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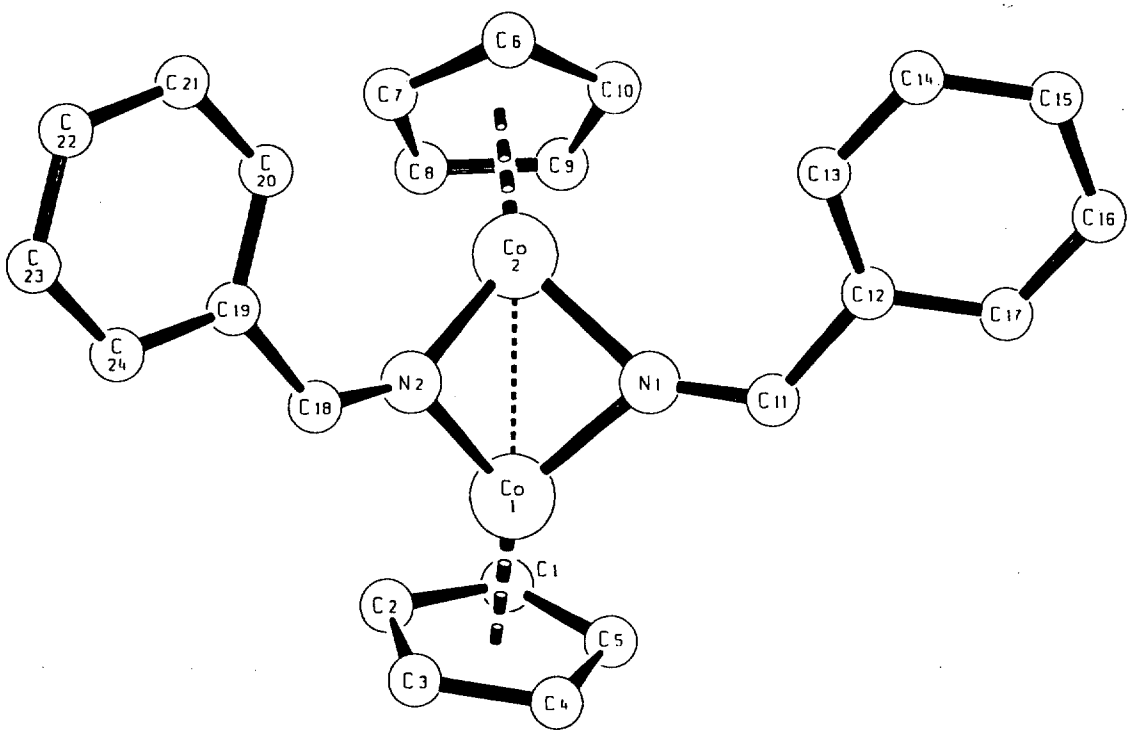

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Table 1. Crystal data and structure refinement for 12.

Identification code	755o
Empirical formula	C24 H22 Co2 N2
Formula weight	456.30
Crystal system	Orthorhombic
Space group	Pca2(1)
Unit cell dimensions	a= 21.602(4) A alpha= 90 deg. b= 10.129(2) A beta= 90 deg. c= 9.660(2) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	5000
Theta for cell determination	4 to 20 deg
Volume	2113.7(7) A^3
Z	4
Density (calculated)	1.434 Mg/m^3
Absorption coefficient	1.580 mm^-1
F(000)	936
Crystal colour	brown
Crystal description	prism
Crystal size	0.3 x 0.2 x 0.2 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	laser scanned imaging plate
Standards (intensity + orient.)	50-200
Intensity after	360 sec
Theta range for data collection	1.89 to 24.22 deg.
Index ranges	0<=h<=24, -11<=k<=11, -10<=l<=10
Reflections collected	6010
Independent reflections	3224 [R(int) = 0.0232]

Reflections unique	3224
Reflections observed	2761
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	3224 / 1 / 261
Final R indices [I>2sigma(I)]	R1 = 0.0273, wR2 = 0.0642
R indices (all data)	R1 = 0.0350, wR2 = 0.0728
Goodness-of-fit on F^2(all)	1.012
Goodness-of-fit on F^2(obs)	0.971
Shift/esd(max)	0.000
Shift/esd(mean)	0.000
Absolute structure parameter	0.43(2)
Weighting scheme	
calc w=1/[\s^2^(Fo^2^)+(0.0412P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	0.178 and -0.218 e.A^-3
Diff. density rms	0.049
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 12. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Co(1)	1733(1)	1200(1)	321(1)	40(1)
Co(2)	1250(1)	3137(1)	1099(1)	42(1)
N(1)	2089(1)	2792(3)	800(4)	44(1)
N(2)	1306(1)	1484(3)	1949(4)	37(1)
C(1)	1572(2)	621(6)	-1743(6)	64(1)
C(2)	1298(3)	-244(6)	-803(7)	73(2)
C(3)	1761(4)	-802(5)	18(7)	86(2)
C(4)	2336(3)	-242(5)	-392(6)	67(1)
C(5)	2205(2)	644(5)	-1449(6)	60(1)
C(6)	772(3)	4832(6)	1755(8)	84(2)
C(7)	357(2)	3831(6)	1383(7)	73(2)
C(8)	433(3)	3496(6)	14(7)	76(2)
C(9)	905(3)	4281(6)	-534(6)	79(2)
C(10)	1119(3)	5085(5)	570(9)	79(2)
C(11)	2631(2)	3277(4)	735(5)	48(1)
C(12)	2826(2)	4607(4)	1185(6)	46(1)
C(13)	2517(3)	5295(5)	2241(6)	68(2)
C(14)	2715(3)	6522(6)	2617(8)	95(2)
C(15)	3217(3)	7108(6)	1967(8)	90(2)
C(16)	3533(3)	6423(5)	999(9)	84(2)
C(17)	3343(2)	5168(4)	621(5)	59(2)
C(18)	1154(2)	716(4)	2935(4)	39(1)
C(19)	784(2)	1013(4)	4181(4)	40(1)
C(20)	622(2)	2291(5)	4566(6)	57(1)
C(21)	253(2)	2509(6)	5702(6)	73(2)
C(22)	50(2)	1466(7)	6491(6)	75(2)
C(23)	212(2)	210(5)	6141(7)	65(1)
C(24)	581(2)	-15(5)	5003(5)	53(1)

Table 3. Bond lengths [A] and angles [deg] for 12.

Co(1)-N(1)	1.846(3)
Co(1)-N(2)	1.846(3)
Co(1)-C(3)	2.049(5)
Co(1)-C(2)	2.050(5)
Co(1)-C(5)	2.068(5)
Co(1)-C(4)	2.075(5)
Co(1)-C(1)	2.107(5)
Co(1)-Co(2)	2.3472(8)
Co(2)-N(2)	1.869(3)
Co(2)-N(1)	1.870(3)
Co(2)-C(10)	2.057(5)
Co(2)-C(7)	2.070(5)
Co(2)-C(8)	2.085(5)
Co(2)-C(9)	2.094(5)
Co(2)-C(6)	2.100(5)
N(1)-C(11)	1.271(5)
N(2)-C(18)	1.272(5)
C(1)-C(2)	1.395(8)
C(1)-C(5)	1.395(7)
C(2)-C(3)	1.396(9)
C(3)-C(4)	1.423(8)
C(4)-C(5)	1.388(8)
C(6)-C(10)	1.393(9)
C(6)-C(7)	1.399(8)
C(7)-C(8)	1.376(9)
C(8)-C(9)	1.397(8)
C(9)-C(10)	1.420(8)
C(11)-C(12)	1.477(6)
C(12)-C(17)	1.367(6)
C(12)-C(13)	1.404(7)
C(13)-C(14)	1.363(7)
C(14)-C(15)	1.386(9)
C(15)-C(16)	1.351(9)
C(16)-C(17)	1.384(7)
C(18)-C(19)	1.476(5)
C(19)-C(24)	1.381(6)
C(19)-C(20)	1.391(6)
C(20)-C(21)	1.374(7)
C(21)-C(22)	1.374(8)
C(22)-C(23)	1.363(8)
C(23)-C(24)	1.377(7)
N(1)-Co(1)-N(2)	81.87(14)
N(1)-Co(1)-C(3)	152.6(3)
N(2)-Co(1)-C(3)	106.9(2)
N(1)-Co(1)-C(2)	161.3(2)
N(2)-Co(1)-C(2)	109.4(2)
C(3)-Co(1)-C(2)	39.8(3)
N(1)-Co(1)-C(5)	103.9(2)
N(2)-Co(1)-C(5)	173.1(2)
C(3)-Co(1)-C(5)	66.3(2)
C(2)-Co(1)-C(5)	66.0(2)
N(1)-Co(1)-C(4)	115.9(2)
N(2)-Co(1)-C(4)	135.0(2)
C(3)-Co(1)-C(4)	40.4(2)
C(2)-Co(1)-C(4)	67.1(2)
C(5)-Co(1)-C(4)	39.2(2)
N(1)-Co(1)-C(1)	123.3(2)
N(2)-Co(1)-C(1)	140.1(2)
C(3)-Co(1)-C(1)	66.1(3)
C(2)-Co(1)-C(1)	39.2(2)

C(4)-Co(1)-C(1)	66.0(2)
N(1)-Co(1)-Co(2)	51.28(10)
N(2)-Co(1)-Co(2)	51.26(10)
C(3)-Co(1)-Co(2)	152.4(2)
C(2)-Co(1)-Co(2)	124.2(2)
C(5)-Co(1)-Co(2)	135.4(2)
C(4)-Co(1)-Co(2)	167.0(2)
C(1)-Co(1)-Co(2)	117.5(2)
N(2)-Co(2)-N(1)	80.62(13)
N(2)-Co(2)-C(10)	167.8(3)
N(1)-Co(2)-C(10)	105.9(2)
N(2)-Co(2)-C(7)	107.9(2)
N(1)-Co(2)-C(7)	170.9(2)
C(10)-Co(2)-C(7)	65.2(2)
N(2)-Co(2)-C(8)	115.6(2)
N(1)-Co(2)-C(8)	140.9(2)
C(10)-Co(2)-C(8)	65.9(2)
C(7)-Co(2)-C(8)	38.7(2)
N(2)-Co(2)-C(9)	148.2(2)
N(1)-Co(2)-C(9)	109.4(2)
C(10)-Co(2)-C(9)	40.0(2)
C(7)-Co(2)-C(9)	65.2(2)
C(8)-Co(2)-C(9)	39.1(2)
N(2)-Co(2)-C(6)	129.2(2)
N(1)-Co(2)-C(6)	132.6(2)
C(10)-Co(2)-C(6)	39.1(2)
C(7)-Co(2)-C(6)	39.2(2)
C(8)-Co(2)-C(6)	66.0(2)
C(9)-Co(2)-C(6)	66.5(3)
N(2)-Co(2)-Co(1)	50.39(10)
N(1)-Co(2)-Co(1)	50.36(9)
C(10)-Co(2)-Co(1)	141.5(2)
C(7)-Co(2)-Co(1)	137.8(2)
C(8)-Co(2)-Co(1)	111.2(2)
C(9)-Co(2)-Co(1)	112.3(2)
C(6)-Co(2)-Co(1)	176.9(2)
C(11)-N(1)-Co(1)	135.2(3)
C(11)-N(1)-Co(2)	146.0(3)
Co(1)-N(1)-Co(2)	78.36(12)
C(18)-N(2)-Co(1)	132.2(3)
C(18)-N(2)-Co(2)	149.2(3)
Co(1)-N(2)-Co(2)	78.34(14)
C(2)-C(1)-C(5)	107.1(5)
C(2)-C(1)-Co(1)	68.2(3)
C(5)-C(1)-Co(1)	69.0(3)
C(1)-C(2)-C(3)	108.6(5)
C(1)-C(2)-Co(1)	72.6(3)
C(3)-C(2)-Co(1)	70.1(3)
C(2)-C(3)-C(4)	107.9(5)
C(2)-C(3)-Co(1)	70.1(3)
C(4)-C(3)-Co(1)	70.8(3)
C(5)-C(4)-C(3)	106.4(5)
C(5)-C(4)-Co(1)	70.2(3)
C(3)-C(4)-Co(1)	68.9(3)
C(4)-C(5)-C(1)	109.9(5)
C(4)-C(5)-Co(1)	70.7(3)
C(1)-C(5)-Co(1)	72.0(3)
C(10)-C(6)-C(7)	105.5(6)
C(10)-C(6)-Co(2)	68.7(3)
C(7)-C(6)-Co(2)	69.2(3)
C(8)-C(7)-C(6)	110.5(6)
C(8)-C(7)-Co(2)	71.2(3)
C(6)-C(7)-Co(2)	71.6(3)
C(7)-C(8)-C(9)	108.1(5)
C(7)-C(8)-Co(2)	70.1(3)

C(8)-C(9)-C(10)	106.3(6)
C(8)-C(9)-Co(2)	70.1(3)
C(10)-C(9)-Co(2)	68.6(3)
C(6)-C(10)-C(9)	109.6(6)
C(6)-C(10)-Co(2)	72.1(3)
C(9)-C(10)-Co(2)	71.4(3)
N(1)-C(11)-C(12)	126.9(4)
C(17)-C(12)-C(13)	118.1(4)
C(17)-C(12)-C(11)	119.6(4)
C(13)-C(12)-C(11)	122.1(4)
C(14)-C(13)-C(12)	119.8(5)
C(13)-C(14)-C(15)	121.0(6)
C(16)-C(15)-C(14)	119.3(5)
C(15)-C(16)-C(17)	120.3(6)
C(12)-C(17)-C(16)	121.2(5)
N(2)-C(18)-C(19)	128.7(4)
C(24)-C(19)-C(20)	117.9(4)
C(24)-C(19)-C(18)	119.1(4)
C(20)-C(19)-C(18)	122.9(4)
C(21)-C(20)-C(19)	120.6(5)
C(22)-C(21)-C(20)	120.3(5)
C(23)-C(22)-C(21)	119.9(5)
C(22)-C(23)-C(24)	120.1(5)
C(23)-C(24)-C(19)	121.2(4)

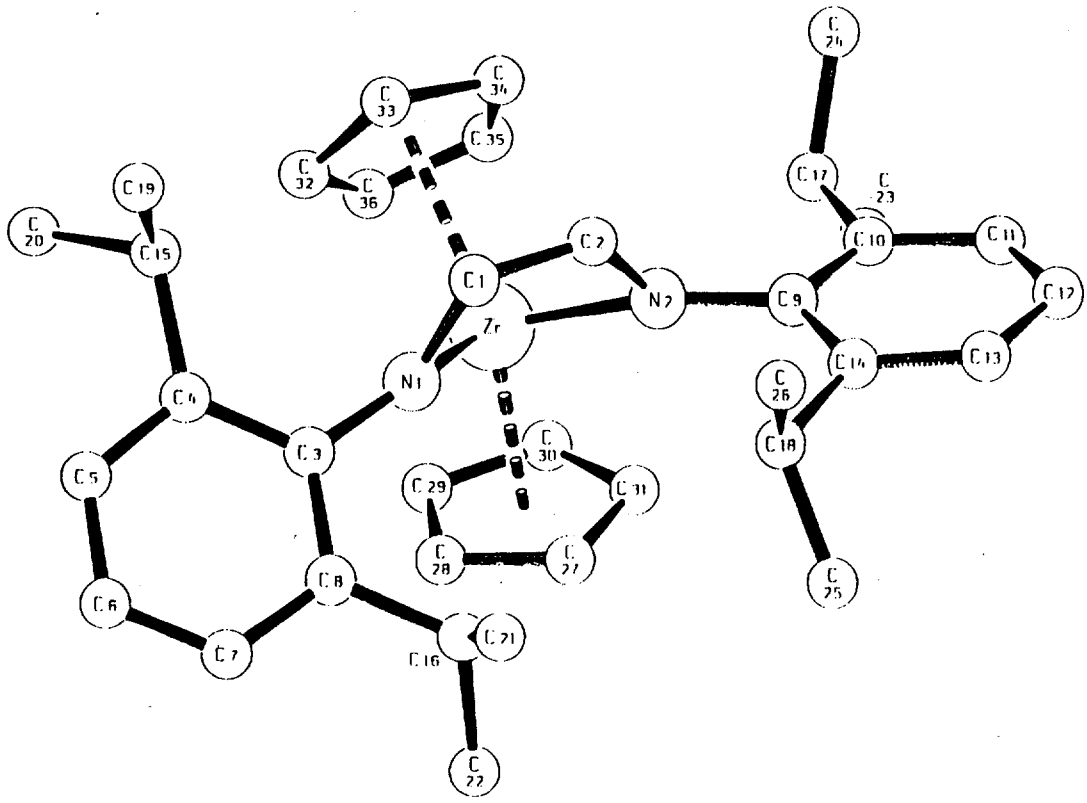
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 12. 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)	41(1)	38(1)	42(1)	-7(1)	7(1)	-3(1)
Co(2)	41(1)	39(1)	46(1)	-1(1)	1(1)	3(1)
N(1)	44(2)	38(2)	50(3)	0(2)	6(2)	-3(1)
N(2)	34(2)	37(2)	39(2)	-5(2)	3(2)	-2(1)
C(1)	59(3)	77(3)	55(4)	-19(3)	4(2)	2(3)
C(2)	74(4)	80(4)	64(4)	-36(3)	20(3)	-23(3)
C(3)	153(6)	35(3)	71(5)	-10(3)	40(4)	-9(3)
C(4)	83(4)	65(3)	54(4)	-16(3)	-1(3)	27(3)
C(5)	52(3)	63(3)	66(4)	-15(3)	18(2)	-9(2)
C(6)	91(4)	59(4)	103(6)	-16(3)	-19(4)	40(3)
C(7)	50(3)	83(4)	87(5)	9(3)	1(3)	21(3)
C(8)	63(3)	79(4)	85(6)	2(3)	-21(3)	12(3)
C(9)	99(4)	92(4)	47(4)	11(3)	-1(3)	36(4)
C(10)	72(3)	58(3)	107(7)	23(3)	-9(4)	14(3)
C(11)	46(2)	42(2)	55(4)	-4(2)	10(2)	-4(2)
C(12)	47(2)	45(2)	47(3)	-5(2)	-4(2)	-5(2)
C(13)	76(3)	62(3)	67(4)	-23(3)	1(3)	-8(3)
C(14)	111(5)	76(4)	98(6)	-40(4)	-3(4)	-3(4)
C(15)	126(5)	59(4)	86(5)	-19(3)	-27(4)	-22(4)
C(16)	82(3)	64(3)	104(5)	1(4)	-8(4)	-34(3)
C(17)	62(3)	56(3)	61(5)	-7(2)	4(2)	-14(2)
C(18)	36(2)	40(2)	40(3)	-9(2)	-2(2)	-1(2)
C(19)	33(2)	45(2)	42(3)	-5(2)	-2(2)	-3(2)
C(20)	56(3)	53(3)	60(3)	-4(2)	6(2)	2(2)
C(21)	69(3)	80(3)	71(6)	-29(3)	10(3)	11(3)
C(22)	54(3)	119(5)	51(4)	-3(3)	15(2)	-17(3)
C(23)	61(3)	87(4)	45(3)	6(3)	8(3)	-20(2)
C(24)	45(2)	57(2)	57(4)	2(2)	-1(2)	-8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 12.

	x	y	z	U(eq)
H(1)	1372(2)	1094(6)	-2436(6)	76
H(2)	876(3)	-420(6)	-734(7)	87
H(3)	1704(4)	-1428(5)	710(7)	104
H(4)	2724(3)	-431(5)	-25(6)	81
H(5)	2494(2)	1173(5)	-1895(6)	72
H(6)	808(3)	5241(6)	2613(8)	101
H(7)	71(2)	3447(6)	1978(7)	88
H(8)	208(3)	2859(6)	-464(7)	91
H(9)	1050(3)	4277(6)	-1441(6)	95
H(10)	1443(3)	5688(5)	512(9)	95
H(11)	2956(15)	2696(33)	262(45)	36(9)
H(13)	2180(3)	4914(5)	2685(6)	82
H(14)	2510(3)	6973(6)	3318(8)	114
H(15)	3335(3)	7964(6)	2196(8)	108
H(16)	3880(3)	6795(5)	584(9)	100
H(17)	3572(2)	4698(4)	-29(5)	71
H(18)	1240(19)	-224(50)	2748(53)	55(14)
H(20)	764(2)	3004(5)	4049(6)	68
H(21)	141(2)	3366(6)	5939(6)	87
H(22)	-197(2)	1618(7)	7263(6)	90
H(23)	73(2)	-497(5)	6671(7)	77
H(24)	696(2)	-875(5)	4784(5)	63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C 13
N 1
C 4
C 26
C 18
C 30
C 3
C 5
C 29
C 31
C 28
C 27
C 25
C 8
C 6
C 21
C 7
C 16
C 22

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Table 1. Crystal data and structure refinement for 4a.

Identification code	726m
Empirical formula	C36 H46 N2 Zr
Formula weight	597.97
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a= 13.789(3) A alpha= 90 deg. b= 15.397(3) A beta= 102.70(3) deg. c= 15.188(3) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	2000
Theta for cell determination	4 to 20 deg
Volume	3145.7(11) A^3
Z	4
Density (calculated)	1.263 Mg/m^3
Absorption coefficient	0.375 mm^-1
F(000)	1264
Crystal colour	yellow-orange
Crystal description	prism
Crystal size	0.4 x 0.4 x 0.4 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	laser scanned imaging plate
Standards (intensity + orient.)	2000
Intensity after	360 sec
Theta range for data collection	1.91 to 24.34 deg.
Index ranges	-15<=h<=15, -17<=k<=17, 0<=l<=17
Reflections collected	9267
Independent reflections	5035 [R(int) = 0.0253]

Reflections unique	5035
Reflections observed	3746
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	5035 / 0 / 352
Final R indices [I>2sigma(I)]	R1 = 0.0359, wR2 = 0.0845
R indices (all data)	R1 = 0.0561, wR2 = 0.0949
Goodness-of-fit on F^2(all)	0.999
Goodness-of-fit on F^2(obs)	1.043
Shift/esd(max)	0.000
Shift/esd(mean)	0.000

Weighting scheme

calc w=1/[\s^2^(Fo^2^)+(0.0546P)^2^+0.3595P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.196 and -0.487 e.A^-3
Diff. density rms	0.055
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 4a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr	1561(1)	1311(1)	2672(1)	38(1)
N(1)	2489(2)	187(1)	2834(2)	36(1)
N(2)	2847(2)	1943(2)	2464(2)	38(1)
C(1)	3297(2)	636(2)	3331(2)	38(1)
C(2)	3464(2)	1481(2)	3152(2)	41(1)
C(3)	2488(2)	-747(2)	2810(2)	37(1)
C(4)	2364(2)	-1256(2)	3549(2)	44(1)
C(5)	2259(2)	-2153(2)	3440(2)	52(1)
C(6)	2278(2)	-2545(2)	2638(3)	58(1)
C(7)	2450(2)	-2058(2)	1934(2)	57(1)
C(8)	2590(2)	-1166(2)	2014(2)	46(1)
C(9)	3278(2)	2626(2)	2043(2)	42(1)
C(10)	2941(2)	3488(2)	2034(2)	47(1)
C(11)	3424(3)	4129(2)	1657(2)	59(1)
C(12)	4229(3)	3945(3)	1302(3)	76(1)
C(13)	4546(3)	3100(3)	1276(3)	70(1)
C(14)	4076(2)	2425(2)	1622(2)	50(1)
C(15)	2403(2)	-890(2)	4480(2)	50(1)
C(16)	2938(3)	-702(2)	1266(2)	63(1)
C(17)	2080(3)	3764(2)	2443(2)	54(1)
C(18)	4397(2)	1503(2)	1493(2)	57(1)
C(19)	3388(3)	-1145(2)	5118(2)	64(1)
C(20)	1522(3)	-1192(2)	4879(3)	73(1)
C(21)	4046(3)	-934(3)	1347(3)	101(2)
C(22)	2324(4)	-908(3)	324(3)	112(2)
C(23)	1251(3)	4224(3)	1765(3)	74(1)
C(24)	2432(3)	4337(3)	3271(3)	85(1)
C(25)	4294(4)	1320(3)	481(3)	113(2)
C(26)	5421(3)	1301(3)	2028(4)	119(2)
C(27)	1207(3)	1035(2)	979(2)	58(1)
C(28)	604(3)	466(2)	1338(2)	70(1)
C(29)	-83(2)	957(3)	1667(3)	73(1)
C(30)	78(2)	1825(3)	1504(2)	63(1)
C(31)	877(2)	1872(2)	1081(2)	53(1)
C(32)	919(3)	1003(3)	4111(2)	64(1)
C(33)	1835(3)	1425(2)	4416(2)	58(1)
C(34)	1730(3)	2277(2)	4102(2)	64(1)
C(35)	757(3)	2388(3)	3619(3)	75(1)
C(36)	257(3)	1610(3)	3633(3)	73(1)

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

Zr-N(2)	2.107(2)
Zr-N(1)	2.134(2)
Zr-C(29)	2.499(3)
Zr-C(28)	2.523(3)
Zr-C(30)	2.522(3)
Zr-C(31)	2.544(3)
Zr-C(27)	2.545(3)
Zr-C(32)	2.578(3)
Zr-C(2)	2.577(3)
Zr-C(36)	2.595(3)
Zr-C(35)	2.597(4)
Zr-C(33)	2.598(3)
N(1)-C(1)	1.386(3)
N(1)-C(3)	1.439(3)
N(2)-C(2)	1.390(3)
N(2)-C(9)	1.425(4)
C(1)-C(2)	1.358(4)
C(3)-C(8)	1.404(4)
C(3)-C(4)	1.409(4)
C(4)-C(5)	1.394(4)
C(4)-C(15)	1.512(4)
C(5)-C(6)	1.364(5)
C(6)-C(7)	1.369(5)
C(7)-C(8)	1.390(4)
C(8)-C(16)	1.508(5)
C(9)-C(10)	1.405(4)
C(9)-C(14)	1.422(4)
C(10)-C(11)	1.384(4)
C(10)-C(17)	1.517(5)
C(11)-C(12)	1.366(5)
C(12)-C(13)	1.375(5)
C(13)-C(14)	1.389(4)
C(14)-C(18)	1.513(4)
C(15)-C(19)	1.536(4)
C(15)-C(20)	1.543(4)
C(16)-C(22)	1.527(5)
C(16)-C(21)	1.547(5)
C(17)-C(24)	1.526(5)
C(17)-C(23)	1.533(5)
C(18)-C(26)	1.498(5)
C(18)-C(25)	1.539(5)
C(27)-C(31)	1.386(5)
C(27)-C(28)	1.399(5)
C(28)-C(29)	1.388(5)
C(29)-C(30)	1.387(5)
C(30)-C(31)	1.395(5)
C(32)-C(36)	1.394(5)
C(32)-C(33)	1.406(5)
C(33)-C(34)	1.393(5)
C(34)-C(35)	1.391(5)
C(35)-C(36)	1.384(5)
N(2)-Zr-N(1)	83.63(8)
N(2)-Zr-C(29)	133.64(11)
N(1)-Zr-C(29)	109.49(12)
N(2)-Zr-C(28)	115.29(12)
N(1)-Zr-C(28)	82.47(11)
C(29)-Zr-C(28)	32.08(12)
N(2)-Zr-C(30)	109.21(11)
N(1)-Zr-C(30)	135.12(11)
C(29)-Zr-C(30)	32.06(12)

N(2)-Zr-C(31)	81.35(10)
N(1)-Zr-C(31)	118.20(10)
C(29)-Zr-C(31)	52.92(12)
C(28)-Zr-C(31)	52.62(12)
C(30)-Zr-C(31)	31.95(11)
N(2)-Zr-C(27)	84.65(11)
N(1)-Zr-C(27)	87.60(10)
C(29)-Zr-C(27)	53.13(13)
C(28)-Zr-C(27)	32.04(11)
C(30)-Zr-C(27)	52.86(12)
C(31)-Zr-C(27)	31.61(11)
N(2)-Zr-C(32)	132.07(11)
N(1)-Zr-C(32)	93.53(10)
C(29)-Zr-C(32)	92.44(14)
C(28)-Zr-C(32)	111.67(14)
C(30)-Zr-C(32)	106.11(12)
C(31)-Zr-C(32)	138.03(11)
C(27)-Zr-C(32)	143.20(13)
N(2)-Zr-C(2)	32.59(8)
N(1)-Zr-C(2)	60.15(9)
C(29)-Zr-C(2)	157.72(13)
C(28)-Zr-C(2)	126.86(12)
C(30)-Zr-C(2)	141.73(11)
C(31)-Zr-C(2)	112.10(10)
C(27)-Zr-C(2)	105.07(11)
C(32)-Zr-C(2)	107.29(11)
N(2)-Zr-C(36)	135.47(13)
N(1)-Zr-C(36)	123.42(11)
C(29)-Zr-C(36)	74.6(2)
C(28)-Zr-C(36)	103.8(2)
C(30)-Zr-C(36)	77.58(13)
C(31)-Zr-C(36)	108.44(11)
C(27)-Zr-C(36)	126.54(13)
C(32)-Zr-C(36)	31.26(11)
C(2)-Zr-C(36)	127.68(12)
N(2)-Zr-C(35)	105.32(12)
N(1)-Zr-C(35)	140.49(11)
C(29)-Zr-C(35)	92.1(2)
C(28)-Zr-C(35)	124.2(2)
C(30)-Zr-C(35)	79.06(13)
C(31)-Zr-C(35)	101.26(12)
C(27)-Zr-C(35)	130.97(12)
C(32)-Zr-C(35)	51.65(12)
C(2)-Zr-C(35)	108.11(12)
C(36)-Zr-C(35)	30.92(12)
N(2)-Zr-C(33)	100.57(11)
N(1)-Zr-C(33)	89.30(10)
C(29)-Zr-C(33)	123.09(13)
C(28)-Zr-C(33)	141.85(13)
C(30)-Zr-C(33)	127.55(12)
C(31)-Zr-C(33)	152.38(11)
C(27)-Zr-C(33)	173.61(12)
C(32)-Zr-C(33)	31.51(11)
C(2)-Zr-C(33)	78.12(11)
C(36)-Zr-C(33)	51.50(12)
C(35)-Zr-C(33)	51.42(11)
C(1)-N(1)-C(3)	120.5(2)
C(1)-N(1)-Zr	92.8(2)
C(3)-N(1)-Zr	144.2(2)
C(2)-N(2)-C(9)	117.9(2)
C(2)-N(2)-Zr	92.7(2)
C(9)-N(2)-Zr	148.8(2)
C(2)-C(1)-N(1)	121.3(3)
C(2)-C(1)-Zr	73.9(2)
N(1)-C(1)-Zr	55.05(13)

C(1)-C(2)-Zr	75.7(2)
N(2)-C(2)-Zr	54.74(13)
C(8)-C(3)-C(4)	118.9(3)
C(8)-C(3)-N(1)	118.7(3)
C(4)-C(3)-N(1)	122.4(3)
C(5)-C(4)-C(3)	118.9(3)
C(5)-C(4)-C(15)	117.5(3)
C(3)-C(4)-C(15)	123.5(3)
C(6)-C(5)-C(4)	121.5(3)
C(5)-C(6)-C(7)	119.7(3)
C(6)-C(7)-C(8)	121.1(3)
C(7)-C(8)-C(3)	119.4(3)
C(7)-C(8)-C(16)	117.6(3)
C(3)-C(8)-C(16)	122.8(3)
C(10)-C(9)-C(14)	119.2(3)
C(10)-C(9)-N(2)	122.1(3)
C(14)-C(9)-N(2)	118.7(3)
C(11)-C(10)-C(9)	119.3(3)
C(11)-C(10)-C(17)	117.4(3)
C(9)-C(10)-C(17)	123.3(3)
C(12)-C(11)-C(10)	121.4(3)
C(11)-C(12)-C(13)	119.9(3)
C(12)-C(13)-C(14)	121.3(3)
C(13)-C(14)-C(9)	118.6(3)
C(13)-C(14)-C(18)	118.6(3)
C(9)-C(14)-C(18)	122.7(3)
C(4)-C(15)-C(19)	109.8(3)
C(4)-C(15)-C(20)	112.7(3)
C(19)-C(15)-C(20)	109.8(3)
C(8)-C(16)-C(22)	113.9(3)
C(8)-C(16)-C(21)	107.6(3)
C(22)-C(16)-C(21)	111.2(4)
C(10)-C(17)-C(24)	111.4(3)
C(10)-C(17)-C(23)	113.0(3)
C(24)-C(17)-C(23)	110.0(3)
C(26)-C(18)-C(14)	113.1(3)
C(26)-C(18)-C(25)	111.9(4)
C(14)-C(18)-C(25)	109.6(3)
C(31)-C(27)-C(28)	107.5(3)
C(31)-C(27)-Zr	74.1(2)
C(28)-C(27)-Zr	73.1(2)
C(29)-C(28)-C(27)	108.1(3)
C(29)-C(28)-Zr	73.0(2)
C(27)-C(28)-Zr	74.9(2)
C(30)-C(29)-C(28)	108.2(3)
C(30)-C(29)-Zr	74.9(2)
C(28)-C(29)-Zr	74.9(2)
C(29)-C(30)-C(31)	107.8(3)
C(29)-C(30)-Zr	73.0(2)
C(31)-C(30)-Zr	74.9(2)
C(27)-C(31)-C(30)	108.4(3)
C(27)-C(31)-Zr	74.3(2)
C(30)-C(31)-Zr	73.2(2)
C(36)-C(32)-C(33)	107.4(4)
C(36)-C(32)-Zr	75.0(2)
C(33)-C(32)-Zr	75.0(2)
C(34)-C(33)-C(32)	107.8(3)
C(34)-C(33)-Zr	74.6(2)
C(32)-C(33)-Zr	73.4(2)
C(35)-C(34)-C(33)	108.1(4)
C(35)-C(34)-Zr	74.3(2)
C(33)-C(34)-Zr	74.4(2)
C(36)-C(35)-C(34)	108.2(3)
C(36)-C(35)-Zr	74.4(2)
C(34)-C(35)-Zr	74.6(2)

C(35)-C(36)-Zr	74.6(2)
C(32)-C(36)-Zr	73.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 4a. 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
Zr	38(1)	41(1)	36(1)	5(1)	13(1)	4(1)
N(1)	38(1)	39(1)	32(1)	0(1)	9(1)	0(1)
N(2)	43(1)	36(1)	36(1)	2(1)	9(1)	1(1)
C(1)	40(2)	40(2)	32(2)	4(1)	5(1)	6(1)
C(2)	36(2)	46(2)	40(2)	-1(1)	5(1)	-2(1)
C(3)	36(2)	35(2)	38(2)	1(1)	6(1)	0(1)
C(4)	47(2)	39(2)	46(2)	5(1)	13(1)	3(1)
C(5)	46(2)	47(2)	63(2)	10(2)	15(2)	-1(2)
C(6)	51(2)	38(2)	80(3)	-5(2)	7(2)	-4(2)
C(7)	66(2)	47(2)	55(2)	-10(2)	4(2)	-1(2)
C(8)	50(2)	41(2)	45(2)	-3(1)	5(1)	2(1)
C(9)	48(2)	43(2)	35(2)	2(1)	7(1)	-9(1)
C(10)	60(2)	39(2)	40(2)	1(1)	5(2)	-4(2)
C(11)	71(2)	45(2)	61(2)	8(2)	13(2)	-5(2)
C(12)	77(3)	60(3)	92(3)	19(2)	20(2)	-23(2)
C(13)	55(2)	76(3)	84(3)	17(2)	30(2)	-7(2)
C(14)	46(2)	55(2)	50(2)	7(2)	12(2)	-7(2)
C(15)	62(2)	45(2)	46(2)	10(2)	22(2)	6(2)
C(16)	101(3)	52(2)	39(2)	-4(2)	22(2)	5(2)
C(17)	70(2)	43(2)	50(2)	2(2)	17(2)	5(2)
C(18)	56(2)	54(2)	66(2)	3(2)	27(2)	2(2)
C(19)	78(2)	61(2)	49(2)	4(2)	7(2)	10(2)
C(20)	92(3)	65(2)	75(3)	16(2)	48(2)	8(2)
C(21)	116(4)	100(4)	111(4)	21(3)	77(3)	22(3)
C(22)	213(6)	75(3)	41(2)	-8(2)	9(3)	12(3)
C(23)	80(3)	72(3)	69(3)	3(2)	19(2)	19(2)
C(24)	124(4)	72(3)	59(3)	-15(2)	18(2)	0(3)
C(25)	181(5)	92(4)	86(3)	2(3)	69(4)	33(3)
C(26)	49(2)	97(4)	199(6)	24(4)	0(3)	13(2)
C(27)	56(2)	75(2)	37(2)	-4(2)	-1(2)	7(2)
C(28)	79(3)	53(2)	60(2)	-1(2)	-23(2)	-9(2)
C(29)	38(2)	93(3)	82(3)	23(2)	-1(2)	-10(2)
C(30)	45(2)	75(3)	65(2)	19(2)	2(2)	18(2)
C(31)	54(2)	63(2)	40(2)	14(2)	3(2)	4(2)
C(32)	82(3)	69(2)	53(2)	19(2)	41(2)	16(2)
C(33)	77(2)	66(2)	38(2)	3(2)	25(2)	17(2)
C(34)	91(3)	61(2)	47(2)	-11(2)	33(2)	3(2)
C(35)	107(3)	68(3)	67(3)	18(2)	53(2)	39(2)
C(36)	62(2)	98(3)	70(3)	25(2)	39(2)	28(2)

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

	x	y	z	U(eq)
H(1)	3735(2)	354(2)	3796(2)	45
H(2)	4012(2)	1760(2)	3503(2)	50
H(5)	2175(2)	-2491(2)	3924(2)	62
H(6)	2175(2)	-3140(2)	2571(3)	69
H(7)	2473(2)	-2330(2)	1392(2)	69
H(11)	3196(3)	4698(2)	1645(2)	71
H(12)	4562(3)	4390(3)	1077(3)	91
H(13)	5086(3)	2979(3)	1021(3)	83
H(15)	2379(2)	-255(2)	4434(2)	59
H(16)	2894(3)	-76(2)	1365(2)	75
H(17)	1794(3)	3237(2)	2643(2)	64
H(18)	3935(2)	1115(2)	1708(2)	68
H(19A)	3408(3)	-911(2)	5707(2)	96
H(19B)	3933(3)	-918(2)	4890(2)	96
H(19C)	3437(3)	-1767(2)	5154(2)	96
H(20A)	1581(3)	-942(2)	5468(3)	110
H(20B)	1529(3)	-1814(2)	4925(3)	110
H(20C)	909(3)	-1007(2)	4493(3)	110
H(21A)	4289(3)	-647(3)	877(3)	152
H(21B)	4112(3)	-1551(3)	1290(3)	152
H(21C)	4425(3)	-749(3)	1924(3)	152
H(22A)	2585(4)	-592(3)	-118(3)	168
H(22B)	1645(4)	-741(3)	286(3)	168
H(22C)	2355(4)	-1519(3)	211(3)	168
H(23A)	727(3)	4384(3)	2058(3)	110
H(23B)	993(3)	3840(3)	1271(3)	110
H(23C)	1513(3)	4736(3)	1541(3)	110
H(24A)	1872(3)	4501(3)	3515(3)	128
H(24B)	2745(3)	4848(3)	3102(3)	128
H(24C)	2899(3)	4021(3)	3719(3)	128
H(25A)	3630(4)	1456(3)	161(3)	170
H(25B)	4428(4)	718(3)	395(3)	170
H(25C)	4759(4)	1672(3)	253(3)	170
H(26A)	5585(3)	710(3)	1919(4)	179
H(26B)	5442(3)	1379(3)	2659(4)	179
H(26C)	5891(3)	1684(3)	1847(4)	179
H(27)	1733(3)	880(2)	719(2)	69
H(28)	654(3)	-137(2)	1353(2)	84
H(29)	-567(2)	740(3)	1949(3)	88
H(30)	-284(2)	2293(3)	1650(2)	76
H(31)	1144(2)	2378(2)	898(2)	64
H(32)	779(3)	425(3)	4211(2)	77
H(33)	2409(3)	1179(2)	4764(2)	70
H(34)	2225(3)	2699(2)	4199(2)	76
H(35)	489(3)	2896(3)	3335(3)	90
H(36)	-408(3)	1510(3)	3368(3)	87

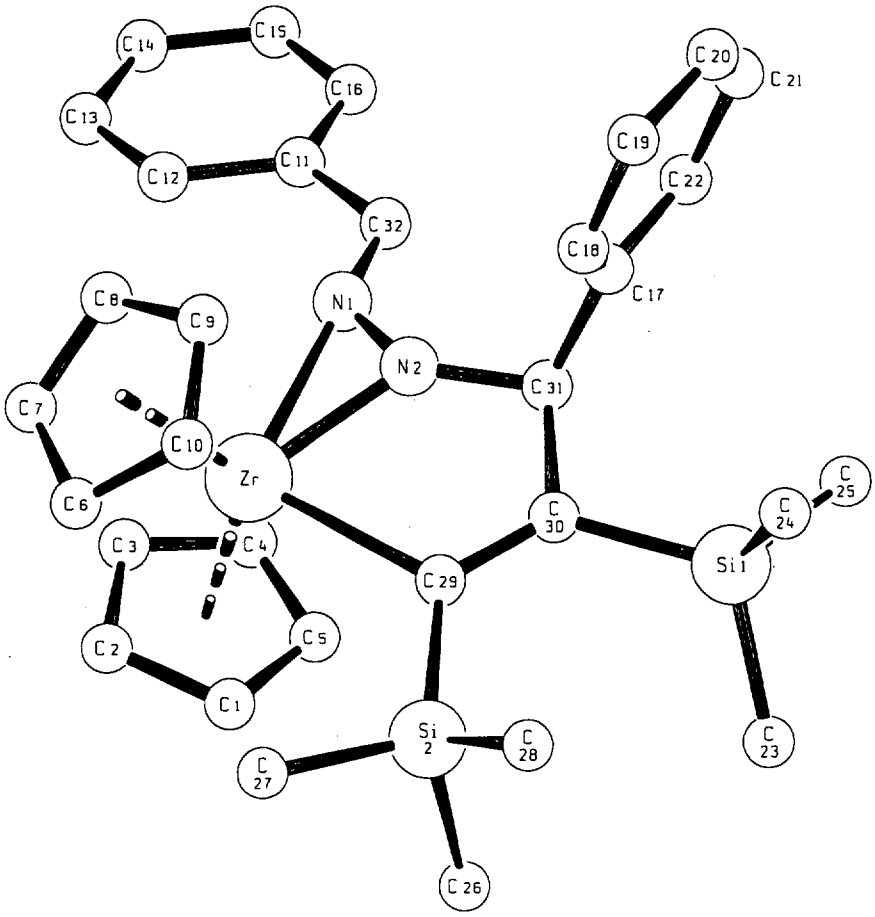

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Table 1. Crystal data and structure refinement for 8.

Identification code	708
Empirical formula	C32 H40 N2 Si2 Zr
Formula weight	600.06
Crystal system	Orthorombic
Space group	P212121
Unit cell dimensions	a= 7.900(2) A alpha= 90 deg. b= 14.012(3) A beta= 90 deg. c= 28.718(6) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	2000
Theta for cell determination	4 to 20 deg
Volume	3178.9(12) A^3
Z	4
Density (calculated)	1.254 Mg/m^3
Absorption coefficient	0.443 mm^-1
F(000)	1256
Crystal colour	yellow
Crystal description	prism
Crystal size	0.4 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	laser scanned imaging plate
Standards (intensity + orient.)	50-200
Intensity after	360 sec
Theta range for data collection	2.03 to 24.36 deg.
Index ranges	-9<=h<=9, -16<=k<=16, 0<=l<=33
Reflections collected	9477
Independent reflections	4859 [R(int) = 0.0376]

Reflections unique	4859
Reflections observed	3501
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	4859 / 0 / 334
Final R indices [I>2sigma(I)]	R1 = 0.0410, wR2 = 0.0979
R indices (all data)	R1 = 0.0698, wR2 = 0.1076
Goodness-of-fit on F^2(all)	0.973
Goodness-of-fit on F^2(obs)	1.056
Shift/esd(max)	0.004
Shift/esd(mean)	0.001
Absolute structure parameter	0.68(6)

Weighting scheme

calc w=1/[\s^2^(Fo^2^)+(0.0582P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.323 and -0.670 e.A^-3
Diff. density rms	0.063
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 8. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr	90(1)	9571(1)	8053(1)	46(1)
Si(1)	2970(2)	10638(1)	9571(1)	73(1)
Si(2)	-324(2)	8866(1)	9315(1)	77(1)
N(1)	1937(5)	10708(3)	7754(2)	42(1)
N(2)	1581(5)	10700(3)	8207(1)	54(1)
C(1)	974(14)	7862(5)	8202(3)	99(3)
C(2)	90(14)	7843(5)	7784(5)	126(3)
C(3)	1100(14)	8347(6)	7475(3)	99(3)
C(4)	2503(10)	8639(5)	7702(4)	87(3)
C(5)	2413(10)	8362(5)	8142(3)	87(2)
C(6)	-3084(7)	9320(7)	8031(4)	105(3)
C(7)	-2609(9)	9611(9)	7587(3)	108(3)
C(8)	-2056(8)	10527(8)	7587(3)	91(3)
C(9)	-2168(8)	10855(6)	8031(4)	89(2)
C(10)	-2778(8)	10144(8)	8308(3)	96(3)
C(11)	3413(6)	11046(3)	7044(2)	43(1)
C(12)	2241(7)	10579(4)	6753(2)	59(2)
C(13)	2540(8)	10519(5)	6281(2)	76(2)
C(14)	3985(9)	10914(5)	6095(2)	79(2)
C(15)	5137(10)	11357(4)	6373(2)	75(2)
C(16)	4840(7)	11426(4)	6840(2)	57(1)
C(17)	2384(8)	12065(4)	8674(2)	56(2)
C(18)	852(9)	12420(5)	8841(2)	80(2)
C(19)	620(13)	13386(6)	8894(3)	111(3)
C(20)	1902(17)	14009(7)	8802(4)	130(4)
C(21)	3394(16)	13672(6)	8642(3)	119(3)
C(22)	3663(9)	12697(5)	8572(2)	77(2)
C(23)	3567(9)	9561(6)	9917(2)	99(2)
C(24)	1726(12)	11490(6)	9938(3)	133(4)
C(25)	5076(11)	11222(5)	9464(2)	102(2)
C(26)	1051(11)	7798(5)	9454(3)	119(3)
C(27)	-2345(9)	8323(5)	9110(3)	106(3)
C(28)	-1023(9)	9452(7)	9867(2)	116(3)
C(29)	689(6)	9697(4)	8887(2)	50(1)
C(30)	1893(6)	10360(4)	8995(2)	50(1)
C(31)	2583(7)	10998(4)	8598(2)	47(1)
C(32)	3183(6)	11117(4)	7544(2)	44(1)

Table 3. Bond lengths [A] and angles [deg] for 8.

Zr-N(2)	2.021(5)
Zr-N(1)	2.324(4)
Zr-C(29)	2.447(5)
Zr-C(10)	2.512(6)
Zr-C(3)	2.517(7)
Zr-C(7)	2.519(6)
Zr-C(4)	2.521(6)
Zr-C(5)	2.511(6)
Zr-C(6)	2.533(6)
Zr-C(9)	2.534(6)
Zr-C(1)	2.532(7)
Zr-C(2)	2.542(6)
Si(1)-C(23)	1.868(7)
Si(1)-C(24)	1.871(7)
Si(1)-C(25)	1.880(9)
Si(1)-C(30)	1.902(5)
Si(2)-C(27)	1.864(7)
Si(2)-C(28)	1.868(7)
Si(2)-C(29)	1.874(5)
Si(2)-C(26)	1.891(7)
N(1)-C(32)	1.289(6)
N(1)-N(2)	1.331(6)
N(2)-C(31)	1.435(6)
C(1)-C(5)	1.346(11)
C(1)-C(2)	1.388(12)
C(2)-C(3)	1.388(12)
C(3)-C(4)	1.350(11)
C(4)-C(5)	1.322(10)
C(6)-C(7)	1.392(10)
C(6)-C(10)	1.422(11)
C(7)-C(8)	1.355(12)
C(8)-C(9)	1.358(11)
C(9)-C(10)	1.363(10)
C(11)-C(16)	1.378(7)
C(11)-C(12)	1.408(7)
C(11)-C(32)	1.452(7)
C(12)-C(13)	1.378(7)
C(13)-C(14)	1.378(9)
C(14)-C(15)	1.361(9)
C(15)-C(16)	1.365(7)
C(17)-C(22)	1.375(8)
C(17)-C(18)	1.393(8)
C(17)-C(31)	1.520(7)
C(18)-C(19)	1.373(10)
C(19)-C(20)	1.364(12)
C(20)-C(21)	1.351(13)
C(21)-C(22)	1.397(11)
C(29)-C(30)	1.366(7)
C(30)-C(31)	1.547(7)
N(2)-Zr-N(1)	34.8(2)
N(2)-Zr-C(29)	67.5(2)
N(1)-Zr-C(29)	101.0(2)
N(2)-Zr-C(10)	102.2(3)
N(1)-Zr-C(10)	117.1(3)
C(29)-Zr-C(10)	82.3(2)
N(2)-Zr-C(3)	119.5(3)
N(1)-Zr-C(3)	91.4(3)
C(29)-Zr-C(3)	129.3(2)
C(10)-Zr-C(3)	134.1(4)
N(2)-Zr-C(7)	126.3(3)

C(29)-Zr-C(7)	133.0(2)
C(10)-Zr-C(7)	52.0(3)
C(3)-Zr-C(7)	86.1(3)
N(2)-Zr-C(4)	93.0(2)
N(1)-Zr-C(4)	74.5(2)
C(29)-Zr-C(4)	106.4(3)
C(10)-Zr-C(4)	164.5(3)
C(3)-Zr-C(4)	31.1(3)
C(7)-Zr-C(4)	116.0(3)
N(2)-Zr-C(5)	94.6(2)
N(1)-Zr-C(5)	92.3(3)
C(29)-Zr-C(5)	78.9(2)
C(10)-Zr-C(5)	147.7(3)
C(3)-Zr-C(5)	51.3(3)
C(7)-Zr-C(5)	133.4(3)
C(4)-Zr-C(5)	30.5(2)
N(2)-Zr-C(6)	133.7(3)
N(1)-Zr-C(6)	135.0(2)
C(29)-Zr-C(6)	103.0(3)
C(10)-Zr-C(6)	32.7(3)
C(3)-Zr-C(6)	101.7(4)
C(7)-Zr-C(6)	32.0(2)
C(4)-Zr-C(6)	131.8(3)
C(5)-Zr-C(6)	129.2(3)
N(2)-Zr-C(9)	82.0(2)
N(1)-Zr-C(9)	86.9(2)
C(29)-Zr-C(9)	96.3(3)
C(10)-Zr-C(9)	31.3(2)
C(3)-Zr-C(9)	133.7(3)
C(7)-Zr-C(9)	51.3(3)
C(4)-Zr-C(9)	152.9(3)
C(5)-Zr-C(9)	175.0(3)
C(6)-Zr-C(9)	53.2(3)
N(2)-Zr-C(1)	122.9(3)
N(1)-Zr-C(1)	122.5(3)
C(29)-Zr-C(1)	81.3(3)
C(10)-Zr-C(1)	120.1(3)
C(3)-Zr-C(1)	51.6(3)
C(7)-Zr-C(1)	110.2(4)
C(4)-Zr-C(1)	50.8(2)
C(5)-Zr-C(1)	31.0(2)
C(6)-Zr-C(1)	98.4(3)
C(9)-Zr-C(1)	150.5(3)
N(2)-Zr-C(2)	144.3(3)
N(1)-Zr-C(2)	122.7(3)
C(29)-Zr-C(2)	111.4(3)
C(10)-Zr-C(2)	113.1(4)
C(3)-Zr-C(2)	31.8(3)
C(7)-Zr-C(2)	81.9(4)
C(4)-Zr-C(2)	52.1(3)
C(5)-Zr-C(2)	52.2(3)
C(6)-Zr-C(2)	81.9(4)
C(9)-Zr-C(2)	132.0(3)
C(1)-Zr-C(2)	31.8(3)
C(23)-Si(1)-C(24)	110.4(4)
C(23)-Si(1)-C(25)	102.5(3)
C(24)-Si(1)-C(25)	106.2(4)
C(23)-Si(1)-C(30)	114.2(3)
C(24)-Si(1)-C(30)	112.7(3)
C(25)-Si(1)-C(30)	110.0(3)
C(27)-Si(2)-C(28)	101.2(4)
C(27)-Si(2)-C(29)	114.2(3)
C(28)-Si(2)-C(29)	114.2(4)
C(27)-Si(2)-C(26)	103.7(4)
C(28)-Si(2)-C(26)	109.8(4)

C(32)-N(1)-N(2)	128.5(4)
C(32)-N(1)-Zr	163.2(4)
N(2)-N(1)-Zr	60.0(3)
N(1)-N(2)-C(31)	130.2(4)
N(1)-N(2)-Zr	85.2(3)
C(31)-N(2)-Zr	136.0(3)
C(5)-C(1)-C(2)	108.9(8)
C(5)-C(1)-Zr	73.7(4)
C(2)-C(1)-Zr	74.5(4)
C(3)-C(2)-C(1)	104.7(8)
C(3)-C(2)-Zr	73.1(4)
C(1)-C(2)-Zr	73.7(4)
C(4)-C(3)-C(2)	108.5(8)
C(4)-C(3)-Zr	74.6(4)
C(2)-C(3)-Zr	75.1(4)
C(5)-C(4)-C(3)	109.1(7)
C(5)-C(4)-Zr	74.3(4)
C(3)-C(4)-Zr	74.3(4)
C(4)-C(5)-C(1)	108.8(8)
C(4)-C(5)-Zr	75.2(4)
C(1)-C(5)-Zr	75.4(4)
C(7)-C(6)-C(10)	103.2(8)
C(7)-C(6)-Zr	73.5(4)
C(10)-C(6)-Zr	72.8(3)
C(8)-C(7)-C(6)	111.3(9)
C(8)-C(7)-Zr	75.4(4)
C(6)-C(7)-Zr	74.5(3)
C(7)-C(8)-C(9)	107.5(8)
C(7)-C(8)-Zr	73.6(4)
C(9)-C(8)-Zr	74.2(4)
C(8)-C(9)-C(10)	108.8(9)
C(8)-C(9)-Zr	74.8(4)
C(10)-C(9)-Zr	73.4(4)
C(9)-C(10)-C(6)	109.2(7)
C(9)-C(10)-Zr	75.2(3)
C(6)-C(10)-Zr	74.4(4)
C(16)-C(11)-C(12)	117.8(5)
C(16)-C(11)-C(32)	119.8(5)
C(12)-C(11)-C(32)	122.4(4)
C(13)-C(12)-C(11)	119.9(5)
C(14)-C(13)-C(12)	120.0(6)
C(15)-C(14)-C(13)	120.6(6)
C(14)-C(15)-C(16)	119.6(6)
C(15)-C(16)-C(11)	122.1(6)
C(22)-C(17)-C(18)	118.8(6)
C(22)-C(17)-C(31)	121.8(6)
C(18)-C(17)-C(31)	119.4(6)
C(19)-C(18)-C(17)	120.3(8)
C(20)-C(19)-C(18)	120.7(9)
C(21)-C(20)-C(19)	119.3(9)
C(20)-C(21)-C(22)	121.6(10)
C(17)-C(22)-C(21)	119.2(8)
C(30)-C(29)-Si(2)	124.9(4)
C(30)-C(29)-Zr	113.9(4)
Si(2)-C(29)-Zr	121.0(3)
C(29)-C(30)-C(31)	118.2(4)
C(29)-C(30)-Si(1)	130.4(4)
C(31)-C(30)-Si(1)	111.4(4)
N(2)-C(31)-C(17)	110.0(4)
N(2)-C(31)-C(30)	102.3(4)
C(17)-C(31)-C(30)	115.2(5)
N(1)-C(32)-C(11)	121.9(5)

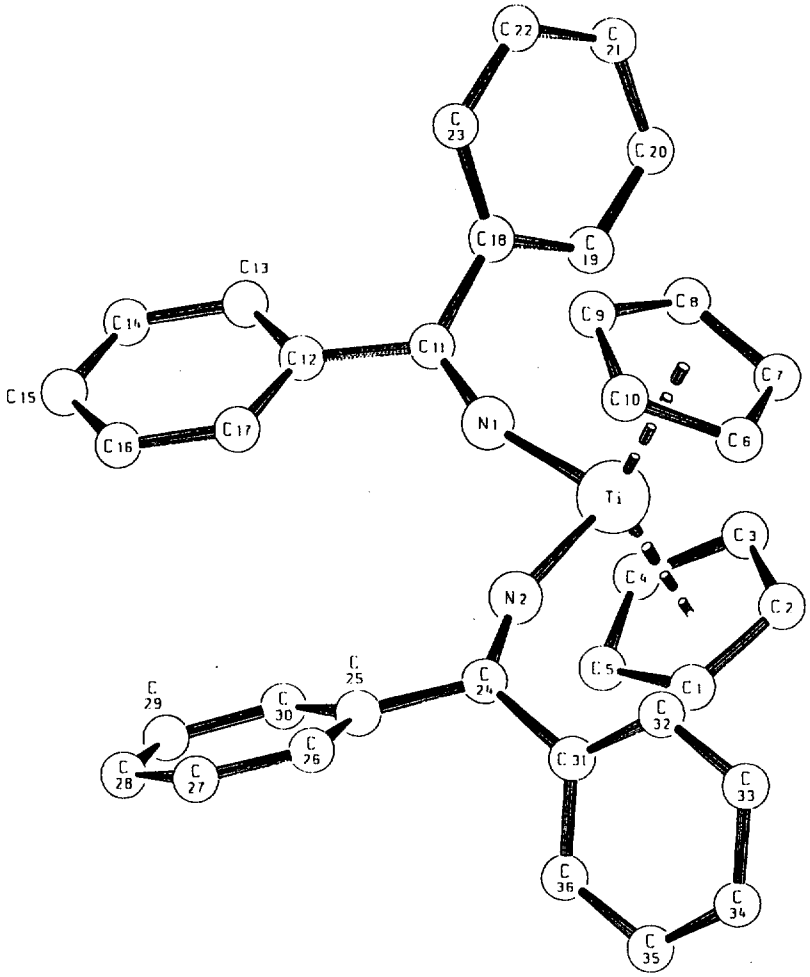
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 8. 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
Zr	41(1)	50(1)	46(1)	1(1)	-1(1)	-2(1)
Si(1)	90(1)	89(2)	40(1)	-11(1)	-13(1)	27(1)
Si(2)	77(1)	91(1)	62(1)	30(1)	12(1)	6(1)
N(1)	50(2)	39(3)	38(3)	-1(2)	-1(2)	-11(2)
N(2)	60(3)	70(4)	31(3)	2(2)	2(2)	-17(2)
C(1)	139(8)	48(5)	112(7)	20(5)	42(6)	24(5)
C(2)	108(6)	53(5)	216(11)	-52(6)	-17(10)	-19(6)
C(3)	165(9)	74(6)	59(5)	-24(4)	-11(5)	26(6)
C(4)	87(5)	49(4)	126(8)	-13(5)	52(5)	2(4)
C(5)	86(5)	68(5)	105(7)	-21(5)	-13(5)	30(4)
C(6)	46(3)	150(8)	119(7)	33(7)	-13(4)	-39(4)
C(7)	62(4)	190(10)	71(6)	-7(7)	-32(4)	13(6)
C(8)	52(4)	121(7)	99(7)	48(7)	-9(4)	19(5)
C(9)	68(4)	103(6)	96(7)	9(6)	-1(5)	40(4)
C(10)	38(3)	172(9)	78(5)	21(6)	9(3)	42(5)
C(11)	46(3)	44(3)	39(3)	5(2)	0(2)	6(2)
C(12)	65(3)	69(4)	43(3)	-1(3)	1(3)	-23(3)
C(13)	94(5)	82(5)	52(4)	-9(4)	-6(3)	-27(4)
C(14)	109(5)	87(5)	42(4)	-4(4)	20(4)	-8(4)
C(15)	80(4)	90(4)	55(4)	8(3)	24(4)	-15(5)
C(16)	60(3)	63(3)	49(3)	10(2)	-1(3)	-5(3)
C(17)	75(4)	44(3)	49(3)	-4(3)	-15(3)	-4(3)
C(18)	103(5)	61(4)	75(5)	-6(4)	2(4)	28(4)
C(19)	152(9)	75(6)	106(7)	-11(5)	13(6)	27(6)
C(20)	193(12)	62(6)	134(9)	-18(6)	-7(8)	-6(8)
C(21)	184(10)	68(6)	104(7)	8(5)	-33(7)	-27(6)
C(22)	95(5)	64(5)	72(5)	-6(4)	-11(4)	-18(4)
C(23)	94(5)	144(7)	60(4)	30(5)	-9(3)	24(5)
C(24)	176(9)	154(8)	69(5)	-48(6)	-18(5)	75(7)
C(25)	125(6)	103(5)	77(5)	-9(4)	-51(5)	-11(7)
C(26)	145(7)	90(6)	122(7)	57(6)	13(6)	9(5)
C(27)	116(6)	108(7)	93(6)	18(5)	20(5)	-41(5)
C(28)	98(5)	199(9)	50(4)	26(6)	18(4)	28(6)
C(29)	55(3)	56(4)	38(3)	6(3)	2(2)	11(3)
C(30)	58(3)	49(3)	42(3)	1(3)	0(2)	13(3)
C(31)	53(3)	55(4)	33(3)	-6(3)	-5(2)	-1(3)
C(32)	47(3)	44(3)	40(3)	-3(3)	-6(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 8.

	x	y	z	U(eq)
H(1)	630(14)	7575(5)	8478(3)	119
H(2)	-950(14)	7556(5)	7725(5)	151
H(3)	852(14)	8464(6)	7164(3)	119
H(4)	3392(10)	8981(5)	7571(4)	105
H(5)	3211(10)	8491(5)	8371(3)	104
H(6)	-3500(7)	8729(7)	8125(4)	126
H(7)	-2664(9)	9227(9)	7323(3)	129
H(8)	-1671(8)	10868(8)	7330(3)	109
H(9)	-1876(8)	11465(6)	8130(4)	107
H(10)	-2965(8)	10190(8)	8627(3)	115
H(12)	1267(7)	10311(4)	6879(2)	71
H(13)	1765(8)	10212(5)	6089(2)	91
H(14)	4175(9)	10878(5)	5775(2)	95
H(15)	6121(10)	11612(4)	6245(2)	90
H(16)	5627(7)	11739(4)	7026(2)	69
H(18)	-18(9)	12001(5)	8917(2)	96
H(19)	-424(13)	13616(6)	8993(3)	133
H(20)	1751(17)	14660(7)	8850(4)	156
H(21)	4264(16)	14099(6)	8577(3)	142
H(22)	4694(9)	12478(5)	8459(2)	92
H(23A)	4210(9)	9132(6)	9725(2)	149
H(23B)	2561(9)	9245(6)	10024(2)	149
H(23C)	4238(9)	9751(6)	10180(2)	149
H(24A)	1424(12)	12038(6)	9756(3)	200
H(24B)	2398(12)	11687(6)	10199(3)	200
H(24C)	717(12)	11181(6)	10048(3)	200
H(25A)	4914(11)	11794(5)	9285(2)	152
H(25B)	5796(11)	10792(5)	9295(2)	152
H(25C)	5593(11)	11380(5)	9756(2)	152
H(26A)	2133(11)	8013(5)	9565(3)	179
H(26B)	1203(11)	7421(5)	9179(3)	179
H(26C)	515(11)	7419(5)	9691(3)	179
H(27A)	-2150(9)	7989(5)	8823(3)	159
H(27B)	-3168(9)	8817(5)	9060(3)	159
H(27C)	-2757(9)	7884(5)	9340(3)	159
H(28A)	-78(9)	9770(7)	10008(2)	173
H(28B)	-1455(9)	8978(7)	10077(2)	173
H(28C)	-1894(9)	9909(7)	9799(2)	173
H(31)	3776(7)	10846(4)	8541(2)	56
H(32)	3957(6)	11468(4)	7718(2)	52


C 22
C 21
C 23
C 20
C 18
C 19
C 13
C 14
C 9
C 8
C 12
C 11
C 7
C 15
C 10
N 1
C 16
C 17
C 6
Ti
C 3
C 4
N 2
C 2
C 5
C 1
C 25
C 24
C 29
C 30
C 32
C 26
C 31
C 28
C 27
C 33
C 36
C 34
C 35

SCHAKAL

Table 1. Crystal data and structure refinement for 10.

Identification code	728
Empirical formula	C36 H30 N2 Ti
Formula weight	538.52
Crystal system	P2(1)2(1)2(1)
Space group	Orthorhombic
Unit cell dimensions	a= 13.698(3) A alpha= 90 deg. b= 13.784(3) A beta= 90 deg. c= 15.102(3) A gamma= 90 deg.
Temperature for cell	293(2)
Number of reflecions for cell	2000
Theta for cell determination	4 to 20 deg
Volume	2851.5(10) A^3
Z	4
Density (calculated)	1.254 Mg/m^3
Absorption coefficient	0.327 mm^-1
F(000)	1128
Crystal colour	dark red
Crystal description	prism
Crystal size	0.2 x 0.2 x 0.2 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	laser scanned imaging plate
Standards (intensity + orient.)	50-200
Intensity after	360 sec
Theta range for data collection	2.00 to 24.31 deg.
Index ranges	-15<=h<=15, -15<=k<=15, 0<=l<=17
Reflections collected	8593
Independent reflections	4593 [R(int) = 0.0345]

Reflections unique	4593
Reflections observed	3038
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	4593 / 0 / 352
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0677
R indices (all data)	R1 = 0.0715, wR2 = 0.0746
Goodness-of-fit on F^2(all)	0.893
Goodness-of-fit on F^2(obs)	1.017
Shift/esd(max)	0.001
Shift/esd(mean)	0.000
Absolute structure parameter	0.53(3)

Weighting scheme

calc w=1/[\s^2^(Fo^2^)+(0.0326P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.125 and -0.213 e.A^-3
Diff. density rms	0.034
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 10. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	10(1)	7694(1)	9730(1)	48(1)
N(1)	-692(2)	8283(2)	8748(2)	61(1)
N(2)	-708(2)	6471(2)	9814(2)	62(1)
C(1)	1288(2)	6557(3)	9552(3)	75(1)
C(2)	1704(2)	7402(4)	9896(3)	87(1)
C(3)	1607(2)	8138(3)	9260(3)	84(1)
C(4)	1170(2)	7741(3)	8528(2)	74(1)
C(5)	960(2)	6782(3)	8698(2)	68(1)
C(6)	40(3)	7888(2)	11293(2)	71(1)
C(7)	463(3)	8717(3)	10942(2)	69(1)
C(8)	-232(3)	9217(2)	10460(2)	71(1)
C(9)	-1111(2)	8703(3)	10526(2)	68(1)
C(10)	-950(3)	7898(3)	11043(2)	69(1)
C(11)	-1081(2)	8918(2)	8256(2)	56(1)
C(12)	-1829(2)	8637(2)	7573(2)	53(1)
C(13)	-2021(3)	9202(3)	6845(3)	87(1)
C(14)	-2668(3)	8905(3)	6199(3)	104(2)
C(15)	-3145(3)	8056(3)	6289(3)	95(1)
C(16)	-2985(3)	7481(3)	7014(3)	82(1)
C(17)	-2319(2)	7773(2)	7646(2)	68(1)
C(18)	-834(3)	9970(2)	8359(2)	61(1)
C(19)	121(3)	10288(2)	8326(2)	78(1)
C(20)	357(3)	11248(3)	8475(3)	97(1)
C(21)	-371(5)	11889(3)	8680(3)	110(2)
C(22)	-1311(4)	11592(3)	8716(3)	104(2)
C(23)	-1547(3)	10634(2)	8547(2)	78(1)
C(24)	-899(2)	5589(2)	9961(2)	59(1)
C(25)	-1684(2)	5070(2)	9462(2)	57(1)
C(26)	-2280(3)	4390(2)	9851(3)	80(1)
C(27)	-2997(3)	3925(3)	9386(3)	97(1)
C(28)	-3118(3)	4105(3)	8510(4)	94(1)
C(29)	-2547(3)	4774(3)	8098(3)	83(1)
C(30)	-1835(3)	5263(2)	8578(2)	71(1)
C(31)	-326(2)	4981(2)	10616(2)	62(1)
C(32)	-137(3)	5285(2)	11446(2)	91(1)
C(33)	439(4)	4749(4)	12016(3)	119(2)
C(34)	818(4)	3896(4)	11737(4)	123(2)
C(35)	641(4)	3596(3)	10922(5)	143(2)
C(36)	47(3)	4113(2)	10357(3)	117(1)

Table 3. Bond lengths [A] and angles [deg] for 10.

Ti-N(1)	1.944(3)
Ti-N(2)	1.956(2)
Ti-C(1)	2.366(3)
Ti-C(2)	2.369(3)
Ti-C(6)	2.376(3)
Ti-C(3)	2.381(3)
Ti-C(5)	2.389(3)
Ti-C(7)	2.394(3)
Ti-C(8)	2.394(3)
Ti-C(9)	2.396(3)
Ti-C(10)	2.396(3)
Ti-C(4)	2.413(3)
N(1)-C(11)	1.265(3)
N(2)-C(24)	1.263(3)
C(1)-C(2)	1.396(5)
C(1)-C(5)	1.401(5)
C(2)-C(3)	1.403(5)
C(3)-C(4)	1.372(4)
C(4)-C(5)	1.377(4)
C(6)-C(7)	1.387(4)
C(6)-C(10)	1.407(5)
C(7)-C(8)	1.382(4)
C(8)-C(9)	1.401(4)
C(9)-C(10)	1.376(4)
C(11)-C(18)	1.497(4)
C(11)-C(12)	1.505(4)
C(12)-C(17)	1.372(4)
C(12)-C(13)	1.372(4)
C(13)-C(14)	1.380(5)
C(14)-C(15)	1.347(5)
C(15)-C(16)	1.370(5)
C(16)-C(17)	1.380(5)
C(18)-C(23)	1.367(4)
C(18)-C(19)	1.381(5)
C(19)-C(20)	1.380(4)
C(20)-C(21)	1.367(6)
C(21)-C(22)	1.353(6)
C(22)-C(23)	1.384(5)
C(24)-C(25)	1.495(4)
C(24)-C(31)	1.516(4)
C(25)-C(26)	1.375(4)
C(25)-C(30)	1.378(4)
C(26)-C(27)	1.366(5)
C(27)-C(28)	1.356(5)
C(28)-C(29)	1.361(5)
C(29)-C(30)	1.390(5)
C(31)-C(32)	1.346(4)
C(31)-C(36)	1.358(4)
C(32)-C(33)	1.382(5)
C(33)-C(34)	1.354(6)
C(34)-C(35)	1.322(6)
C(35)-C(36)	1.378(6)
N(1)-Ti-N(2)	99.27(11)
N(1)-Ti-C(1)	123.81(12)
N(2)-Ti-C(1)	78.95(12)
N(1)-Ti-C(2)	129.51(13)
N(2)-Ti-C(2)	109.80(14)
C(1)-Ti-C(2)	34.29(12)
N(1)-Ti-C(6)	135.97(12)
N(2)-Ti-C(6)	92.36(12)

C(2)-Ti-C(6)	84.08(14)
N(1)-Ti-C(3)	96.90(14)
N(2)-Ti-C(3)	134.66(12)
C(1)-Ti-C(3)	57.03(13)
C(2)-Ti-C(3)	34.37(12)
C(6)-Ti-C(3)	104.5(2)
N(1)-Ti-C(5)	89.55(12)
N(2)-Ti-C(5)	82.10(11)
C(1)-Ti-C(5)	34.27(11)
C(2)-Ti-C(5)	56.31(12)
C(6)-Ti-C(5)	134.25(13)
C(3)-Ti-C(5)	55.92(12)
N(1)-Ti-C(7)	117.75(12)
N(2)-Ti-C(7)	126.07(13)
C(1)-Ti-C(7)	106.54(14)
C(2)-Ti-C(7)	76.39(13)
C(6)-Ti-C(7)	33.81(10)
C(3)-Ti-C(7)	80.66(13)
C(5)-Ti-C(7)	131.88(12)
N(1)-Ti-C(8)	85.25(12)
N(2)-Ti-C(8)	131.03(11)
C(1)-Ti-C(8)	137.32(14)
C(2)-Ti-C(8)	103.63(13)
C(6)-Ti-C(8)	56.35(11)
C(3)-Ti-C(8)	92.23(12)
C(5)-Ti-C(8)	146.87(12)
C(7)-Ti-C(8)	33.56(10)
N(1)-Ti-C(9)	79.81(12)
N(2)-Ti-C(9)	98.40(12)
C(1)-Ti-C(9)	156.38(14)
C(2)-Ti-C(9)	132.35(12)
C(6)-Ti-C(9)	56.44(12)
C(3)-Ti-C(9)	126.12(12)
C(5)-Ti-C(9)	169.30(12)
C(7)-Ti-C(9)	55.96(12)
C(8)-Ti-C(9)	34.01(10)
N(1)-Ti-C(10)	108.11(12)
N(2)-Ti-C(10)	76.80(11)
C(1)-Ti-C(10)	125.28(14)
C(2)-Ti-C(10)	118.02(13)
C(6)-Ti-C(10)	34.30(11)
C(3)-Ti-C(10)	136.13(13)
C(5)-Ti-C(10)	154.27(13)
C(7)-Ti-C(10)	55.95(11)
C(8)-Ti-C(10)	55.94(11)
C(9)-Ti-C(10)	33.37(10)
N(1)-Ti-C(4)	74.99(11)
N(2)-Ti-C(4)	113.75(12)
C(1)-Ti-C(4)	56.29(12)
C(2)-Ti-C(4)	55.88(13)
C(6)-Ti-C(4)	137.12(14)
C(3)-Ti-C(4)	33.25(11)
C(5)-Ti-C(4)	33.31(10)
C(7)-Ti-C(4)	112.87(13)
C(8)-Ti-C(4)	114.47(13)
C(9)-Ti-C(4)	141.63(13)
C(10)-Ti-C(4)	168.74(13)
C(11)-N(1)-Ti	160.8(2)
C(24)-N(2)-Ti	161.0(2)
C(2)-C(1)-C(5)	106.8(3)
C(2)-C(1)-Ti	73.0(2)
C(5)-C(1)-Ti	73.8(2)
C(1)-C(2)-C(3)	108.1(3)
C(1)-C(2)-Ti	72.7(2)
C(3)-C(2)-Ti	73.3(2)

C(4)-C(3)-Ti	74.7(2)
C(2)-C(3)-Ti	72.3(2)
C(3)-C(4)-C(5)	108.9(4)
C(3)-C(4)-Ti	72.1(2)
C(5)-C(4)-Ti	72.4(2)
C(4)-C(5)-C(1)	108.5(3)
C(4)-C(5)-Ti	74.3(2)
C(1)-C(5)-Ti	72.0(2)
C(7)-C(6)-C(10)	107.0(3)
C(7)-C(6)-Ti	73.8(2)
C(10)-C(6)-Ti	73.6(2)
C(8)-C(7)-C(6)	108.9(3)
C(8)-C(7)-Ti	73.2(2)
C(6)-C(7)-Ti	72.4(2)
C(7)-C(8)-C(9)	107.7(3)
C(7)-C(8)-Ti	73.2(2)
C(9)-C(8)-Ti	73.1(2)
C(10)-C(9)-C(8)	108.0(3)
C(10)-C(9)-Ti	73.3(2)
C(8)-C(9)-Ti	72.9(2)
C(9)-C(10)-C(6)	108.4(3)
C(9)-C(10)-Ti	73.3(2)
C(6)-C(10)-Ti	72.1(2)
N(1)-C(11)-C(18)	121.0(3)
N(1)-C(11)-C(12)	120.7(3)
C(18)-C(11)-C(12)	118.3(3)
C(17)-C(12)-C(13)	117.6(3)
C(17)-C(12)-C(11)	120.1(3)
C(13)-C(12)-C(11)	122.3(3)
C(12)-C(13)-C(14)	121.4(3)
C(15)-C(14)-C(13)	119.9(4)
C(14)-C(15)-C(16)	120.3(4)
C(15)-C(16)-C(17)	119.4(3)
C(12)-C(17)-C(16)	121.4(3)
C(23)-C(18)-C(19)	118.2(3)
C(23)-C(18)-C(11)	120.5(3)
C(19)-C(18)-C(11)	121.1(3)
C(20)-C(19)-C(18)	121.3(4)
C(21)-C(20)-C(19)	119.1(4)
C(22)-C(21)-C(20)	120.5(4)
C(21)-C(22)-C(23)	120.2(4)
C(18)-C(23)-C(22)	120.7(4)
N(2)-C(24)-C(25)	121.4(3)
N(2)-C(24)-C(31)	122.6(3)
C(25)-C(24)-C(31)	115.9(2)
C(26)-C(25)-C(30)	117.2(3)
C(26)-C(25)-C(24)	122.6(3)
C(30)-C(25)-C(24)	120.3(3)
C(27)-C(26)-C(25)	121.8(4)
C(28)-C(27)-C(26)	120.2(4)
C(27)-C(28)-C(29)	120.0(4)
C(28)-C(29)-C(30)	119.6(4)
C(25)-C(30)-C(29)	121.1(3)
C(32)-C(31)-C(36)	118.1(3)
C(32)-C(31)-C(24)	122.3(3)
C(36)-C(31)-C(24)	119.5(3)
C(31)-C(32)-C(33)	121.6(4)
C(34)-C(33)-C(32)	119.3(5)
C(35)-C(34)-C(33)	119.5(5)
C(34)-C(35)-C(36)	121.5(5)
C(31)-C(36)-C(35)	120.0(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 10. 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
Ti	41(1)	49(1)	55(1)	-10(1)	-6(1)	0(1)
N(1)	55(2)	64(2)	63(2)	4(2)	5(1)	13(1)
N(2)	64(2)	48(1)	74(2)	-9(1)	9(2)	5(1)
C(1)	58(2)	76(2)	90(3)	4(2)	7(2)	25(2)
C(2)	44(2)	137(3)	79(3)	-37(3)	-15(2)	23(2)
C(3)	47(2)	92(3)	114(3)	-29(3)	16(2)	-14(2)
C(4)	61(2)	82(3)	79(3)	-10(2)	14(2)	4(2)
C(5)	58(2)	67(2)	78(3)	-21(2)	3(2)	6(2)
C(6)	72(2)	85(2)	56(2)	-17(2)	-9(2)	4(3)
C(7)	52(2)	85(3)	69(2)	-35(2)	-7(2)	-10(2)
C(8)	77(3)	57(2)	79(3)	-26(2)	3(2)	-4(2)
C(9)	50(2)	75(2)	81(3)	-32(2)	-4(2)	10(2)
C(10)	55(2)	85(3)	67(2)	-26(2)	10(2)	-13(2)
C(11)	53(2)	60(2)	55(2)	3(2)	7(2)	5(2)
C(12)	53(2)	50(2)	58(2)	5(2)	2(2)	4(2)
C(13)	110(3)	62(2)	89(3)	12(2)	-31(3)	-17(2)
C(14)	143(4)	76(3)	91(3)	10(3)	-52(3)	-2(3)
C(15)	92(3)	93(3)	99(3)	-21(3)	-26(3)	11(3)
C(16)	75(3)	78(3)	93(3)	-18(2)	13(2)	-16(2)
C(17)	74(2)	63(2)	66(2)	1(2)	16(2)	0(2)
C(18)	72(2)	56(2)	55(2)	7(2)	-1(2)	2(2)
C(19)	81(3)	66(2)	85(2)	14(2)	1(2)	-14(2)
C(20)	121(4)	89(3)	82(3)	19(3)	-16(3)	-38(3)
C(21)	186(6)	67(3)	76(3)	-11(2)	-19(3)	-32(3)
C(22)	150(5)	74(3)	89(3)	-17(2)	0(3)	16(3)
C(23)	89(3)	64(2)	81(3)	-3(2)	0(2)	5(2)
C(24)	64(2)	49(2)	63(2)	-4(2)	10(2)	2(2)
C(25)	63(2)	40(2)	66(2)	0(2)	3(2)	5(2)
C(26)	105(3)	52(2)	82(3)	2(2)	-7(2)	-13(2)
C(27)	106(3)	63(2)	121(4)	-2(3)	-5(3)	-21(2)
C(28)	89(3)	70(3)	123(4)	-22(3)	-21(3)	1(2)
C(29)	86(3)	92(3)	72(3)	-9(2)	-12(2)	17(3)
C(30)	71(3)	70(2)	72(3)	0(2)	8(2)	7(2)
C(31)	63(2)	56(2)	68(2)	5(2)	2(2)	2(2)
C(32)	117(4)	90(2)	66(2)	21(2)	4(3)	2(3)
C(33)	130(4)	149(4)	78(3)	41(3)	0(3)	-15(3)
C(34)	88(4)	152(5)	129(5)	71(4)	-1(4)	7(4)
C(35)	160(5)	106(4)	164(6)	23(4)	-21(4)	66(3)
C(36)	151(4)	84(2)	116(3)	-5(2)	-31(4)	49(3)

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

	x	y	z	U(eq)
H(1)	1239(2)	5960(3)	9836(3)	90
H(2)	1994(2)	7465(4)	10450(3)	105
H(3)	1805(2)	8780(3)	9324(3)	101
H(4)	1036(2)	8066(3)	8002(2)	89
H(5)	653(2)	6355(3)	8311(2)	81
H(6)	351(3)	7415(2)	11630(2)	85
H(7)	1110(3)	8906(3)	11019(2)	82
H(8)	-133(3)	9790(2)	10149(2)	85
H(9)	-1701(2)	8877(3)	10265(2)	82
H(10)	-1416(3)	7438(3)	11200(2)	82
H(13)	-1708(3)	9797(3)	6785(3)	105
H(14)	-2774(3)	9290(3)	5703(3)	124
H(15)	-3585(3)	7859(3)	5856(3)	114
H(16)	-3321(3)	6899(3)	7080(3)	98
H(17)	-2200(2)	7376(2)	8132(2)	81
H(19)	616(3)	9847(2)	8200(2)	93
H(20)	1001(3)	11456(3)	8436(3)	117
H(21)	-218(5)	12534(3)	8795(3)	131
H(22)	-1801(4)	12034(3)	8854(3)	125
H(23)	-2196(3)	10439(2)	8562(2)	94
H(26)	-2193(3)	4242(2)	10447(3)	96
H(27)	-3403(3)	3484(3)	9672(3)	116
H(28)	-3592(3)	3770(3)	8192(4)	113
H(29)	-2633(3)	4903(3)	7498(3)	100
H(30)	-1454(3)	5729(2)	8297(2)	85
H(32)	-400(3)	5870(2)	11640(2)	109
H(33)	565(4)	4973(4)	12586(3)	143
H(34)	1201(4)	3523(4)	12116(4)	147
H(35)	924(4)	3021(3)	10724(5)	172
H(36)	-99(3)	3869(2)	9798(3)	140