	-3(1)
Ti(2)	51(1)	53(1)	55(1)	-4(1)	5(1)	-5(1)
N(3)	69(7)	49(7)	59(6)	10(5)	6(5)	11(5)
N(4)	63(7)	54(6)	55(6)	-2(5)	8(5)	-9(5)
C(30)	126(18)	63(10)	134(20)	22(11)	85(17)	15(11)
C(31)	176(29)	165(28)	72(15)	7(17)	44(17)	-65(24)
C(32)	143(20)	117(16)	112(18)	76(14)	66(17)	39(14)
C(33)	179(22)	57(10)	91(15)	3(9)	53(15)	-37(12)
C(34)	71(12)	129(20)	149(22)	49(17)	17(12)	-28(12)
C(35)	97(12)	79(10)	55(9)	12(7)	4(8)	18(9)
C(36)	115(15)	85(10)	57(10)	10(7)	11(9)	-24(10)
C(37)	86(11)	78(10)	87(12)	-10(8)	29(9)	-16(9)
C(38)	77(11)	104(11)	50(8)	-12(7)	23(7)	-5(8)
C(39)	58(9)	111(13)	47(8)	-3(8)	2(6)	-13(8)
C(40)	77(10)	62(9)	102(13)	-4(8)	-13(10)	-23(8)
C(41)	74(10)	65(9)	93(12)	-32(8)	-1(9)	-22(7)
C(42)	87(12)	51(8)	88(11)	-13(7)	-14(9)	-23(7)
C(43)	62(9)	74(10)	84(11)	-26(8)	-26(8)	-3(7)
C(44)	58(8)	36(7)	122(14)	-18(7)	6(8)	-10(6)
C(45)	63(9)	94(11)	60(9)	19(8)	17(7)	-15(8)
C(46)	69(9)	38(7)	80(9)	8(6)	6(7)	6(6)
C(47)	68(9)	76(10)	105(13)	4(9)	22(9)	2(8)
C(48)	100(14)	75(11)	109(14)	3(9)	-1(11)	25(10)

C(49)	75(11)	82(12)	166(20)	-28(11)	24(12)	-5(9)
C(50)	65(10)	78(12)	173(19)	-22(11)	52(12)	-16(8)
C(51)	83(10)	51(9)	106(13)	-12(8)	27(9)	-12(7)
C(52)	54(8)	52(7)	65(9)	5(6)	10(6)	-5(6)
C(53)	63(8)	61(8)	49(7)	-4(6)	13(6)	-7(6)
C(54)	63(9)	64(8)	73(9)	-5(7)	9(7)	13(6)
C(55)	94(12)	65(10)	93(12)	-3(8)	28(10)	-22(8)
C(56)	99(12)	36(7)	94(12)	14(6)	9(9)	24(7)
C(57)	78(11)	110(14)	107(14)	-1(11)	15(10)	24(10)
C(58)	57(8)	67(8)	83(10)	0(7)	6(7)	15(6)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 4.

	x	y	z	U(eq)
H(1)	-1079(10)	4858(10)	550(19)	94
H(2)	254(10)	5208(11)	1666(19)	94
H(3)	541(8)	4238(7)	3944(15)	72
H(4)	-617(12)	3480(13)	4421(18)	106
H(5)	-1675(8)	3958(8)	2379(18)	76
H(6)	-1614(9)	1475(10)	-748(18)	86
H(7)	-1109(10)	1703(9)	1992(20)	87
H(8)	58(12)	881(10)	2637(21)	102
H(9)	372(10)	141(10)	189(19)	97
H(10)	-677(10)	632(9)	-1914(18)	94
H(11)	901(8)	3669(9)	-813(18)	76
H(12)	-3(8)	3073(11)	-3000(17)	82
H(13)	232(10)	1454(10)	-3124(19)	92
H(14)	1276(10)	1075(10)	-1080(22)	103
H(15)	1684(9)	2425(9)	467(19)	84
H(16)	845(7)	2950(9)	4052(15)	73
H(18)	1357(9)	1060(9)	1835(18)	86
H(19)	2309(10)	117(12)	2778(23)	110
H(20)	2995(10)	278(12)	5133(22)	104
H(21)	2757(10)	1457(12)	6688(23)	110
H(22)	1776(8)	2371(11)	5887(19)	91
H(23)	-1487(8)	3927(10)	-948(16)	85
H(25)	-1117(8)	1993(8)	-3135(15)	76
H(26)	-1777(12)	1657(12)	-5546(18)	107
H(27)	-2743(11)	2576(16)	-6692(21)	124
H(28)	-3028(11)	3776(12)	-5473(21)	108
H(29)	-2386(8)	4175(14)	-3089(18)	96
H(30)	6539(16)	2931(11)	-1453(33)	121
H(31)	5419(21)	3523(24)	-2820(28)	162
H(32)	5049(15)	4783(15)	-1385(32)	143
H(33)	6021(16)	5081(12)	818(28)	127
H(34)	6954(11)	3770(18)	886(31)	139
H(35)	5826(10)	1682(10)	4194(17)	93
H(36)	4557(12)	1046(11)	4265(19)	103
H(37)	3635(10)	2242(11)	4180(19)	99
H(38)	4291(9)	3666(12)	3970(16)	91
H(39)	5650(8)	3334(11)	4048(15)	87
H(40)	3997(9)	549(10)	1674(22)	99
H(41)	4828(9)	801(10)	-327(20)	94
H(42)	4343(10)	2196(10)	-1765(20)	93
H(43)	3251(8)	2745(10)	-550(19)	92
H(44)	3045(8)	1684(8)	1585(21)	87
H(45)	4422(8)	4783(10)	488(17)	86
H(47)	3604(9)	5835(10)	1300(20)	98
H(48)	2505(11)	6249(11)	2102(22)	116
H(49)	1672(11)	5252(11)	2788(28)	128
H(50)	1982(9)	3780(12)	2724(26)	122
H(51)	3091(9)	3329(9)	1912(20)	94
H(52)	6641(8)	2036(8)	644(16)	68
H(54)	5425(8)	455(9)	2260(17)	80
H(55)	5773(10)	-971(10)	2758(19)	99
H(56)	6927(9)	-1480(9)	2380(18)	92
H(57)	7789(10)	-532(13)	1553(22)	118
H(58)	7455(8)	937(9)	1095(18)	83