ORGANOMETALLICS
Organometallics, 1998, 17(18), 3900-3907, DOI:10.1021/om971050o

dl-12b

Table 1. Crystal data and structure refinement for 1.

Identification code	rh02a
Empirical formula	C26 H28 Cl2 Zr
Formula weight	502.60
Temperature	153(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 21.671(9) A alpha = 90 deg. b = 17.383(9) A beta = 98.46(3) deg. c = 12.063(6) A gamma = 90 deg.
Volume, Z	4495(4) A^3, 8
Density (calculated)	1.485 Mg/m^3
Absorption coefficient	0.737 mm^-1
F(000)	2064
Crystal size	0.06 x 0.14 x 0.52 mm
Theta range for data collection	1.51 to 23.00 deg.
Limiting indices	0<=h<=23, 0<=k<=19, -13<=l<=13
Reflections collected	3213
Independent reflections	3089 [R(int) = 0.0820]
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3080 / 305 / 262
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0754, wR2 = 0.1730
R indices (all data)	R1 = 0.1334, wR2 = 0.2276
Largest diff. peak and hole	1.699 and -1.914 e.A^-3

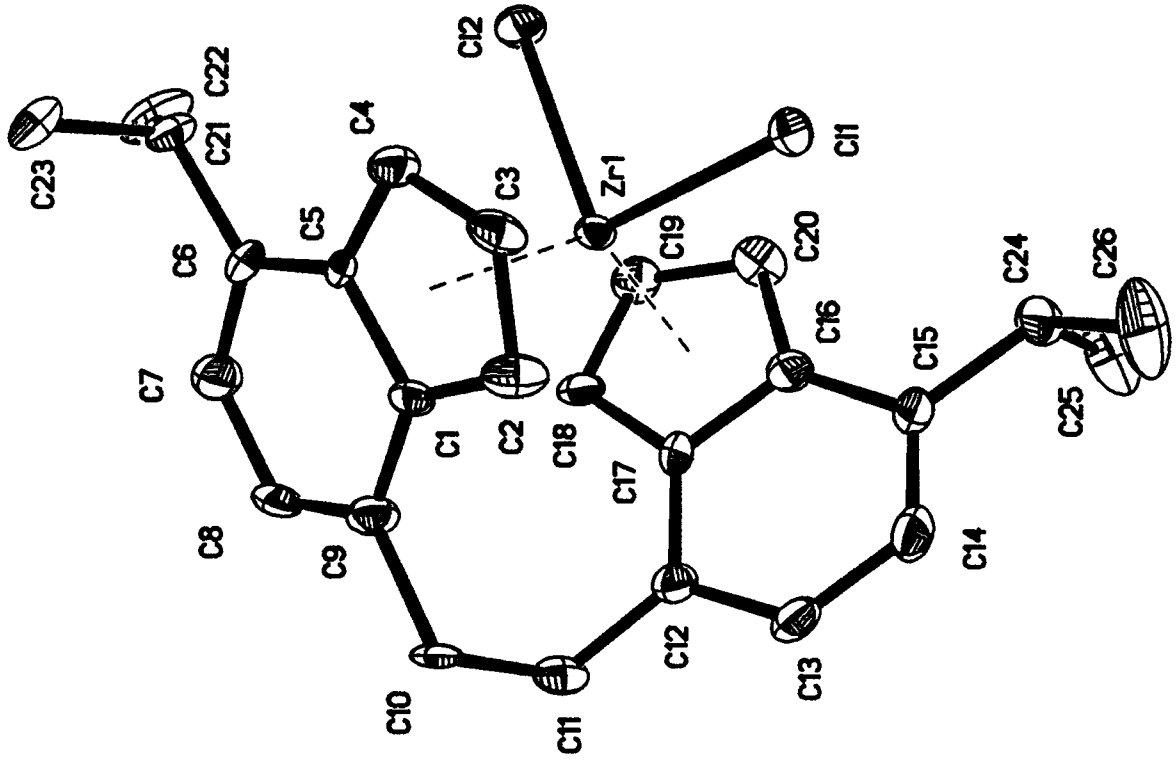

C12
C22
C21
C4
C23
C3
Zr1
Cl1
C5
C19
C20
C24
C26
C6
C16
C15
C7
C1
C2
C18
C17
C25
C8
C9
C14
C12
C13
C10
C11

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	7074(1)	3420(1)	7686(1)	16(1)
Cl(1)	6511(1)	2225(2)	7873(2)	25(1)
Cl(2)	8116(1)	2849(2)	7872(2)	27(1)
C(1)	6931(4)	4670(5)	8731(8)	17(2)
C(2)	6482(4)	4113(6)	8967(9)	24(2)
C(3)	6806(4)	3527(6)	9630(8)	22(2)
C(4)	7450(4)	3668(5)	9720(8)	23(2)
C(5)	7538(4)	4380(5)	9189(8)	17(2)
C(6)	8087(4)	4805(6)	9024(9)	23(2)
C(7)	7995(5)	5510(6)	8516(10)	27(2)
C(8)	7390(5)	5807(6)	8138(10)	26(2)
C(9)	6861(4)	5402(6)	8242(9)	23(2)
C(10)	6222(5)	5751(6)	7837(9)	23(2)
C(11)	5997(5)	5552(6)	6610(9)	21(2)
C(12)	5917(4)	4728(6)	6328(9)	21(2)
C(13)	5337(5)	4382(6)	6167(9)	24(2)
C(14)	5234(5)	3600(7)	5880(9)	30(3)
C(15)	5697(5)	3121(6)	5669(9)	24(2)
C(16)	6319(4)	3442(6)	5801(8)	21(2)
C(17)	6426(4)	4225(5)	6128(9)	21(2)
C(18)	7082(4)	4374(6)	6159(9)	23(2)
C(19)	7353(4)	3712(6)	5799(9)	25(2)
C(20)	6908(4)	3124(6)	5614(9)	24(2)
C(21)	8728(4)	4511(7)	9534(9)	24(2)
C(22)	9219(5)	4670(9)	8782(11)	43(3)
C(23)	8896(5)	4826(7)	10683(10)	35(3)
C(24)	5598(5)	2291(6)	5261(10)	28(2)
C(25)	5498(7)	2266(8)	3992(12)	48(3)
C(26)	5058(7)	1904(9)	5724(13)	56(4)

Table 3. Bond lengths [A] and angles [deg] for 1.

Zr(1)-Cl(1)	2.436(3)
Zr(1)-Cl(2)	2.446(3)
Zr(1)-C(2)	2.463(10)
Zr(1)-C(18)	2.480(10)
Zr(1)-C(19)	2.492(11)
Zr(1)-C(3)	2.505(10)
Zr(1)-C(4)	2.507(10)
Zr(1)-C(20)	2.526(10)
Zr(1)-C(1)	2.554(10)
Zr(1)-C(5)	2.558(9)
Zr(1)-C(17)	2.585(10)
Zr(1)-C(16)	2.599(10)
C(1)-C(9)	1.401(14)
C(1)-C(2)	1.431(12)
C(1)-C(5)	1.442(12)
C(2)-C(3)	1.416(12)
C(3)-C(4)	1.406(12)
C(4)-C(5)	1.419(12)
C(5)-C(6)	1.438(14)
C(6)-C(7)	1.37(2)
C(6)-C(21)	1.524(13)
C(7)-C(8)	1.42(2)
C(8)-C(9)	1.37(2)
C(9)-C(10)	1.525(13)
C(10)-C(11)	1.53(2)
C(11)-C(12)	1.48(2)
C(12)-C(13)	1.38(2)
C(12)-C(17)	1.455(13)
C(13)-C(14)	1.41(2)
C(14)-C(15)	1.36(2)
C(15)-C(16)	1.446(14)
C(15)-C(24)	1.53(2)
C(16)-C(17)	1.426(13)
C(16)-C(20)	1.438(13)
C(17)-C(18)	1.441(12)
C(18)-C(19)	1.389(13)
C(19)-C(20)	1.401(13)
C(21)-C(23)	1.48(2)
C(21)-C(22)	1.52(2)
C(24)-C(25)	1.51(2)
C(24)-C(26)	1.53(2)
Cl(1)-Zr(1)-Cl(2)	96.46(10)
Cl(1)-Zr(1)-C(2)	92.6(2)
Cl(2)-Zr(1)-C(2)	134.4(2)
Cl(1)-Zr(1)-C(18)	134.2(2)
Cl(2)-Zr(1)-C(18)	103.4(2)
C(2)-Zr(1)-C(18)	101.6(3)
Cl(1)-Zr(1)-C(19)	116.8(2)
Cl(2)-Zr(1)-C(19)	79.8(2)
C(2)-Zr(1)-C(19)	133.8(3)
C(18)-Zr(1)-C(19)	32.5(3)
Cl(1)-Zr(1)-C(3)	77.8(2)
Cl(2)-Zr(1)-C(3)	106.4(2)
C(2)-Zr(1)-C(3)	33.1(3)
C(18)-Zr(1)-C(3)	132.4(3)

C(19)-Zr(1)-C(3)	164.0(3)
Cl(1)-Zr(1)-C(4)	98.7(2)
Cl(2)-Zr(1)-C(4)	79.5(2)
C(2)-Zr(1)-C(4)	55.0(3)
C(18)-Zr(1)-C(4)	125.1(3)
C(19)-Zr(1)-C(4)	140.5(3)
C(3)-Zr(1)-C(4)	32.6(3)
Cl(1)-Zr(1)-C(20)	85.3(2)
Cl(2)-Zr(1)-C(20)	90.2(2)
C(2)-Zr(1)-C(20)	135.2(3)
C(18)-Zr(1)-C(20)	54.3(3)
C(19)-Zr(1)-C(20)	32.4(3)
C(3)-Zr(1)-C(20)	157.3(3)
C(4)-Zr(1)-C(20)	169.2(3)
Cl(1)-Zr(1)-C(1)	125.5(2)
Cl(2)-Zr(1)-C(1)	118.5(2)
C(2)-Zr(1)-C(1)	33.1(3)
C(18)-Zr(1)-C(1)	79.2(3)
C(19)-Zr(1)-C(1)	109.9(3)
C(3)-Zr(1)-C(1)	54.1(3)
C(4)-Zr(1)-C(1)	54.3(3)
C(20)-Zr(1)-C(1)	130.7(3)
Cl(1)-Zr(1)-C(5)	129.8(2)
Cl(2)-Zr(1)-C(5)	86.5(2)
C(2)-Zr(1)-C(5)	54.8(3)
C(18)-Zr(1)-C(5)	92.6(3)
C(19)-Zr(1)-C(5)	113.1(3)
C(3)-Zr(1)-C(5)	53.8(3)
C(4)-Zr(1)-C(5)	32.5(3)
C(20)-Zr(1)-C(5)	144.9(3)
C(1)-Zr(1)-C(5)	32.8(3)
Cl(1)-Zr(1)-C(17)	107.6(2)
Cl(2)-Zr(1)-C(17)	133.0(2)
C(2)-Zr(1)-C(17)	85.1(3)
C(18)-Zr(1)-C(17)	33.0(3)
C(19)-Zr(1)-C(17)	53.5(3)
C(3)-Zr(1)-C(17)	117.7(3)
C(4)-Zr(1)-C(17)	133.0(3)
C(20)-Zr(1)-C(17)	53.7(3)
C(1)-Zr(1)-C(17)	78.8(3)
C(5)-Zr(1)-C(17)	106.1(3)
Cl(1)-Zr(1)-C(16)	80.5(2)
Cl(2)-Zr(1)-C(16)	122.7(2)
C(2)-Zr(1)-C(16)	102.9(3)
C(18)-Zr(1)-C(16)	54.0(3)
C(19)-Zr(1)-C(16)	53.4(3)
C(3)-Zr(1)-C(16)	128.0(3)
C(4)-Zr(1)-C(16)	157.9(3)
C(20)-Zr(1)-C(16)	32.6(3)
C(1)-Zr(1)-C(16)	108.3(3)
C(5)-Zr(1)-C(16)	137.9(3)
C(17)-Zr(1)-C(16)	31.9(3)
C(9)-C(1)-C(2)	131.7(8)
C(9)-C(1)-C(5)	121.0(8)
C(2)-C(1)-C(5)	107.2(7)
C(9)-C(1)-Zr(1)	125.3(7)
C(2)-C(1)-Zr(1)	70.0(5)
C(5)-C(1)-Zr(1)	73.8(5)
C(3)-C(2)-C(1)	107.8(8)
C(3)-C(2)-Zr(1)	75.1(6)

C(1)-C(2)-Zr(1)	76.9(5)
C(4)-C(3)-C(2)	108.8(8)
C(4)-C(3)-Zr(1)	73.8(6)
C(2)-C(3)-Zr(1)	71.8(6)
C(3)-C(4)-C(5)	108.4(8)
C(3)-C(4)-Zr(1)	73.6(6)
C(5)-C(4)-Zr(1)	75.7(5)
C(4)-C(5)-C(6)	132.8(9)
C(4)-C(5)-C(1)	107.6(7)
C(6)-C(5)-C(1)	119.6(8)
C(4)-C(5)-Zr(1)	71.8(5)
C(6)-C(5)-Zr(1)	119.0(7)
C(1)-C(5)-Zr(1)	73.5(5)
C(7)-C(6)-C(5)	117.0(9)
C(7)-C(6)-C(21)	122.9(10)
C(5)-C(6)-C(21)	119.7(9)
C(6)-C(7)-C(8)	122.3(10)
C(9)-C(8)-C(7)	122.0(10)
C(8)-C(9)-C(1)	117.8(9)
C(8)-C(9)-C(10)	120.1(10)
C(1)-C(9)-C(10)	122.1(9)
C(9)-C(10)-C(11)	111.5(9)
C(12)-C(11)-C(10)	116.9(9)
C(13)-C(12)-C(17)	114.2(10)
C(13)-C(12)-C(11)	121.9(10)
C(17)-C(12)-C(11)	123.7(9)
C(12)-C(13)-C(14)	124.2(10)
C(15)-C(14)-C(13)	122.8(10)
C(14)-C(15)-C(16)	116.5(10)
C(14)-C(15)-C(24)	124.5(10)
C(16)-C(15)-C(24)	118.9(9)
C(17)-C(16)-C(20)	107.4(7)
C(17)-C(16)-C(15)	120.6(9)
C(20)-C(16)-C(15)	131.9(9)
C(17)-C(16)-Zr(1)	73.5(5)
C(20)-C(16)-Zr(1)	70.9(6)
C(15)-C(16)-Zr(1)	123.2(7)
C(16)-C(17)-C(18)	107.3(8)
C(16)-C(17)-C(12)	121.6(8)
C(18)-C(17)-C(12)	131.0(9)
C(16)-C(17)-Zr(1)	74.6(6)
C(18)-C(17)-Zr(1)	69.5(5)
C(12)-C(17)-Zr(1)	123.2(7)
C(19)-C(18)-C(17)	107.6(8)
C(19)-C(18)-Zr(1)	74.2(6)
C(17)-C(18)-Zr(1)	77.5(6)
C(18)-C(19)-C(20)	110.0(8)
C(18)-C(19)-Zr(1)	73.3(6)
C(20)-C(19)-Zr(1)	75.1(6)
C(19)-C(20)-C(16)	107.4(8)
C(19)-C(20)-Zr(1)	72.5(6)
C(16)-C(20)-Zr(1)	76.5(6)
C(23)-C(21)-C(22)	113.1(10)
C(23)-C(21)-C(6)	109.7(9)
C(22)-C(21)-C(6)	112.0(9)
C(25)-C(24)-C(26)	110.7(11)
C(25)-C(24)-C(15)	110.1(10)
C(26)-C(24)-C(15)	112.1(10)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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(1)	12(1)	13(1)	23(1)	0(1)	3(1)	2(1)
Cl(1)	21(1)	17(1)	34(2)	3(1)	-2(1)	-4(1)
Cl(2)	13(1)	24(2)	44(2)	-4(1)	2(1)	7(1)
C(1)	15(4)	14(4)	22(6)	-2(4)	4(4)	5(3)
C(2)	20(4)	26(5)	30(6)	9(5)	14(4)	7(4)
C(3)	25(5)	14(5)	28(6)	6(4)	11(4)	1(4)
C(4)	20(4)	22(5)	25(6)	-2(4)	1(4)	7(4)
C(5)	18(4)	13(5)	16(5)	-2(4)	-8(4)	0(3)
C(6)	14(4)	24(5)	28(6)	-2(4)	-8(4)	0(4)
C(7)	20(5)	21(5)	37(7)	2(5)	1(5)	-1(4)
C(8)	25(5)	10(5)	43(7)	3(5)	-2(5)	4(4)
C(9)	16(4)	20(5)	34(6)	1(4)	5(4)	5(4)
C(10)	17(4)	14(5)	37(6)	2(4)	0(4)	10(4)
C(11)	21(5)	17(5)	26(5)	9(4)	9(4)	3(4)
C(12)	18(4)	18(5)	27(6)	4(4)	-1(4)	0(4)
C(13)	13(4)	29(5)	30(6)	2(5)	-1(4)	2(4)
C(14)	16(5)	32(6)	41(7)	-11(5)	0(5)	-4(4)
C(15)	21(4)	21(5)	27(6)	1(4)	-6(4)	-3(4)
C(16)	16(4)	22(5)	27(6)	-1(5)	4(4)	3(4)
C(17)	13(4)	19(5)	29(6)	-4(5)	-2(4)	-3(3)
C(18)	17(4)	18(5)	33(6)	5(5)	-1(5)	5(4)
C(19)	17(4)	30(6)	28(6)	-5(5)	8(4)	3(4)
C(20)	25(5)	25(5)	25(6)	0(5)	16(5)	0(4)
C(21)	17(4)	27(6)	25(6)	2(5)	-5(4)	8(4)
C(22)	20(5)	64(9)	43(7)	16(7)	1(5)	11(6)
C(23)	29(6)	41(7)	29(6)	1(5)	-14(5)	6(5)
C(24)	18(5)	20(5)	46(6)	4(5)	8(5)	-5(4)
C(25)	63(9)	33(8)	51(7)	-14(6)	14(7)	-16(7)
C(26)	54(8)	54(9)	65(9)	-11(8)	26(7)	-40(7)

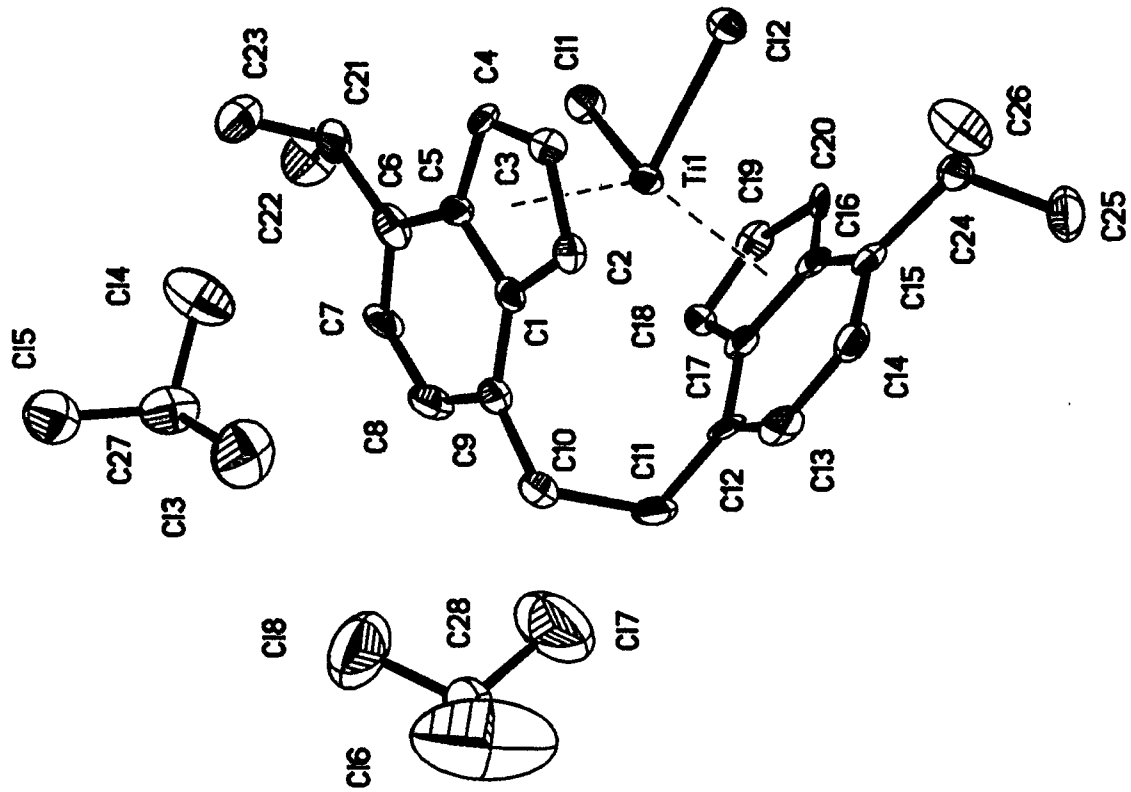
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	6054(4)	4132(6)	8727(9)	29
H(3A)	6622(4)	3116(6)	9954(8)	26
H(4A)	7765(4)	3349(5)	10069(8)	27
H(7A)	8341(5)	5803(6)	8414(10)	32
H(8A)	7353(5)	6292(6)	7810(10)	32
H(10A)	6245(5)	6305(6)	7922(9)	28
H(10B)	5924(5)	5559(6)	8296(9)	28
H(11A)	5601(5)	5808(6)	6385(9)	25
H(12A)	6292(5)	5767(6)	6162(9)	25
H(13A)	4992(5)	4683(6)	6252(9)	29
H(14A)	4831(5)	3404(7)	5835(9)	36
H(18A)	7288(4)	4831(6)	6380(9)	27
H(19A)	7768(4)	3667(6)	5695(9)	30
H(20A)	6980(4)	2620(6)	5408(9)	28
H(21A)	8696(4)	3951(7)	9604(9)	29
H(22A)	9086(5)	4454(9)	8054(11)	64
H(22B)	9607(5)	4441(9)	9102(11)	64
H(22C)	9272(5)	5215(9)	8716(11)	64
H(23A)	8571(5)	4709(7)	11118(10)	52
H(23B)	8946(5)	5374(7)	10643(10)	52
H(23C)	9280(5)	4599(7)	11030(10)	52
H(24A)	5979(5)	2002(6)	5529(10)	33
H(25C)	5842(7)	2512(8)	3717(12)	73
H(25D)	5118(7)	2530(8)	3710(12)	73
H(25A)	5469(7)	1740(8)	3746(12)	73
H(26C)	5129(7)	1926(9)	6528(13)	84
H(26D)	5027(7)	1377(9)	5486(13)	84
H(26A)	4676(7)	2167(9)	5450(13)	84

dl-13

Table 1. Crystal data and structure refinement for 1.

Identification code	rh06b
Empirical formula	C28 H30 Cl8 Ti
Formula weight	698.02
Temperature	188(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 15.822(3) A alpha = 90 deg. b = 17.255(3) A beta = 107.180(10) de c = 11.681(2) A gamma = 90 deg.
Volume, Z	3046.7(9) A^3, 4
Density (calculated)	1.522 Mg/m^3
Absorption coefficient	1.001 mm^-1
F(000)	1424
Crystal size	0.02 x 0.34 x 0.26 mm
Theta range for data collection	1.79 to 24.99 deg.
Limiting indices	-14<=h<=16, -1<=k<=16, -16<=l<=0
Reflections collected	3479
Independent reflections	3244 [R(int) = 0.0631]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.6847 and 0.4776
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3239 / 0 / 334
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0658, wR2 = 0.1447
R indices (all data)	R1 = 0.1144, wR2 = 0.1781
Largest diff. peak and hole	0.909 and -0.735 e.A^-3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C21
C4
Cl1
Cl2
C26
C22
C6
C5
C3
Ti1
C19
C20
C16
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C14
C2
C15
C7
C1
C18
C17
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C17
C16

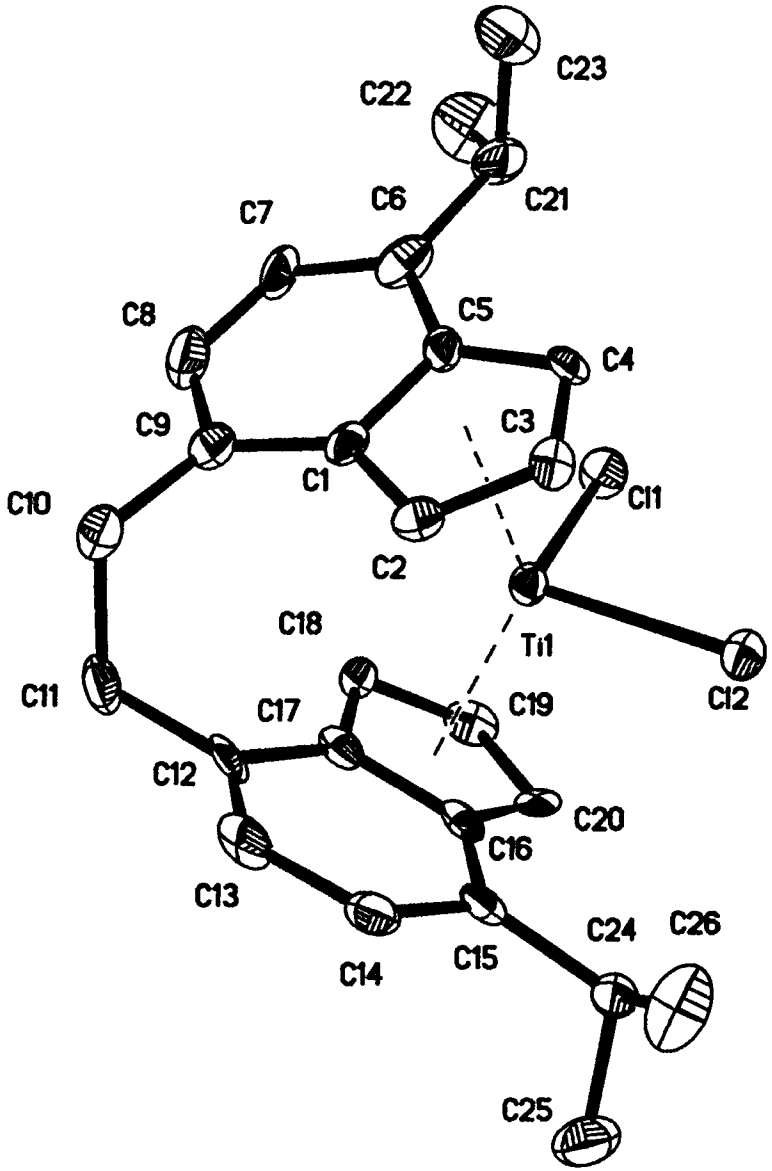

Table 2.. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti(1)	4290(1)	4110(1)	6861(1)	17(1)
Cl(1)	3569(1)	5317(1)	6281(2)	26(1)
Cl(2)	5719(1)	4652(1)	7450(2)	25(1)
C(1)	3398(5)	3367(5)	7890(7)	20(2)
C(2)	4322(5)	3205(5)	8346(7)	21(2)
C(3)	4745(6)	3850(5)	8941(6)	18(2)
C(4)	4140(6)	4454(5)	8791(7)	20(2)
C(5)	3282(5)	4165(5)	8170(7)	20(2)
C(6)	2426(6)	4512(5)	7874(8)	27(2)
C(7)	1732(6)	4044(5)	7297(8)	30(2)
C(8)	1847(6)	3261(6)	7055(8)	37(3)
C(9)	2652(6)	2891(5)	7327(7)	23(2)
C(10)	2724(6)	2037(5)	7145(8)	32(2)
C(11)	3032(6)	1814(5)	6037(8)	31(2)
C(12)	3942(6)	2111(5)	6141(7)	24(2)
C(13)	4700(6)	1707(5)	6627(7)	27(2)
C(14)	5544(6)	2007(5)	6716(7)	24(2)
C(15)	5677(6)	2723(5)	6303(7)	22(2)
C(16)	4899(5)	3172(5)	5748(7)	18(2)
C(17)	4048(5)	2876(5)	5720(7)	20(2)
C(18)	3425(6)	3467(5)	5187(7)	22(2)
C(19)	3880(6)	4040(5)	4741(7)	23(2)
C(20)	4768(6)	3890(5)	5112(6)	18(2)
C(21)	2320(6)	5331(5)	8277(8)	32(2)
C(22)	1513(7)	5733(6)	7504(9)	52(3)
C(23)	2353(7)	5324(6)	9597(8)	46(3)
C(24)	6579(5)	3019(5)	6260(7)	22(2)
C(25)	6781(6)	2697(6)	5157(8)	39(3)
C(26)	7312(6)	2840(6)	7404(9)	50(3)
Cl(5)	-1944(2)	4922(2)	7396(3)	63(1)
Cl(4)	-1013(2)	5842(2)	6101(3)	79(1)
Cl(3)	-861(2)	4169(2)	6144(3)	83(1)
Cl(8)	-699(3)	2289(3)	5275(5)	148(2)
Cl(7)	266(4)	2218(4)	3652(5)	175(3)
Cl(6)	368(4)	1031(3)	5270(7)	208(4)
C(28)	-292(6)	1700(6)	4421(9)	46(3)
C(27)	-1578(7)	4957(6)	6135(10)	53(3)

Table 3. Bond lengths [A] and angles [deg] for 1.

Ti(1)-C(18)	2.312(8)
Ti(1)-C(2)	2.323(8)
Ti(1)-Cl(2)	2.354(2)
Ti(1)-C(3)	2.364(7)
Ti(1)-C(19)	2.370(7)
Ti(1)-Cl(1)	2.374(2)
Ti(1)-C(20)	2.409(7)
Ti(1)-C(4)	2.410(7)
Ti(1)-C(16)	2.446(8)
Ti(1)-C(1)	2.465(8)
Ti(1)-C(17)	2.482(8)
Ti(1)-C(5)	2.515(7)
C(1)-C(9)	1.429(12)
C(1)-C(2)	1.429(11)
C(1)-C(5)	1.439(11)
C(2)-C(3)	1.377(11)
C(3)-C(4)	1.390(11)
C(4)-C(5)	1.426(11)
C(5)-C(6)	1.427(12)
C(6)-C(7)	1.370(12)
C(6)-C(21)	1.514(12)
C(7)-C(8)	1.403(13)
C(8)-C(9)	1.376(12)
C(9)-C(10)	1.497(12)
C(10)-C(11)	1.561(11)
C(11)-C(12)	1.499(12)
C(12)-C(13)	1.358(12)
C(12)-C(17)	1.435(12)
C(13)-C(14)	1.407(12)
C(14)-C(15)	1.364(11)
C(15)-C(16)	1.436(12)
C(15)-C(24)	1.530(11)
C(16)-C(20)	1.428(11)
C(16)-C(17)	1.433(11)
C(17)-C(18)	1.427(12)
C(18)-C(19)	1.409(11)
C(19)-C(20)	1.367(11)
C(21)-C(22)	1.499(13)
C(21)-C(23)	1.527(12)
C(24)-C(26)	1.520(13)
C(24)-C(25)	1.521(11)
Cl(5)-C(27)	1.735(11)
Cl(4)-C(27)	1.776(11)
Cl(3)-C(27)	1.770(10)
Cl(8)-C(28)	1.680(10)
Cl(7)-C(28)	1.689(10)
Cl(6)-C(28)	1.672(11)

C(18)-Ti(1)-C(2)	100.7(3)
C(18)-Ti(1)-Cl(2)	135.6(2)
C(2)-Ti(1)-Cl(2)	104.0(2)
C(18)-Ti(1)-C(3)	134.7(3)
C(2)-Ti(1)-C(3)	34.2(3)
Cl(2)-Ti(1)-C(3)	78.5(2)
C(18)-Ti(1)-C(19)	35.0(3)
C(2)-Ti(1)-C(19)	133.2(3)

Cl(2)-Ti(1)-C(19)	105.6(2)
C(3)-Ti(1)-C(19)	166.0(3)
C(18)-Ti(1)-Cl(1)	93.7(2)
C(2)-Ti(1)-Cl(1)	134.9(2)
Cl(2)-Ti(1)-Cl(1)	94.22(9)
C(3)-Ti(1)-Cl(1)	115.7(2)
C(19)-Ti(1)-Cl(1)	77.7(2)
C(18)-Ti(1)-C(20)	57.5(3)
C(2)-Ti(1)-C(20)	125.7(3)
Cl(2)-Ti(1)-C(20)	78.2(2)
C(3)-Ti(1)-C(20)	139.9(3)
C(19)-Ti(1)-C(20)	33.2(3)
Cl(1)-Ti(1)-C(20)	98.1(2)
C(18)-Ti(1)-C(4)	135.4(3)
C(2)-Ti(1)-C(4)	56.9(3)
Cl(2)-Ti(1)-C(4)	88.9(2)
C(3)-Ti(1)-C(4)	33.8(3)
C(19)-Ti(1)-C(4)	156.6(3)
Cl(1)-Ti(1)-C(4)	83.1(2)
C(20)-Ti(1)-C(4)	167.1(3)
C(18)-Ti(1)-C(16)	57.4(3)
C(2)-Ti(1)-C(16)	91.5(3)
Cl(2)-Ti(1)-C(16)	85.6(2)
C(3)-Ti(1)-C(16)	111.9(3)
C(19)-Ti(1)-C(16)	55.9(3)
Cl(1)-Ti(1)-C(16)	131.3(2)
C(20)-Ti(1)-C(16)	34.2(3)
C(4)-Ti(1)-C(16)	145.4(3)
C(18)-Ti(1)-C(1)	83.2(3)
C(2)-Ti(1)-C(1)	34.6(3)
Cl(2)-Ti(1)-C(1)	134.6(2)
C(3)-Ti(1)-C(1)	56.3(3)
C(19)-Ti(1)-C(1)	117.6(3)
Cl(1)-Ti(1)-C(1)	107.4(2)
C(20)-Ti(1)-C(1)	134.4(3)
C(4)-Ti(1)-C(1)	56.2(3)
C(16)-Ti(1)-C(1)	106.7(3)
C(18)-Ti(1)-C(17)	34.4(3)
C(2)-Ti(1)-C(17)	77.9(3)
Cl(2)-Ti(1)-C(17)	118.7(2)
C(3)-Ti(1)-C(17)	110.0(3)
C(19)-Ti(1)-C(17)	56.2(3)
Cl(1)-Ti(1)-C(17)	127.9(2)
C(20)-Ti(1)-C(17)	56.4(3)
C(4)-Ti(1)-C(17)	132.2(3)
C(16)-Ti(1)-C(17)	33.8(3)
C(1)-Ti(1)-C(17)	78.2(3)
C(18)-Ti(1)-C(5)	102.1(3)
C(2)-Ti(1)-C(5)	56.6(3)
Cl(2)-Ti(1)-C(5)	122.3(2)
C(3)-Ti(1)-C(5)	55.8(3)
C(19)-Ti(1)-C(5)	127.6(3)
Cl(1)-Ti(1)-C(5)	78.6(2)
C(20)-Ti(1)-C(5)	159.3(3)
C(4)-Ti(1)-C(5)	33.6(3)
C(16)-Ti(1)-C(5)	140.2(3)
C(1)-Ti(1)-C(5)	33.6(3)
C(17)-Ti(1)-C(5)	109.5(3)
C(9)-C(1)-C(2)	132.3(8)
C(9)-C(1)-C(5)	120.8(8)

C(2)-C(1)-C(5)	106.7(7)
C(9)-C(1)-Ti(1)	126.0(5)
C(2)-C(1)-Ti(1)	67.3(4)
C(5)-C(1)-Ti(1)	75.1(4)
C(3)-C(2)-C(1)	108.7(7)
C(3)-C(2)-Ti(1)	74.6(4)
C(1)-C(2)-Ti(1)	78.2(5)
C(2)-C(3)-C(4)	109.1(7)
C(2)-C(3)-Ti(1)	71.3(4)
C(4)-C(3)-Ti(1)	74.9(4)
C(3)-C(4)-C(5)	108.6(7)
C(3)-C(4)-Ti(1)	71.3(4)
C(5)-C(4)-Ti(1)	77.3(4)
C(4)-C(5)-C(6)	132.0(8)
C(4)-C(5)-C(1)	106.5(7)
C(6)-C(5)-C(1)	121.4(8)
C(4)-C(5)-Ti(1)	69.2(4)
C(6)-C(5)-Ti(1)	126.6(5)
C(1)-C(5)-Ti(1)	71.3(4)
C(7)-C(6)-C(5)	116.0(8)
C(7)-C(6)-C(21)	123.8(8)
C(5)-C(6)-C(21)	120.1(8)
C(6)-C(7)-C(8)	122.3(8)
C(9)-C(8)-C(7)	124.5(9)
C(8)-C(9)-C(1)	114.9(8)
C(8)-C(9)-C(10)	121.8(8)
C(1)-C(9)-C(10)	123.0(8)
C(9)-C(10)-C(11)	114.5(7)
C(12)-C(11)-C(10)	112.1(7)
C(13)-C(12)-C(17)	116.0(8)
C(13)-C(12)-C(11)	124.5(8)
C(17)-C(12)-C(11)	119.5(8)
C(12)-C(13)-C(14)	122.8(8)
C(15)-C(14)-C(13)	123.3(8)
C(14)-C(15)-C(16)	116.5(8)
C(14)-C(15)-C(24)	123.8(8)
C(16)-C(15)-C(24)	119.2(7)
C(20)-C(16)-C(17)	107.8(7)
C(20)-C(16)-C(15)	132.6(8)
C(17)-C(16)-C(15)	119.5(7)
C(20)-C(16)-Ti(1)	71.5(4)
C(17)-C(16)-Ti(1)	74.5(4)
C(15)-C(16)-Ti(1)	122.5(5)
C(18)-C(17)-C(16)	106.2(7)
C(18)-C(17)-C(12)	132.2(8)
C(16)-C(17)-C(12)	121.6(8)
C(18)-C(17)-Ti(1)	66.3(4)
C(16)-C(17)-Ti(1)	71.7(4)
C(12)-C(17)-Ti(1)	128.3(5)
C(19)-C(18)-C(17)	107.5(7)
C(19)-C(18)-Ti(1)	74.8(5)
C(17)-C(18)-Ti(1)	79.3(5)
C(20)-C(19)-C(18)	109.8(8)
C(20)-C(19)-Ti(1)	74.9(4)
C(18)-C(19)-Ti(1)	70.2(4)
C(19)-C(20)-C(16)	107.9(7)
C(19)-C(20)-Ti(1)	71.8(4)
C(16)-C(20)-Ti(1)	74.3(4)
C(22)-C(21)-C(6)	113.5(8)
C(22)-C(21)-C(23)	112.4(8)

C(6)-C(21)-C(23)	109.4(7)
C(26)-C(24)-C(25)	112.0(7)
C(26)-C(24)-C(15)	112.4(7)
C(25)-C(24)-C(15)	109.7(7)
Cl(6)-C(28)-Cl(8)	110.3(7)
Cl(6)-C(28)-Cl(7)	110.4(6)
Cl(8)-C(28)-Cl(7)	110.4(6)
Cl(5)-C(27)-Cl(3)	110.0(6)
Cl(5)-C(27)-Cl(4)	110.2(6)
Cl(3)-C(27)-Cl(4)	109.6(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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(1)	17(1)	15(1)	20(1)	1(1)	6(1)	-1(1)
Cl(1)	25(1)	20(1)	33(1)	4(1)	8(1)	4(1)
Cl(2)	20(1)	25(1)	32(1)	-4(1)	8(1)	-3(1)
C(1)	20(6)	29(6)	13(4)	-1(4)	8(4)	-7(5)
C(2)	22(6)	24(6)	19(4)	1(4)	9(4)	2(5)
C(3)	20(5)	26(5)	4(4)	3(4)	-3(4)	-4(5)
C(4)	29(6)	18(5)	16(4)	-9(4)	11(4)	-5(5)
C(5)	27(6)	19(6)	17(4)	-2(4)	10(4)	-8(5)
C(6)	18(6)	33(6)	32(5)	11(5)	9(5)	7(5)
C(7)	13(5)	29(6)	49(6)	-4(5)	13(5)	-5(5)
C(8)	31(7)	41(7)	41(6)	-7(5)	13(5)	-18(5)
C(9)	25(6)	25(6)	22(4)	2(4)	11(4)	-3(5)
C(10)	33(6)	34(6)	35(5)	-7(5)	17(5)	-13(5)
C(11)	43(6)	23(5)	29(5)	-10(4)	12(5)	-16(5)
C(12)	43(7)	15(5)	19(4)	-12(4)	14(5)	-11(5)
C(13)	48(7)	7(5)	30(5)	6(4)	17(5)	5(5)
C(14)	29(6)	20(6)	26(5)	-4(4)	12(5)	4(5)
C(15)	29(6)	15(5)	24(5)	-9(4)	11(4)	-2(5)
C(16)	29(6)	13(5)	11(4)	-4(4)	6(4)	-1(5)
C(17)	28(6)	17(5)	16(4)	-5(4)	7(4)	-1(5)
C(18)	24(5)	21(5)	24(5)	-4(4)	13(4)	-7(5)
C(19)	28(6)	29(6)	11(4)	0(4)	1(4)	5(5)
C(20)	30(6)	19(5)	14(4)	-1(4)	19(4)	0(4)
C(21)	23(5)	30(6)	47(6)	-3(5)	19(5)	5(5)
C(22)	52(7)	40(7)	59(7)	9(6)	9(6)	25(6)
C(23)	59(7)	38(6)	44(6)	-12(5)	22(6)	-5(6)
C(24)	20(5)	18(5)	31(5)	-3(4)	9(5)	3(4)
C(25)	33(6)	53(7)	38(6)	-7(5)	20(5)	3(5)
C(26)	35(7)	57(7)	57(7)	9(6)	11(6)	-9(6)
Cl(5)	54(2)	58(2)	77(2)	2(2)	21(2)	4(2)
Cl(4)	53(2)	83(2)	93(2)	29(2)	7(2)	-10(2)
Cl(3)	58(2)	86(2)	105(3)	-4(2)	23(2)	27(2)
Cl(8)	101(3)	173(5)	195(5)	-105(4)	81(4)	-25(3)
Cl(7)	233(6)	208(6)	119(4)	-46(4)	108(4)	-133(5)
Cl(6)	125(4)	97(4)	324(9)	60(5)	-58(5)	27(3)
C(28)	32(6)	49(7)	54(7)	-2(6)	9(5)	2(5)
C(27)	32(6)	50(7)	64(7)	-1(6)	-6(6)	7(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	4599(5)	2730(5)	8254(7)	25
H(3A)	5354(6)	3879(5)	9384(6)	22
H(4A)	4274(6)	4972(5)	9059(7)	24
H(7A)	1152(6)	4257(5)	7052(8)	35
H(8A)	1333(6)	2966(6)	6677(8)	45
H(10A)	2139(6)	1797(5)	7055(8)	39
H(10B)	3146(6)	1815(5)	7873(8)	39
H(11A)	3027(6)	1243(5)	5956(8)	38
H(11B)	2610(6)	2030(5)	5304(8)	38
H(13A)	4659(6)	1199(5)	6920(7)	33
H(14A)	6046(6)	1696(5)	7081(7)	29
H(18A)	2816(6)	3474(5)	5141(7)	26
H(19A)	3610(6)	4466(5)	4256(7)	28
H(20A)	5217(6)	4207(5)	4971(6)	22
H(21A)	2844(6)	5633(5)	8217(8)	38
H(21B)	1482(7)	6258(6)	7811(9)	78
H(21C)	984(7)	5442(6)	7515(9)	78
H(21D)	1546(7)	5764(6)	6680(9)	78
H(23A)	2889(7)	5054(6)	10065(8)	68
H(23B)	1831(7)	5054(6)	9687(8)	68
H(23C)	2360(7)	5857(6)	9886(8)	68
H(24A)	6537(5)	3595(5)	6173(7)	27
H(25A)	6294(6)	2823(6)	4441(8)	59
H(25B)	6848(6)	2133(6)	5230(8)	59
H(25C)	7330(6)	2926(6)	5090(8)	59
H(26A)	7158(6)	3057(6)	8092(9)	75
H(26B)	7867(6)	3072(6)	7359(9)	75
H(26C)	7385(6)	2278(6)	7499(9)	75
H(28A)	-797(6)	1432(6)	3834(9)	55
H(27A)	-2100(7)	4923(6)	5403(10)	64

dl-12a

Table 1. Crystal data and structure refinement for 1.

Identification code	rh08a
Empirical formula	C22 H20 Cl2 Zr
Formula weight	446.50
Temperature	188(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 6.7670(10) A alpha = 90 deg. b = 16.921(3) A beta = 95.770(10) de c = 16.123(3) A gamma = 90 deg.
Volume, Z	1836.8(5) A^3, 4
Density (calculated)	1.615 Mg/m^3
Absorption coefficient	0.891 mm^-1
F(000)	904
Crystal size	0.14 x 0.60 x 0.20 mm
Theta range for data collection	2.41 to 24.99 deg.
Limiting indices	0<=h<=8, -20<=k<=0, -19<=l<=19
Reflections collected	3511
Independent reflections	3220 [R(int) = 0.0331]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.2765 and 0.2489
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3214 / 265 / 227
Goodness-of-fit on F^2	1.011
Final R indices [I>2sigma(I)]	R1 = 0.0384, wR2 = 0.0909
R indices (all data)	R1 = 0.0520, wR2 = 0.1010
Extinction coefficient	0.0000(5)
Largest diff. peak and hole	0.547 and -0.628 e.A^-3

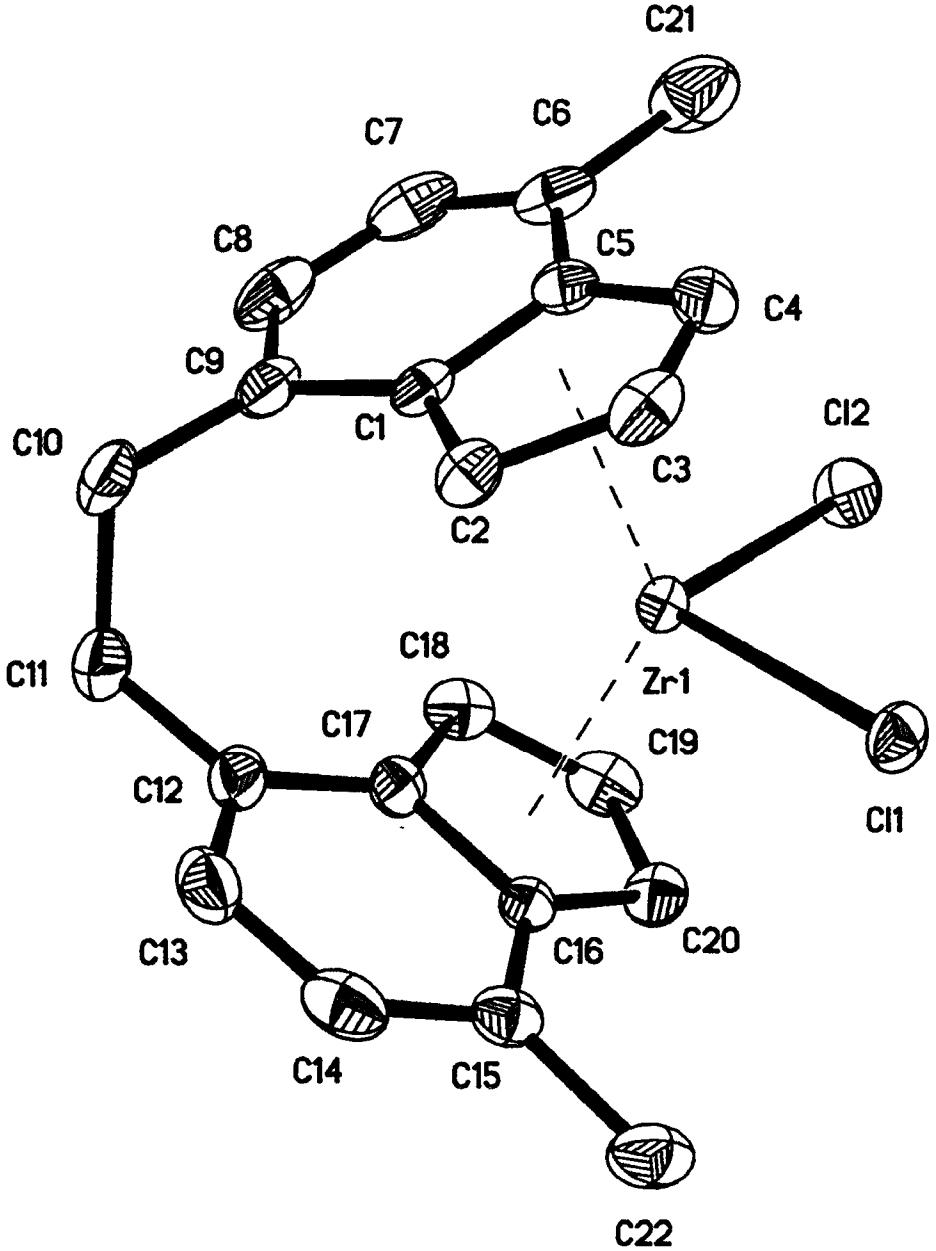

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	337(1)	3474(1)	8713(1)	17(1)
Cl(1)	3012(1)	3982(1)	9682(1)	25(1)
Cl(2)	-1668(1)	3043(1)	9799(1)	30(1)
C(1)	311(5)	2456(2)	7540(2)	21(1)
C(2)	2249(5)	2796(2)	7706(2)	23(1)
C(3)	3062(5)	2515(2)	8490(2)	26(1)
C(4)	1643(6)	2074(2)	8849(3)	28(1)
C(5)	-86(5)	2017(2)	8256(2)	23(1)
C(6)	-1911(6)	1595(2)	8283(3)	33(1)
C(7)	-3207(6)	1632(3)	7580(3)	38(1)
C(8)	-2797(6)	2039(3)	6855(3)	37(1)
C(9)	-1072(6)	2457(2)	6806(2)	28(1)
C(10)	-585(7)	2843(3)	6015(3)	38(1)
C(11)	-1126(7)	3726(3)	5962(3)	38(1)
C(12)	46(6)	4217(2)	6625(2)	28(1)
C(13)	1793(6)	4577(3)	6480(3)	33(1)
C(14)	2918(6)	5037(2)	7091(3)	33(1)
C(15)	2289(5)	5182(2)	7856(2)	24(1)
C(16)	456(5)	4833(2)	8027(2)	20(1)
C(17)	-635(5)	4331(2)	7419(2)	22(1)
C(18)	-2375(5)	4068(2)	7781(3)	27(1)
C(19)	-2425(5)	4471(2)	8544(3)	28(1)
C(20)	-692(5)	4904(2)	8723(2)	25(1)
C(21)	-2297(8)	1118(3)	9028(3)	52(1)
C(22)	3368(6)	5725(2)	8482(3)	34(1)

Table 3. Bond lengths [A] and angles [deg] for 1.

Zr(1)-Cl(1)	2.4266(10)
Zr(1)-Cl(2)	2.4327(10)
Zr(1)-C(2)	2.459(4)
Zr(1)-C(18)	2.466(4)
Zr(1)-C(3)	2.509(4)
Zr(1)-C(19)	2.512(4)
Zr(1)-C(20)	2.519(4)
Zr(1)-C(4)	2.529(4)
Zr(1)-C(16)	2.556(4)
Zr(1)-C(1)	2.557(4)
Zr(1)-C(17)	2.571(4)
Zr(1)-C(5)	2.581(4)
C(1)-C(5)	1.420(5)
C(1)-C(2)	1.433(5)
C(1)-C(9)	1.434(5)
C(2)-C(3)	1.409(5)
C(3)-C(4)	1.388(6)
C(4)-C(5)	1.438(5)
C(5)-C(6)	1.431(5)
C(6)-C(7)	1.363(6)
C(6)-C(21)	1.492(6)
C(7)-C(8)	1.407(7)
C(8)-C(9)	1.374(6)
C(9)-C(10)	1.498(6)
C(10)-C(11)	1.539(6)
C(11)-C(12)	1.514(6)
C(12)-C(13)	1.371(6)
C(12)-C(17)	1.416(5)
C(13)-C(14)	1.416(6)
C(14)-C(15)	1.368(6)
C(15)-C(16)	1.426(5)
C(15)-C(22)	1.499(5)
C(16)-C(20)	1.433(5)
C(16)-C(17)	1.443(5)
C(17)-C(18)	1.436(5)
C(18)-C(19)	1.410(6)
C(19)-C(20)	1.388(6)
Cl(1)-Zr(1)-Cl(2)	94.40(4)
Cl(1)-Zr(1)-C(2)	100.49(9)
Cl(2)-Zr(1)-C(2)	134.72(10)
Cl(1)-Zr(1)-C(18)	135.16(10)
Cl(2)-Zr(1)-C(18)	97.24(10)
C(2)-Zr(1)-C(18)	101.37(13)
Cl(1)-Zr(1)-C(3)	79.02(9)
Cl(2)-Zr(1)-C(3)	112.34(10)
C(2)-Zr(1)-C(3)	32.94(13)
C(18)-Zr(1)-C(3)	133.58(13)
Cl(1)-Zr(1)-C(19)	109.29(10)
Cl(2)-Zr(1)-C(19)	79.45(10)
C(2)-Zr(1)-C(19)	132.62(13)
C(18)-Zr(1)-C(19)	32.89(13)
C(3)-Zr(1)-C(19)	165.54(13)
Cl(1)-Zr(1)-C(20)	81.03(9)
Cl(2)-Zr(1)-C(20)	96.25(9)
C(2)-Zr(1)-C(20)	128.09(13)

C(18)-Zr(1)-C(20)	54.76(13)
C(3)-Zr(1)-C(20)	146.08(13)
C(19)-Zr(1)-C(20)	32.03(13)
Cl(1)-Zr(1)-C(4)	92.53(9)
Cl(2)-Zr(1)-C(4)	82.63(10)
C(2)-Zr(1)-C(4)	54.42(13)
C(18)-Zr(1)-C(4)	131.83(13)
C(3)-Zr(1)-C(4)	31.97(13)
C(19)-Zr(1)-C(4)	152.61(13)
C(20)-Zr(1)-C(4)	173.38(13)
Cl(1)-Zr(1)-C(16)	84.60(8)
Cl(2)-Zr(1)-C(16)	128.71(8)
C(2)-Zr(1)-C(16)	95.31(12)
C(18)-Zr(1)-C(16)	54.81(12)
C(3)-Zr(1)-C(16)	117.65(13)
C(19)-Zr(1)-C(16)	53.45(12)
C(20)-Zr(1)-C(16)	32.79(12)
C(4)-Zr(1)-C(16)	148.63(12)
Cl(1)-Zr(1)-C(1)	131.61(8)
Cl(2)-Zr(1)-C(1)	111.55(9)
C(2)-Zr(1)-C(1)	33.13(11)
C(18)-Zr(1)-C(1)	82.82(12)
C(3)-Zr(1)-C(1)	53.77(11)
C(19)-Zr(1)-C(1)	115.02(12)
C(20)-Zr(1)-C(1)	132.16(12)
C(4)-Zr(1)-C(1)	53.82(12)
C(16)-Zr(1)-C(1)	106.53(12)
Cl(1)-Zr(1)-C(17)	115.85(9)
Cl(2)-Zr(1)-C(17)	129.62(9)
C(2)-Zr(1)-C(17)	80.58(12)
C(18)-Zr(1)-C(17)	33.06(12)
C(3)-Zr(1)-C(17)	112.35(13)
C(19)-Zr(1)-C(17)	53.60(12)
C(20)-Zr(1)-C(17)	54.23(12)
C(4)-Zr(1)-C(17)	131.08(12)
C(16)-Zr(1)-C(17)	32.70(11)
C(1)-Zr(1)-C(17)	78.34(12)
Cl(1)-Zr(1)-C(5)	125.19(8)
Cl(2)-Zr(1)-C(5)	82.25(9)
C(2)-Zr(1)-C(5)	54.30(12)
C(18)-Zr(1)-C(5)	99.28(13)
C(3)-Zr(1)-C(5)	53.38(12)
C(19)-Zr(1)-C(5)	123.43(13)
C(20)-Zr(1)-C(5)	153.77(12)
C(4)-Zr(1)-C(5)	32.67(12)
C(16)-Zr(1)-C(5)	138.00(12)
C(1)-Zr(1)-C(5)	32.08(12)
C(17)-Zr(1)-C(5)	107.15(12)
C(5)-C(1)-C(2)	107.6(3)
C(5)-C(1)-C(9)	120.8(3)
C(2)-C(1)-C(9)	131.5(4)
C(5)-C(1)-Zr(1)	74.9(2)
C(2)-C(1)-Zr(1)	69.7(2)
C(9)-C(1)-Zr(1)	124.4(2)
C(3)-C(2)-C(1)	107.4(3)
C(3)-C(2)-Zr(1)	75.5(2)
C(1)-C(2)-Zr(1)	77.2(2)
C(4)-C(3)-C(2)	109.3(3)
C(4)-C(3)-Zr(1)	74.8(2)
C(2)-C(3)-Zr(1)	71.6(2)

C(3)-C(4)-C(5)	108.0(3)
C(3)-C(4)-Zr(1)	73.2(2)
C(5)-C(4)-Zr(1)	75.6(2)
C(1)-C(5)-C(6)	121.3(4)
C(1)-C(5)-C(4)	107.3(3)
C(6)-C(5)-C(4)	131.3(4)
C(1)-C(5)-Zr(1)	73.0(2)
C(6)-C(5)-Zr(1)	122.6(3)
C(4)-C(5)-Zr(1)	71.7(2)
C(7)-C(6)-C(5)	115.9(4)
C(7)-C(6)-C(21)	123.0(4)
C(5)-C(6)-C(21)	121.0(4)
C(6)-C(7)-C(8)	123.2(4)
C(9)-C(8)-C(7)	122.7(4)
C(8)-C(9)-C(1)	116.0(4)
C(8)-C(9)-C(10)	122.4(4)
C(1)-C(9)-C(10)	121.5(4)
C(9)-C(10)-C(11)	113.5(4)
C(12)-C(11)-C(10)	112.9(3)
C(13)-C(12)-C(17)	117.3(4)
C(13)-C(12)-C(11)	121.5(4)
C(17)-C(12)-C(11)	121.2(4)
C(12)-C(13)-C(14)	122.5(4)
C(15)-C(14)-C(13)	122.2(4)
C(14)-C(15)-C(16)	117.1(4)
C(14)-C(15)-C(22)	122.9(4)
C(16)-C(15)-C(22)	119.9(4)
C(15)-C(16)-C(20)	131.8(3)
C(15)-C(16)-C(17)	120.6(3)
C(20)-C(16)-C(17)	107.6(3)
C(15)-C(16)-Zr(1)	121.5(2)
C(20)-C(16)-Zr(1)	72.2(2)
C(17)-C(16)-Zr(1)	74.2(2)
C(12)-C(17)-C(18)	132.9(4)
C(12)-C(17)-C(16)	120.2(3)
C(18)-C(17)-C(16)	106.8(3)
C(12)-C(17)-Zr(1)	125.2(3)
C(18)-C(17)-Zr(1)	69.4(2)
C(16)-C(17)-Zr(1)	73.1(2)
C(19)-C(18)-C(17)	107.3(3)
C(19)-C(18)-Zr(1)	75.4(2)
C(17)-C(18)-Zr(1)	77.5(2)
C(20)-C(19)-C(18)	110.1(3)
C(20)-C(19)-Zr(1)	74.2(2)
C(18)-C(19)-Zr(1)	71.7(2)
C(19)-C(20)-C(16)	107.8(3)
C(19)-C(20)-Zr(1)	73.7(2)
C(16)-C(20)-Zr(1)	75.0(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 1. 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(1)	13(1)	20(1)	17(1)	-2(1)	1(1)	1(1)
Cl(1)	21(1)	29(1)	24(1)	-3(1)	-4(1)	-1(1)
Cl(2)	30(1)	33(1)	29(1)	0(1)	13(1)	-3(1)
C(1)	19(2)	18(2)	25(2)	-7(2)	-1(1)	2(1)
C(2)	20(2)	26(2)	25(2)	-5(2)	6(1)	1(2)
C(3)	16(2)	30(2)	33(2)	-12(2)	-2(2)	8(2)
C(4)	33(2)	25(2)	26(2)	1(2)	-2(2)	12(2)
C(5)	24(2)	18(2)	28(2)	-3(2)	5(2)	4(1)
C(6)	35(2)	22(2)	44(2)	-11(2)	12(2)	-3(2)
C(7)	25(2)	32(2)	58(3)	-21(2)	7(2)	-7(2)
C(8)	26(2)	35(2)	46(2)	-19(2)	-11(2)	4(2)
C(9)	32(2)	22(2)	28(2)	-8(2)	-7(2)	7(2)
C(10)	56(3)	34(2)	22(2)	-11(2)	-6(2)	2(2)
C(11)	58(3)	33(2)	21(2)	-2(2)	-8(2)	2(2)
C(12)	40(2)	24(2)	20(2)	0(2)	-2(2)	8(2)
C(13)	44(2)	31(2)	24(2)	4(2)	12(2)	5(2)
C(14)	32(2)	28(2)	40(2)	8(2)	14(2)	-1(2)
C(15)	20(2)	21(2)	30(2)	5(2)	-1(2)	1(1)
C(16)	21(2)	17(2)	20(2)	1(1)	-1(1)	5(1)
C(17)	21(2)	22(2)	21(2)	2(2)	-5(1)	5(1)
C(18)	17(2)	25(2)	37(2)	3(2)	-5(2)	3(2)
C(19)	19(2)	28(2)	40(2)	5(2)	9(2)	10(2)
C(20)	26(2)	23(2)	27(2)	-3(2)	4(2)	8(2)
C(21)	71(3)	37(3)	52(3)	-9(2)	26(3)	-22(3)
C(22)	30(2)	26(2)	44(3)	4(2)	0(2)	-8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(2A)	2873(5)	3146(2)	7353(2)	28
H(3A)	4375(5)	2613(2)	8735(2)	32
H(4A)	1787(6)	1850(2)	9392(3)	34
H(7A)	-4449(6)	1370(3)	7578(3)	46
H(8A)	-3751(6)	2024(3)	6381(3)	44
H(10A)	-1304(7)	2565(3)	5536(3)	46
H(10B)	855(7)	2785(3)	5969(3)	46
H(11A)	-879(7)	3929(3)	5406(3)	46
H(11B)	-2561(7)	3787(3)	6020(3)	46
H(13A)	2267(6)	4515(3)	5949(3)	39
H(14A)	4150(6)	5252(2)	6965(3)	39
H(18A)	-3318(5)	3693(2)	7550(3)	32
H(19A)	-3488(5)	4450(2)	8886(3)	34
H(20A)	-331(5)	5196(2)	9219(2)	30
H(21A)	-1179(8)	1176(3)	9460(3)	78
H(21B)	-2447(8)	561(3)	8870(3)	78
H(21C)	-3517(8)	1305(3)	9244(3)	78
H(22A)	2668(6)	5744(2)	8985(3)	50
H(22B)	3419(6)	6257(2)	8244(3)	50
H(22C)	4723(6)	5530(2)	8626(3)	50