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Supporting Information

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Reactivity of Permethylzirconocene and -titanocene toward Disubstituted 1,3-Butadiynes: η^4- vs η^2-Complexation or C-C Coupling with the Permethyltitanocene

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Table 32 Atomic coordinates for **7**.

Table 33 Bond lengths [Å] and angles [deg] for **7**.

Table 34 Anisotropic displacement parameters [$Å^2*10^3$] for **7**.

Table 35 Hydrogen coordinates for **7**.

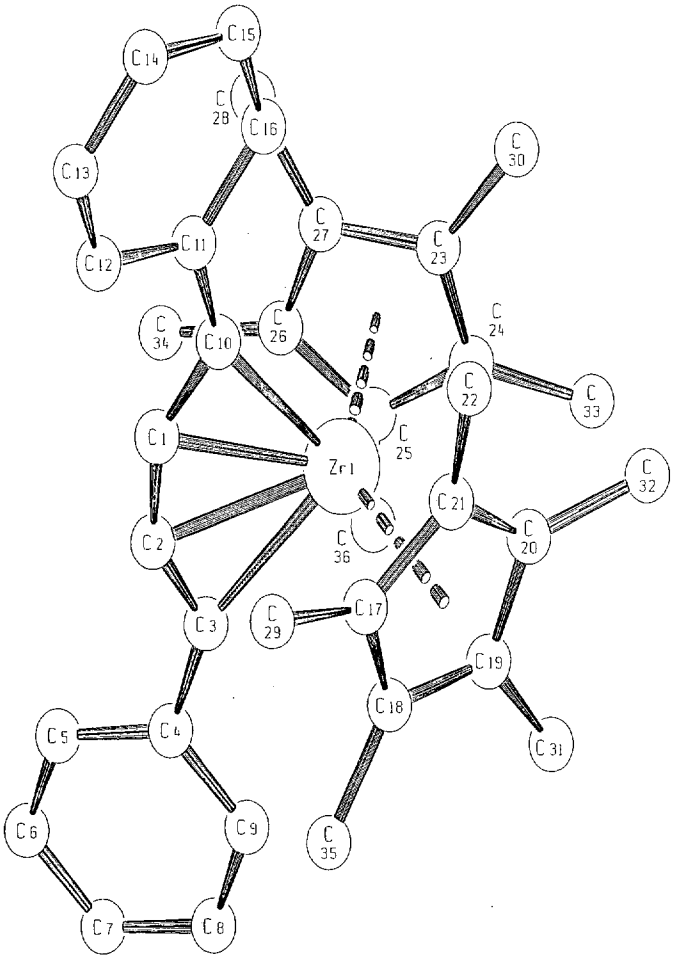


Figure 1: Molecular structure of **2a.**

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Table 1. Crystal data and structure refinement for **2a**.

Identification code	756
Empirical formula	C36 H40 Zr
Formula weight	563.90
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a= 27.086(5) A alpha= 90 deg. b= 15.533(3) A beta= 104.31(3) deg. c= 14.207(3) A gamma= 90 deg.
Temperature for cell	293(2)
Number for reflecions for cell	5000
Theta for cell determination	4 to 20 deg
Volume	5792(2) A^3
Z	8
Density (calculated)	1.293 Mg/m^3
Absorption coefficient	0.402 mm^-1
F(000)	2368
Crystal colour	orange
Crystal description	prism
Crystal size	0.4 x 0.4 x 0.3 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	1.99 to 24.22 deg.

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Index ranges	-31<=h<=25, -16<=k<=17, -15<=l<=16
Reflections collected	12691
Independent reflections	4581 [R(int) = 0.0342]
Reflections unique	4581
Reflections observed	2814
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	4581 / 0 / 334
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0744
R indices (all data)	R1 = 0.0630, wR2 = 0.0801
Goodness-for-fit on F^2(all)	0.919
Goodness-for-fit on F^2(obs)	1.116
Shift/esd(max)	0.000
Shift/esd(mean)	0.000
Weighting scheme	
calc w=1/[\s^2^(Fo^2^)+(0.0440P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	0.270 and -0.339 e.A^-3
Diff. density rms	0.057
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

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

	x	y	z	U(eq)
C(1)	1870(1)	-2094(3)	903(3)	39(1)
C(2)	1866(1)	-2947(3)	948(3)	38(1)
C(3)	1605(1)	-3655(2)	847(2)	37(1)
C(4)	1733(1)	-4557(2)	1031(2)	37(1)
C(5)	2192(1)	-4807(3)	1671(2)	50(1)
C(6)	2296(2)	-5665(3)	1891(3)	61(1)
C(7)	1965(2)	-6298(3)	1469(3)	61(1)
C(8)	1515(2)	-6074(3)	827(3)	58(1)
C(9)	1399(2)	-5216(2)	621(3)	46(1)
C(10)	1611(1)	-1379(2)	743(2)	35(1)
C(11)	1758(1)	-476(2)	683(2)	37(1)
C(12)	2238(1)	-268(2)	549(2)	48(1)
C(13)	2377(2)	582(3)	476(3)	64(1)
C(14)	2048(2)	1235(3)	543(3)	68(1)
C(15)	1578(2)	1052(3)	692(3)	65(1)
C(16)	1429(2)	195(3)	749(3)	53(1)
C(17)	1118(1)	-2271(2)	-1242(2)	39(1)
C(18)	978(1)	-3142(2)	-1211(2)	38(1)
C(19)	481(1)	-3174(2)	-1076(2)	36(1)
C(20)	305(1)	-2316(2)	-1062(2)	37(1)
C(21)	702(2)	-1760(2)	-1144(2)	38(1)
C(22)	654(2)	-807(2)	-1280(3)	70(1)
C(23)	444(1)	-1853(2)	1510(2)	35(1)
C(24)	285(1)	-2719(2)	1333(2)	38(1)
C(25)	685(2)	-3253(2)	1822(2)	39(1)
C(26)	1088(1)	-2718(2)	2325(2)	39(1)
C(27)	936(1)	-1856(2)	2136(2)	37(1)
C(28)	1220(2)	-1094(3)	2663(3)	69(1)
C(29)	1602(2)	-1951(3)	-1465(3)	69(1)
C(30)	119(2)	-1061(3)	1220(3)	69(1)
C(31)	165(2)	-3978(3)	-1117(3)	62(1)
C(32)	-243(1)	-2045(3)	-1205(3)	65(1)
C(33)	-254(2)	-3021(3)	922(3)	70(1)
C(34)	1574(2)	-3000(3)	3033(3)	75(2)
C(35)	1283(2)	-3891(3)	-1450(3)	65(1)
C(36)	653(2)	-4209(2)	1927(3)	75(1)
Zr(1)	1018(1)	-2508(1)	497(1)	25(1)

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Table 3. Bond lengths [A] and angles [deg] for **2a**.

C(1)-C(10)	1.305(5)
C(1)-C(2)	1.327(4)
C(1)-Zr(1)	2.328(4)
C(2)-C(3)	1.296(5)
C(2)-Zr(1)	2.330(4)
C(3)-C(4)	1.453(5)
C(3)-Zr(1)	2.357(4)
C(4)-C(9)	1.395(5)
C(4)-C(5)	1.400(5)
C(5)-C(6)	1.382(5)
C(6)-C(7)	1.366(6)
C(7)-C(8)	1.374(5)
C(8)-C(9)	1.383(5)
C(10)-C(11)	1.466(5)
C(10)-Zr(1)	2.345(4)
C(11)-C(16)	1.389(5)
C(11)-C(12)	1.400(5)
C(12)-C(13)	1.384(5)
C(13)-C(14)	1.369(6)
C(14)-C(15)	1.371(6)
C(15)-C(16)	1.400(5)
C(17)-C(21)	1.413(5)
C(17)-C(18)	1.409(5)
C(17)-C(29)	1.506(5)
C(17)-Zr(1)	2.578(3)
C(18)-C(19)	1.409(5)
C(18)-C(35)	1.512(5)
C(18)-Zr(1)	2.597(3)
C(19)-C(20)	1.417(5)
C(19)-C(31)	1.507(5)
C(19)-Zr(1)	2.564(3)
C(20)-C(21)	1.407(5)
C(20)-C(32)	1.507(5)
C(20)-Zr(1)	2.571(3)
C(21)-C(22)	1.494(5)
C(21)-Zr(1)	2.555(3)
C(23)-C(27)	1.408(5)
C(23)-C(24)	1.414(5)
C(23)-C(30)	1.509(5)
C(23)-Zr(1)	2.575(3)
C(24)-C(25)	1.403(5)
C(24)-C(33)	1.508(5)
C(24)-Zr(1)	2.573(3)
C(25)-C(26)	1.418(5)
C(25)-C(36)	1.497(5)
C(25)-Zr(1)	2.557(3)
C(26)-C(27)	1.408(5)
C(26)-C(34)	1.509(5)
C(26)-Zr(1)	2.578(3)
C(27)-C(28)	1.506(5)
C(27)-Zr(1)	2.598(3)
C(10)-C(1)-C(2)	148.0(4)
C(10)-C(1)-Zr(1)	74.5(2)
C(2)-C(1)-Zr(1)	73.5(3)
C(3)-C(2)-C(1)	148.5(4)

C(3)-C(2)-Zr(1)	75.1(2)
C(1)-C(2)-Zr(1)	73.4(3)
C(2)-C(3)-C(4)	134.3(4)
C(2)-C(3)-Zr(1)	72.8(2)
C(4)-C(3)-Zr(1)	152.4(3)
C(9)-C(4)-C(5)	116.6(3)
C(9)-C(4)-C(3)	122.1(3)
C(5)-C(4)-C(3)	121.3(3)
C(6)-C(5)-C(4)	120.9(4)
C(7)-C(6)-C(5)	121.2(4)
C(6)-C(7)-C(8)	119.2(4)
C(7)-C(8)-C(9)	120.1(4)
C(8)-C(9)-C(4)	121.9(4)
C(1)-C(10)-C(11)	133.0(3)
C(1)-C(10)-Zr(1)	73.1(2)
C(11)-C(10)-Zr(1)	153.2(3)
C(16)-C(11)-C(12)	118.0(4)
C(16)-C(11)-C(10)	121.7(3)
C(12)-C(11)-C(10)	120.3(4)
C(13)-C(12)-C(11)	120.6(4)
C(14)-C(13)-C(12)	120.6(4)
C(15)-C(14)-C(13)	120.2(4)
C(14)-C(15)-C(16)	119.9(4)
C(11)-C(16)-C(15)	120.7(4)
C(21)-C(17)-C(18)	108.0(3)
C(21)-C(17)-C(29)	126.3(3)
C(18)-C(17)-C(29)	125.3(3)
C(21)-C(17)-Zr(1)	73.2(2)
C(18)-C(17)-Zr(1)	74.9(2)
C(29)-C(17)-Zr(1)	123.5(2)
C(19)-C(18)-C(17)	108.1(3)
C(19)-C(18)-C(35)	126.7(4)
C(17)-C(18)-C(35)	124.5(3)
C(19)-C(18)-Zr(1)	72.9(2)
C(17)-C(18)-Zr(1)	73.4(2)
C(35)-C(18)-Zr(1)	127.1(2)
C(18)-C(19)-C(20)	107.8(3)
C(18)-C(19)-C(31)	125.3(4)
C(20)-C(19)-C(31)	126.2(3)
C(18)-C(19)-Zr(1)	75.4(2)
C(20)-C(19)-Zr(1)	74.3(2)
C(31)-C(19)-Zr(1)	124.2(2)
C(21)-C(20)-C(19)	108.0(3)
C(21)-C(20)-C(32)	124.4(3)
C(19)-C(20)-C(32)	125.8(3)
C(21)-C(20)-Zr(1)	73.5(2)
C(19)-C(20)-Zr(1)	73.7(2)
C(32)-C(20)-Zr(1)	130.8(2)
C(17)-C(21)-C(20)	107.9(3)
C(17)-C(21)-C(22)	126.1(4)
C(20)-C(21)-C(22)	125.1(4)
C(17)-C(21)-Zr(1)	74.9(2)
C(20)-C(21)-Zr(1)	74.7(2)
C(22)-C(21)-Zr(1)	124.6(2)
C(27)-C(23)-C(24)	107.9(3)
C(27)-C(23)-C(30)	124.8(4)
C(24)-C(23)-C(30)	126.6(3)
C(27)-C(23)-Zr(1)	75.1(2)
C(24)-C(23)-Zr(1)	74.0(2)
C(30)-C(23)-Zr(1)	124.1(2)

C(25)-C(24)-C(23)	108.1(3)
C(25)-C(24)-C(33)	124.2(3)
C(23)-C(24)-C(33)	125.9(3)
C(25)-C(24)-Zr(1)	73.5(2)
C(23)-C(24)-Zr(1)	74.1(2)
C(33)-C(24)-Zr(1)	130.2(2)
C(24)-C(25)-C(26)	107.9(3)
C(24)-C(25)-C(36)	125.4(4)
C(26)-C(25)-C(36)	125.9(4)
C(24)-C(25)-Zr(1)	74.8(2)
C(26)-C(25)-Zr(1)	74.8(2)
C(36)-C(25)-Zr(1)	124.2(2)
C(27)-C(26)-C(25)	107.9(3)
C(27)-C(26)-C(34)	124.7(3)
C(25)-C(26)-C(34)	127.1(3)
C(27)-C(26)-Zr(1)	75.0(2)
C(25)-C(26)-Zr(1)	73.2(2)
C(34)-C(26)-Zr(1)	122.9(2)
C(23)-C(27)-C(26)	108.1(3)
C(23)-C(27)-C(28)	126.8(4)
C(26)-C(27)-C(28)	124.3(3)
C(23)-C(27)-Zr(1)	73.3(2)
C(26)-C(27)-Zr(1)	73.4(2)
C(28)-C(27)-Zr(1)	127.3(2)
C(1)-Zr(1)-C(2)	33.10(11)
C(1)-Zr(1)-C(10)	32.42(13)
C(2)-Zr(1)-C(10)	65.52(13)
C(1)-Zr(1)-C(3)	65.21(14)
C(2)-Zr(1)-C(3)	32.11(13)
C(10)-Zr(1)-C(3)	97.63(11)
C(1)-Zr(1)-C(21)	100.88(13)
C(2)-Zr(1)-C(21)	117.97(13)
C(10)-Zr(1)-C(21)	81.88(12)
C(3)-Zr(1)-C(21)	126.35(12)
C(1)-Zr(1)-C(25)	116.84(13)
C(2)-Zr(1)-C(25)	99.73(13)
C(10)-Zr(1)-C(25)	125.59(11)
C(3)-Zr(1)-C(25)	81.07(12)
C(21)-Zr(1)-C(25)	141.05(13)
C(1)-Zr(1)-C(19)	129.96(12)
C(2)-Zr(1)-C(19)	115.48(13)
C(10)-Zr(1)-C(19)	130.71(11)
C(3)-Zr(1)-C(19)	95.00(12)
C(21)-Zr(1)-C(19)	53.02(11)
C(25)-Zr(1)-C(19)	103.36(12)
C(1)-Zr(1)-C(20)	132.05(12)
C(2)-Zr(1)-C(20)	138.65(11)
C(10)-Zr(1)-C(20)	112.51(11)
C(3)-Zr(1)-C(20)	126.40(11)
C(21)-Zr(1)-C(20)	31.86(10)
C(25)-Zr(1)-C(20)	111.07(12)
C(19)-Zr(1)-C(20)	32.03(11)
C(1)-Zr(1)-C(23)	116.83(13)
C(2)-Zr(1)-C(23)	130.77(12)
C(10)-Zr(1)-C(23)	96.14(12)
C(3)-Zr(1)-C(23)	130.49(11)
C(21)-Zr(1)-C(23)	102.58(11)
C(25)-Zr(1)-C(23)	52.80(11)
C(19)-Zr(1)-C(23)	110.80(12)
C(20)-Zr(1)-C(23)	90.37(11)

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C(1)-Zr(1)-C(24)	138.71(11)
C(2)-Zr(1)-C(24)	131.05(12)
C(10)-Zr(1)-C(24)	127.14(11)
C(3)-Zr(1)-C(24)	111.29(12)
C(21)-Zr(1)-C(24)	110.87(12)
C(25)-Zr(1)-C(24)	31.75(11)
C(19)-Zr(1)-C(24)	90.83(11)
C(20)-Zr(1)-C(24)	84.91(11)
C(23)-Zr(1)-C(24)	31.89(11)
C(1)-Zr(1)-C(26)	87.89(12)
C(2)-Zr(1)-C(26)	82.16(12)
C(10)-Zr(1)-C(26)	93.84(11)
C(3)-Zr(1)-C(26)	79.23(11)
C(21)-Zr(1)-C(26)	154.35(11)
C(25)-Zr(1)-C(26)	32.06(11)
C(19)-Zr(1)-C(26)	135.37(11)
C(20)-Zr(1)-C(26)	137.33(11)
C(23)-Zr(1)-C(26)	52.52(11)
C(24)-Zr(1)-C(26)	52.57(11)
C(1)-Zr(1)-C(17)	82.27(12)
C(2)-Zr(1)-C(17)	88.56(12)
C(10)-Zr(1)-C(17)	78.81(11)
C(3)-Zr(1)-C(17)	94.89(12)
C(21)-Zr(1)-C(17)	31.96(11)
C(25)-Zr(1)-C(17)	155.53(11)
C(19)-Zr(1)-C(17)	52.70(11)
C(20)-Zr(1)-C(17)	52.60(11)
C(23)-Zr(1)-C(17)	134.46(11)
C(24)-Zr(1)-C(17)	137.43(11)
C(26)-Zr(1)-C(17)	169.99(11)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2a**.
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(1)	25(2)	50(3)	42(2)	-4(2)	9(2)	-7(2)
C(2)	27(2)	45(3)	41(2)	-3(2)	6(2)	6(2)
C(3)	33(2)	43(3)	36(2)	0(2)	10(2)	7(2)
C(4)	38(2)	41(2)	32(2)	0(2)	11(2)	9(2)
C(5)	43(2)	57(3)	45(2)	-7(2)	3(2)	11(2)
C(6)	59(3)	65(3)	54(2)	5(2)	4(2)	33(2)
C(7)	80(3)	49(3)	60(3)	7(2)	27(2)	24(2)
C(8)	61(3)	49(3)	66(3)	-3(2)	20(2)	0(2)
C(9)	44(3)	44(3)	47(2)	2(2)	5(2)	8(2)
C(10)	32(2)	42(2)	32(2)	-2(2)	9(2)	-7(2)
C(11)	41(2)	40(2)	31(2)	-3(2)	9(2)	-9(2)
C(12)	45(2)	50(2)	53(2)	-6(2)	19(2)	-14(2)
C(13)	60(3)	69(3)	69(3)	-9(2)	27(2)	-28(2)
C(14)	92(4)	47(3)	68(3)	-6(2)	25(3)	-31(3)
C(15)	81(4)	40(3)	73(3)	-3(2)	21(3)	1(2)
C(16)	48(3)	49(3)	62(3)	-4(2)	17(2)	-8(2)
C(17)	43(2)	51(3)	26(2)	-1(2)	14(2)	-11(2)
C(18)	46(2)	42(2)	27(2)	-5(2)	8(2)	7(2)
C(19)	47(2)	39(2)	21(2)	-2(2)	5(2)	-10(2)
C(20)	37(2)	47(3)	24(2)	3(2)	4(1)	2(2)
C(21)	52(3)	37(2)	25(2)	5(2)	8(2)	2(2)
C(22)	111(4)	41(2)	46(2)	12(2)	-4(2)	3(2)
C(23)	38(2)	40(2)	32(2)	4(2)	17(2)	14(2)
C(24)	34(2)	54(3)	30(2)	0(2)	16(1)	-4(2)
C(25)	53(3)	34(2)	36(2)	3(2)	24(2)	0(2)
C(26)	39(2)	55(3)	24(2)	3(2)	7(1)	9(2)
C(27)	42(2)	40(2)	33(2)	-9(2)	17(2)	-2(2)
C(28)	85(3)	76(3)	56(3)	-30(2)	34(2)	-26(3)
C(29)	67(3)	102(4)	48(2)	-9(2)	33(2)	-23(3)
C(30)	83(3)	74(3)	61(3)	10(2)	36(2)	40(3)
C(31)	77(3)	61(3)	45(2)	-8(2)	9(2)	-27(2)
C(32)	45(2)	103(3)	42(2)	13(2)	4(2)	18(2)
C(33)	50(3)	116(4)	46(2)	-1(2)	19(2)	-29(3)
C(34)	69(3)	121(4)	31(2)	10(2)	4(2)	40(3)
C(35)	85(3)	69(3)	43(2)	-15(2)	20(2)	22(3)
C(36)	121(4)	44(2)	80(3)	10(2)	67(3)	2(3)
Zr(1)	25(1)	27(1)	24(1)	0(1)	7(1)	0(1)

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

	x	y	z	U(eq)
H(5)	2429(1)	-4390(3)	1951(2)	60
H(6)	2598(2)	-5814(3)	2334(3)	73
H(7)	2042(2)	-6873(3)	1614(3)	73
H(8)	1288(2)	-6500(3)	531(3)	69
H(9)	1089(2)	-5075(2)	197(3)	55
H(12)	2467(1)	-705(2)	508(2)	58
H(13)	2696(2)	711(3)	380(3)	77
H(14)	2144(2)	1805(3)	488(3)	82
H(15)	1358(2)	1497(3)	756(3)	77
H(16)	1106(2)	73(3)	831(3)	63
H(22A)	336(2)	-618(2)	-1169(3)	105
H(22B)	666(2)	-663(2)	-1931(3)	105
H(22C)	930(2)	-527(2)	-828(3)	105
H(28A)	1548(2)	-1276(3)	3040(3)	104
H(28B)	1029(2)	-851(3)	3086(3)	104
H(28C)	1263(2)	-668(3)	2200(3)	104
H(29A)	1821(2)	-2430(3)	-1495(3)	103
H(29B)	1771(2)	-1561(3)	-964(3)	103
H(29C)	1521(2)	-1657(3)	-2079(3)	103
H(30A)	-200(2)	-1222(3)	790(3)	104
H(30B)	293(2)	-664(3)	896(3)	104
H(30C)	58(2)	-793(3)	1789(3)	104
H(31A)	-160(2)	-3832(3)	-1003(3)	93
H(31B)	337(2)	-4375(3)	-627(3)	93
H(31C)	115(2)	-4239(3)	-1745(3)	93
H(32A)	-444(1)	-2532(3)	-1115(3)	97
H(32B)	-368(1)	-1822(3)	-1850(3)	97
H(32C)	-266(1)	-1607(3)	-740(3)	97
H(33A)	-460(2)	-2545(3)	622(3)	104
H(33B)	-388(2)	-3248(3)	1436(3)	104
H(33C)	-257(2)	-3461(3)	447(3)	104
H(34A)	1594(2)	-3617(3)	3037(3)	112
H(34B)	1574(2)	-2799(3)	3672(3)	112
H(34C)	1861(2)	-2764(3)	2840(3)	112
H(35A)	1611(2)	-3690(3)	-1502(3)	97
H(35B)	1105(2)	-4143(3)	-2055(3)	97
H(35C)	1327(2)	-4315(3)	-944(3)	97
H(36A)	976(2)	-4425(2)	2291(3)	112
H(36B)	567(2)	-4471(2)	1295(3)	112
H(36C)	396(2)	-4344(2)	2263(3)	112

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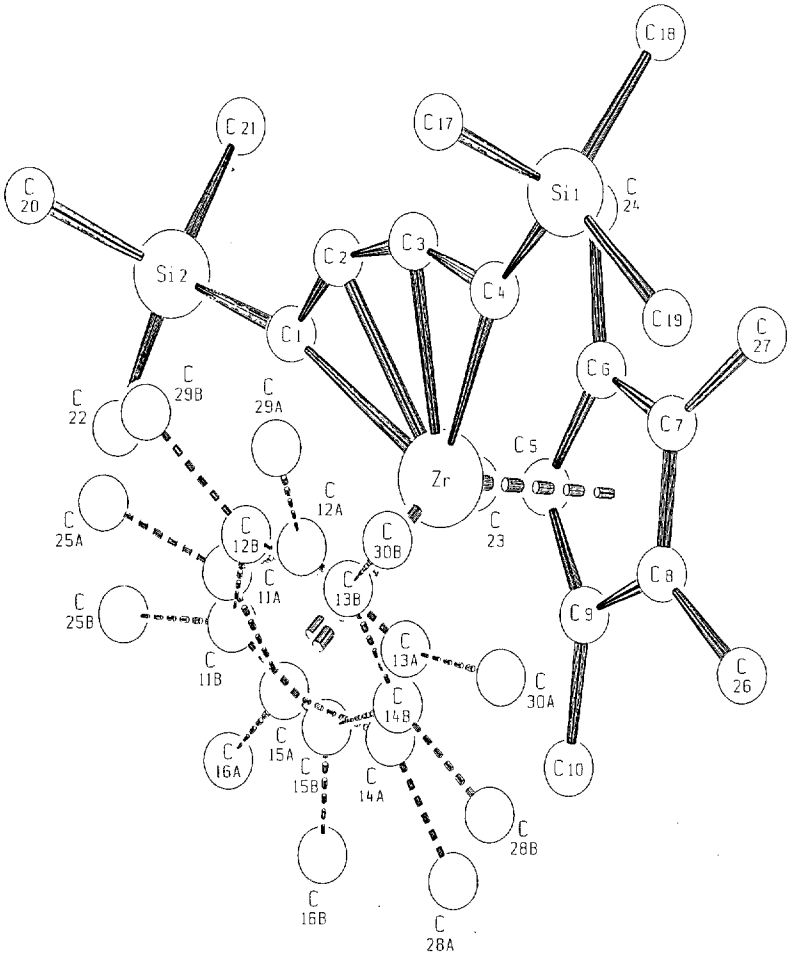


Figure 2: Molecular structure of **2b**

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Table 6. Crystal data and structure refinement for **2b**.

Identification code	770
Empirical formula	C30 H48 Si2 Zr
Formula weight	556.08
Crystal system	MONOCLINIC
Space group	P21/C
Unit cell dimensions	a= 10.595(2) A alpha= 90 deg. b= 18.220(4) A beta= 94.50(3) deg. c= 15.891(3) A gamma= 90 deg.
Temperature for cell	200(2)
Number for reflecions for cell	5000
Theta for cell determination	4 to 20 deg
Volume	3058.2(11) A^3
Z	4
Density (calculated)	1.208 Mg/m^3
Absorption coefficient	0.453 mm^-1
F(000)	1184
Crystal colour	ORANGE
Crystal description	PRISM
Crystal size	0.4 x 0.2 x 0.2 mm
Temperature	200(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	2.23 to 24.23 deg.

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Index ranges	-12<=h<=12, 0<=k<=21, -18<=l<=18
Reflections collected	8957
Independent reflections	4579 [R(int) = 0.0247]
Reflections unique	4579
Reflections observed	3595
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	4579 / 0 / 288
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1266
R indices (all data)	R1 = 0.0653, wR2 = 0.1348
Goodness-for-fit on F^2(all)	1.057
Goodness-for-fit on F^2(obs)	1.128
Shift/esd(max)	-0.001
Shift/esd(mean)	0.000
Weighting scheme	
calc w=1/[\s^2^(Fo^2^)+(0.0783P)^2^+3.0539P] where P=(Fo^2^+2Fc^2^)/3	
Largest diff. peak and hole	0.793 and -0.537 e.A^-3
Diff. density rms	0.091
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

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Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2b**. U(eq) is defined as one third for the trace for the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8142(5)	-364(2)	2251(3)	29(1)
C(2)	7224(4)	-162(2)	1719(3)	27(1)
C(3)	6241(4)	268(2)	1475(3)	26(1)
C(4)	5468(4)	800(2)	1594(3)	26(1)
C(5)	9212(5)	1228(3)	2788(4)	48(2)
C(6)	8571(6)	1426(3)	2017(3)	49(2)
C(7)	7617(6)	1906(3)	2175(4)	50(2)
C(8)	7636(5)	2015(3)	3032(4)	49(2)
C(9)	8639(6)	1600(3)	3420(3)	50(2)
C(23)	10423(7)	788(4)	2923(7)	106(3)
C(24)	8945(10)	1194(5)	1145(5)	119(4)
C(27)	6836(8)	2335(4)	1512(6)	104(3)
C(26)	6863(8)	2597(4)	3453(6)	98(3)
C(10)	9213(9)	1668(5)	4331(4)	107(4)
C(11A)	6114(11)	-422(4)	3594(6)	27(2)
C(12A)	5028(7)	-3(6)	3297(5)	24(2)
C(13A)	5101(8)	698(4)	3721(6)	27(2)
C(14A)	6211(11)	687(4)	4292(5)	27(2)
C(15A)	6853(7)	17(6)	4208(6)	27(2)
C(25A)	6301(10)	-1203(5)	3393(6)	61(3)
C(29A)	3902(9)	-234(6)	2728(6)	61(3)
C(30A)	4125(9)	1292(5)	3696(6)	59(2)
C(28A)	6450(9)	1197(5)	5018(6)	55(2)
C(16A)	7979(9)	-247(5)	4734(6)	59(2)
C(17)	2996(6)	349(3)	628(4)	56(2)
C(18)	4668(7)	1476(4)	-127(4)	71(2)
C(19)	3189(7)	1858(4)	1395(5)	84(2)
C(20)	8441(7)	-2003(3)	1874(5)	79(2)
C(21)	10269(8)	-925(4)	1261(6)	105(3)
C(22)	10296(11)	-1290(5)	3128(6)	154(6)
Si(1)	4097(1)	1123(1)	885(1)	37(1)
Si(2)	9284(2)	-1133(1)	2140(1)	44(1)
Zr	7011(1)	667(1)	2795(1)	20(1)
C(11B)	6754(16)	-350(9)	3904(11)	28(3)
C(12B)	5634(18)	-346(8)	3334(10)	23(3)
C(13B)	5002(13)	307(12)	3459(10)	29(3)
C(14B)	5698(22)	702(7)	4070(12)	27(3)
C(15B)	6760(14)	300(12)	4349(9)	26(4)
C(25B)	7643(23)	-995(13)	4047(15)	93(7)
C(29B)	5291(22)	-1041(12)	2780(14)	84(6)
C(30B)	3737(31)	503(18)	3077(22)	139(12)
C(28B)	5302(25)	1354(13)	4541(15)	97(7)
C(16B)	7729(21)	397(12)	5118(13)	81(6)

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Table 8. Bond lengths [A] and angles [deg] for **2b**.

C(1)-C(2)	1.291(6)
C(1)-Si(2)	1.868(5)
C(1)-Zr	2.422(4)
C(2)-C(3)	1.337(6)
C(2)-Zr	2.305(4)
C(3)-C(4)	1.293(6)
C(3)-Zr	2.307(4)
C(4)-Si(1)	1.863(5)
C(4)-Zr	2.426(5)
C(5)-C(9)	1.389(8)
C(5)-C(6)	1.400(8)
C(5)-C(23)	1.513(9)
C(5)-Zr	2.546(5)
C(6)-C(7)	1.374(9)
C(6)-C(24)	1.530(8)
C(6)-Zr	2.548(5)
C(7)-C(8)	1.376(8)
C(7)-C(27)	1.507(8)
C(7)-Zr	2.566(5)
C(8)-C(9)	1.407(8)
C(8)-C(26)	1.525(8)
C(8)-Zr	2.565(5)
C(9)-C(10)	1.531(8)
C(9)-Zr	2.566(5)
C(11A)-C(12A)	1.429(12)
C(11A)-C(15A)	1.443(13)
C(11A)-C(25A)	1.475(12)
C(11A)-Zr	2.577(7)
C(12A)-C(13A)	1.443(10)
C(12A)-C(29A)	1.500(12)
C(12A)-Zr	2.609(7)
C(13A)-C(14A)	1.428(12)
C(13A)-C(30A)	1.495(12)
C(13A)-Zr	2.596(7)
C(14A)-C(15A)	1.409(12)
C(14A)-C(28A)	1.488(12)
C(14A)-Zr	2.588(7)
C(15A)-C(16A)	1.482(12)
C(15A)-Zr	2.556(7)
C(17)-Si(1)	1.855(6)
C(18)-Si(1)	1.875(6)
C(19)-Si(1)	1.870(6)
C(20)-Si(2)	1.853(7)
C(21)-Si(2)	1.847(7)
C(22)-Si(2)	1.854(8)
Zr-C(13B)	2.536(14)
Zr-C(12B)	2.543(13)
Zr-C(14B)	2.548(13)
C(11B)-C(15B)	1.38(2)
C(11B)-C(12B)	1.44(2)
C(11B)-C(25B)	1.51(3)
C(12B)-C(13B)	1.39(2)
C(12B)-C(29B)	1.57(2)
C(13B)-C(14B)	1.38(3)
C(13B)-C(30B)	1.47(3)

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C(14B)-C(15B)	1.39(2)
C(14B)-C(28B)	1.48(3)
C(15B)-C(16B)	1.54(3)
C(2)-C(1)-Si(2)	127.7(4)
C(2)-C(1)-Zr	69.2(3)
Si(2)-C(1)-Zr	163.1(3)
C(1)-C(2)-C(3)	152.5(4)
C(1)-C(2)-Zr	79.2(3)
C(3)-C(2)-Zr	73.2(2)
C(4)-C(3)-C(2)	152.3(4)
C(4)-C(3)-Zr	79.3(3)
C(2)-C(3)-Zr	73.1(2)
C(3)-C(4)-Si(1)	128.4(3)
C(3)-C(4)-Zr	69.2(3)
Si(1)-C(4)-Zr	162.4(2)
C(9)-C(5)-C(6)	107.3(5)
C(9)-C(5)-C(23)	124.6(7)
C(6)-C(5)-C(23)	127.5(7)
C(9)-C(5)-Zr	75.0(3)
C(6)-C(5)-Zr	74.1(3)
C(23)-C(5)-Zr	123.6(4)
C(7)-C(6)-C(5)	108.6(5)
C(7)-C(6)-C(24)	126.0(7)
C(5)-C(6)-C(24)	125.3(7)
C(7)-C(6)-Zr	75.1(3)
C(5)-C(6)-Zr	74.0(3)
C(24)-C(6)-Zr	120.8(4)
C(8)-C(7)-C(6)	108.6(5)
C(8)-C(7)-C(27)	125.6(7)
C(6)-C(7)-C(27)	125.0(7)
C(8)-C(7)-Zr	74.4(3)
C(6)-C(7)-Zr	73.7(3)
C(27)-C(7)-Zr	125.8(4)
C(7)-C(8)-C(9)	107.9(5)
C(7)-C(8)-C(26)	124.6(7)
C(9)-C(8)-C(26)	126.6(7)
C(7)-C(8)-Zr	74.5(3)
C(9)-C(8)-Zr	74.1(3)
C(26)-C(8)-Zr	126.1(4)
C(5)-C(9)-C(8)	107.7(5)
C(5)-C(9)-C(10)	124.1(7)
C(8)-C(9)-C(10)	126.9(7)
C(5)-C(9)-Zr	73.5(3)
C(8)-C(9)-Zr	74.1(3)
C(10)-C(9)-Zr	128.7(4)
C(12A)-C(11A)-C(15A)	107.9(7)
C(12A)-C(11A)-C(25A)	124.2(11)
C(15A)-C(11A)-C(25A)	127.2(11)
C(12A)-C(11A)-Zr	75.2(4)
C(15A)-C(11A)-Zr	72.9(4)
C(25A)-C(11A)-Zr	125.1(5)
C(11A)-C(12A)-C(13A)	107.8(7)
C(11A)-C(12A)-C(29A)	129.1(10)
C(13A)-C(12A)-C(29A)	122.8(9)
C(11A)-C(12A)-Zr	72.8(4)
C(13A)-C(12A)-Zr	73.4(4)
C(29A)-C(12A)-Zr	124.6(5)
C(14A)-C(13A)-C(12A)	107.1(6)
C(14A)-C(13A)-C(30A)	124.1(9)
C(12A)-C(13A)-C(30A)	128.1(9)

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C(14A)-C(13A)-Zr	73.7(4)
C(12A)-C(13A)-Zr	74.4(4)
C(30A)-C(13A)-Zr	124.7(5)
C(15A)-C(14A)-C(13A)	109.4(7)
C(15A)-C(14A)-C(28A)	124.2(11)
C(13A)-C(14A)-C(28A)	124.4(9)
C(15A)-C(14A)-Zr	72.8(4)
C(13A)-C(14A)-Zr	74.3(4)
C(28A)-C(14A)-Zr	132.4(6)
C(14A)-C(15A)-C(11A)	107.7(7)
C(14A)-C(15A)-C(16A)	126.9(11)
C(11A)-C(15A)-C(16A)	124.9(11)
C(14A)-C(15A)-Zr	75.4(4)
C(11A)-C(15A)-Zr	74.5(4)
C(16A)-C(15A)-Zr	122.7(5)
C(17)-Si(1)-C(4)	109.9(2)
C(17)-Si(1)-C(19)	107.6(3)
C(4)-Si(1)-C(19)	111.5(3)
C(17)-Si(1)-C(18)	108.1(3)
C(4)-Si(1)-C(18)	109.8(3)
C(19)-Si(1)-C(18)	109.8(4)
C(21)-Si(2)-C(20)	107.1(4)
C(21)-Si(2)-C(22)	110.4(5)
C(20)-Si(2)-C(22)	107.3(5)
C(21)-Si(2)-C(1)	109.1(3)
C(20)-Si(2)-C(1)	111.1(3)
C(22)-Si(2)-C(1)	111.8(3)
C(2)-Zr-C(3)	33.7(2)
C(2)-Zr-C(1)	31.6(2)
C(3)-Zr-C(1)	65.3(2)
C(2)-Zr-C(4)	65.3(2)
C(3)-Zr-C(4)	31.6(2)
C(1)-Zr-C(4)	96.8(2)
C(2)-Zr-C(13B)	105.9(5)
C(3)-Zr-C(13B)	92.8(4)
C(1)-Zr-C(13B)	113.8(5)
C(4)-Zr-C(13B)	79.5(3)
C(2)-Zr-C(12B)	82.4(3)
C(3)-Zr-C(12B)	84.7(4)
C(1)-Zr-C(12B)	82.6(4)
C(4)-Zr-C(12B)	88.2(5)
C(13B)-Zr-C(12B)	31.7(5)
C(2)-Zr-C(5)	96.7(2)
C(3)-Zr-C(5)	112.4(2)
C(1)-Zr-C(5)	80.3(2)
C(4)-Zr-C(5)	121.2(2)
C(13B)-Zr-C(5)	154.8(5)
C(12B)-Zr-C(5)	147.4(5)
C(2)-Zr-C(14B)	134.3(4)
C(3)-Zr-C(14B)	123.7(6)
C(1)-Zr-C(14B)	128.3(3)
C(4)-Zr-C(14B)	104.3(6)
C(13B)-Zr-C(14B)	31.4(6)
C(12B)-Zr-C(14B)	52.2(5)
C(5)-Zr-C(14B)	123.4(5)
C(2)-Zr-C(6)	83.8(2)
C(3)-Zr-C(6)	85.8(2)
C(1)-Zr-C(6)	83.7(2)
C(4)-Zr-C(6)	89.3(2)
C(13B)-Zr-C(6)	160.1(4)

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C(12B)-Zr-C(6)	165.6(3)
C(5)-Zr-C(6)	31.9(2)
C(14B)-Zr-C(6)	141.9(4)
C(2)-Zr-C(15A)	111.4(3)
C(3)-Zr-C(15A)	127.6(3)
C(1)-Zr-C(15A)	91.3(3)
C(4)-Zr-C(15A)	130.6(2)
C(5)-Zr-C(15A)	108.2(2)
C(6)-Zr-C(15A)	140.1(2)
C(2)-Zr-C(9)	128.2(2)
C(3)-Zr-C(9)	137.7(2)
C(1)-Zr-C(9)	108.4(2)
C(4)-Zr-C(9)	129.0(2)
C(13B)-Zr-C(9)	124.8(5)
C(12B)-Zr-C(9)	137.4(4)
C(5)-Zr-C(9)	31.5(2)
C(14B)-Zr-C(9)	93.9(5)
C(6)-Zr-C(9)	52.1(2)
C(15A)-Zr-C(9)	93.2(3)
C(2)-Zr-C(7)	104.5(2)
C(3)-Zr-C(7)	90.5(2)
C(1)-Zr-C(7)	113.6(2)
C(4)-Zr-C(7)	77.5(2)
C(13B)-Zr-C(7)	129.1(5)
C(12B)-Zr-C(7)	159.4(5)
C(5)-Zr-C(7)	52.3(2)
C(14B)-Zr-C(7)	116.8(3)
C(6)-Zr-C(7)	31.2(2)
C(15A)-Zr-C(7)	141.3(3)
C(9)-Zr-C(7)	52.0(2)
C(15B)-C(11B)-C(12B)	106.9(12)
C(15B)-C(11B)-C(25B)	128(2)
C(12B)-C(11B)-C(25B)	125(2)
C(15B)-C(11B)-Zr	74.9(7)
C(12B)-C(11B)-Zr	72.1(7)
C(25B)-C(11B)-Zr	124.2(12)
C(13B)-C(12B)-C(11B)	107.3(13)
C(13B)-C(12B)-C(29B)	133(2)
C(11B)-C(12B)-C(29B)	120(2)
C(13B)-C(12B)-Zr	73.9(8)
C(11B)-C(12B)-Zr	75.4(7)
C(29B)-C(12B)-Zr	120.7(11)
C(12B)-C(13B)-C(14B)	108.2(14)
C(12B)-C(13B)-C(30B)	126(2)
C(14B)-C(13B)-C(30B)	126(2)
C(12B)-C(13B)-Zr	74.4(8)
C(14B)-C(13B)-Zr	74.8(8)
C(30B)-C(13B)-Zr	122(2)
C(15B)-C(14B)-C(13B)	108.9(14)
C(15B)-C(14B)-C(28B)	121(2)
C(13B)-C(14B)-C(28B)	128(2)
C(15B)-C(14B)-Zr	76.2(8)
C(13B)-C(14B)-Zr	73.8(8)
C(28B)-C(14B)-Zr	128.0(12)
C(14B)-C(15B)-C(11B)	108.6(13)
C(14B)-C(15B)-C(16B)	132(2)
C(11B)-C(15B)-C(16B)	119(2)
C(14B)-C(15B)-Zr	72.6(8)
C(11B)-C(15B)-Zr	74.3(8)
C(16B)-C(15B)-Zr	127.8(11)

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Table 9. Anisotropic displacement parameters (A^2 x 10^3) for **2b**.
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(1)	33(3)	25(2)	31(2)	1(2)	4(2)	0(2)
C(2)	36(3)	21(2)	26(2)	-6(2)	7(2)	-1(2)
C(3)	30(3)	29(2)	19(2)	-5(2)	-1(2)	-7(2)
C(4)	29(3)	23(2)	26(2)	-1(2)	5(2)	-5(2)
C(5)	21(3)	25(3)	99(5)	9(3)	4(3)	-3(2)
C(6)	69(4)	45(3)	37(3)	-10(2)	29(3)	-37(3)
C(7)	48(4)	36(3)	62(4)	22(3)	-25(3)	-25(3)
C(8)	40(3)	26(3)	84(4)	-13(3)	25(3)	-10(2)
C(9)	69(4)	49(3)	28(3)	9(2)	-9(3)	-39(3)
C(23)	44(5)	64(5)	210(11)	10(6)	6(6)	0(3)
C(24)	181(10)	116(7)	72(5)	-38(5)	82(6)	-91(7)
C(27)	107(7)	57(4)	135(7)	56(5)	-64(6)	-38(4)
C(26)	89(6)	43(4)	170(9)	-23(5)	63(6)	-12(4)
C(10)	127(8)	143(8)	46(4)	19(4)	-26(4)	-91(6)
C(17)	46(4)	69(4)	53(3)	2(3)	-6(3)	-18(3)
C(18)	66(5)	86(5)	56(4)	36(4)	-25(3)	-19(4)
C(19)	60(5)	75(5)	113(6)	-22(4)	-23(4)	35(4)
C(20)	89(6)	38(3)	115(6)	-12(4)	40(5)	9(3)
C(21)	86(6)	68(5)	175(9)	17(5)	91(6)	31(4)
C(22)	186(11)	134(8)	125(8)	-54(7)	-89(8)	129(8)
Si(1)	31(1)	35(1)	43(1)	1(1)	-7(1)	2(1)
Si(2)	46(1)	34(1)	52(1)	-3(1)	3(1)	17(1)
Zr	23(1)	19(1)	19(1)	0(1)	4(1)	-3(1)

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

	x	y	z	U(eq)
H(23A)	10631(7)	583(4)	2395(7)	159
H(23B)	10308(7)	400(4)	3318(7)	159
H(23C)	11097(7)	1104(4)	3141(7)	159
H(24A)	9640(10)	855(5)	1209(5)	179
H(24B)	9194(10)	1619(5)	842(5)	179
H(24C)	8237(10)	962(5)	839(5)	179
H(27A)	6991(8)	2153(4)	962(6)	155
H(27B)	7065(8)	2845(4)	1551(6)	155
H(27C)	5954(8)	2281(4)	1599(6)	155
H(26A)	7032(8)	2568(4)	4054(6)	147
H(26B)	5977(8)	2514(4)	3308(6)	147
H(26C)	7091(8)	3075(4)	3261(6)	147
H(10A)	8653(9)	1947(5)	4654(4)	161
H(10B)	10016(9)	1912(5)	4337(4)	161
H(10C)	9328(9)	1187(5)	4573(4)	161
H(25A)	7094(10)	-1367(5)	3661(6)	91
H(25B)	6305(10)	-1261(5)	2793(6)	91
H(25C)	5625(10)	-1488(5)	3595(6)	91
H(29A)	3328(9)	172(6)	2643(6)	92
H(29B)	3482(9)	-634(6)	2981(6)	92
H(29C)	4177(9)	-387(6)	2194(6)	92
H(30A)	3466(9)	1184(5)	3265(6)	88
H(30B)	4511(9)	1753(5)	3575(6)	88
H(30C)	3772(9)	1321(5)	4234(6)	88
H(28A)	5905(9)	1617(5)	4940(6)	82
H(28B)	7317(9)	1354(5)	5052(6)	82
H(28C)	6281(9)	950(5)	5531(6)	82
H(16A)	8222(9)	-721(5)	4538(6)	88
H(16B)	7780(9)	-283(5)	5311(6)	88
H(16C)	8665(9)	92(5)	4693(6)	88
H(17A)	2292(6)	519(3)	262(4)	84
H(17B)	2693(6)	160(3)	1139(4)	84
H(17C)	3432(6)	-31(3)	350(4)	84
H(18A)	5240(7)	1878(4)	-8(4)	106
H(18B)	3958(7)	1640(4)	-491(4)	106
H(18C)	5098(7)	1090(4)	-400(4)	106
H(19A)	3737(7)	2267(4)	1535(5)	126
H(19B)	2866(7)	1669(4)	1899(5)	126
H(19C)	2496(7)	2016(4)	1011(5)	126
H(20A)	7917(7)	-2130(3)	2318(5)	119
H(20B)	9047(7)	-2387(3)	1809(5)	119
H(20C)	7921(7)	-1944(3)	1355(5)	119
H(21A)	10722(8)	-475(4)	1376(6)	158
H(21B)	9736(8)	-875(4)	747(6)	158
H(21C)	10861(8)	-1317(4)	1202(6)	158
H(22A)	9772(11)	-1397(5)	3579(6)	231
H(22B)	10789(11)	-859(5)	3265(6)	231
H(22C)	10852(11)	-1697(5)	3053(6)	231
H(25D)	7415(23)	-1372(13)	3641(15)	139
H(25E)	7583(23)	-1185(13)	4606(15)	139
H(25F)	8496(23)	-839(13)	3985(15)	139

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H(29D)	5966(22)	-1392(12)	2852(14)	125
H(29E)	5173(22)	-900(12)	2197(14)	125
H(29F)	4525(22)	-1255(12)	2952(14)	125
H(30D)	3514(31)	984(18)	3263(22)	209
H(30E)	3128(31)	153(18)	3245(22)	209
H(30F)	3744(31)	501(18)	2473(22)	209
H(28D)	4553(25)	1562(13)	4255(15)	145
H(28E)	5969(25)	1712(13)	4571(15)	145
H(28F)	5127(25)	1211(13)	5101(15)	145
H(16D)	8353(21)	15(12)	5119(13)	121
H(16E)	7302(21)	371(12)	5628(13)	121
H(16F)	8136(21)	866(12)	5085(13)	121

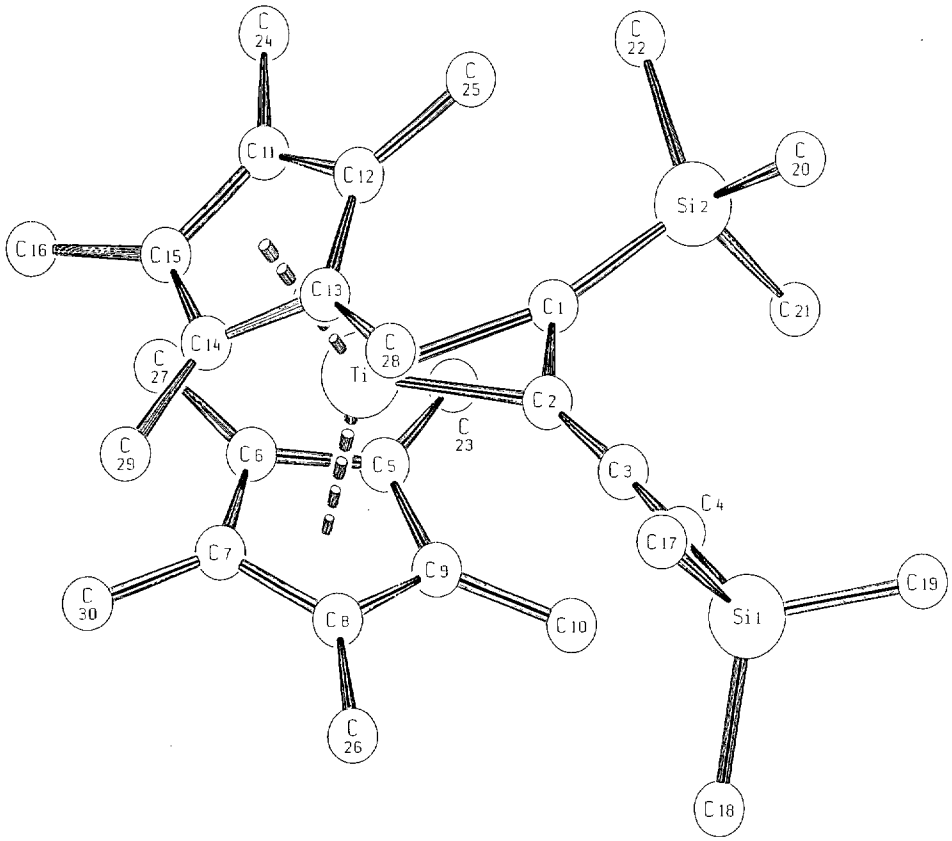


Figure 3: Molecular structure of **3**

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Table 11. Crystal data and structure refinement for **3**.

Identification code	203
Empirical formula	C30 H48 Si2 Ti
Formula weight	512.76
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a= 11.237(2) A alpha= 76.36(3) deg. b= 11.534(2) A beta= 67.09(3) deg. c= 13.691(3) A gamma= 74.46(3) deg.
Temperature for cell	200(2)
Number for reflecions for cell	5000
Theta for cell determination	4 to 20 deg
Volume	1557.3(5) A^3
Z	2
Density (calculated)	1.093 Mg/m^3
Absorption coefficient	0.367 mm^-1
F(000)	556
Crystal colour	red
Crystal description	prism
Crystal size	0.5 x 0.4 x 0.3 mm
Temperature	200(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	1.85 to 24.27 deg.

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Index ranges	-11<=h<=12, -12<=k<=13, 0<=l<=15
Reflections collected	4643
Independent reflections	4643 [R(int) = 0.0000]
Reflections unique	4643
Reflections observed	3685
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	4643 / 0 / 298
Final R indices [I>2sigma(I)]	R1 = 0.0442, wR2 = 0.1280
R indices (all data)	R1 = 0.0564, wR2 = 0.1355
Goodness-for-fit on F^2(all)	0.999
Goodness-for-fit on F^2(obs)	1.067
Shift/esd(max)	-0.001
Shift/esd(mean)	0.000

Weighting scheme

calc w=1/[\s^2^(Fo^2^)+(0.0944P)^2^+0.0247P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.350 and -0.314 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

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Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**. U(eq) is defined as one third for the trace for the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6478(2)	1622(2)	1983(2)	28(1)
C(2)	7238(2)	1265(2)	2565(2)	29(1)
C(3)	7878(3)	214(2)	3057(2)	33(1)
C(4)	8513(3)	-646(3)	3465(3)	44(1)
C(5)	4675(3)	3718(3)	3213(2)	34(1)
C(6)	5227(3)	4767(2)	2924(2)	37(1)
C(7)	6097(3)	4602(3)	3480(3)	41(1)
C(8)	6119(3)	3409(3)	4083(2)	42(1)
C(9)	5198(3)	2893(3)	3950(2)	36(1)
C(10)	4784(3)	1712(3)	4547(3)	55(1)
C(11)	8013(3)	3942(3)	367(2)	35(1)
C(12)	8735(3)	2745(2)	520(2)	31(1)
C(13)	9325(2)	2686(2)	1266(2)	33(1)
C(14)	9035(3)	3856(3)	1538(2)	35(1)
C(15)	8241(3)	4651(2)	969(2)	37(1)
C(16)	7957(4)	6023(3)	829(3)	61(1)
C(17)	11349(3)	-1580(4)	3109(3)	67(1)
C(18)	9340(4)	-1671(4)	5377(3)	72(1)
C(19)	9459(6)	-3344(4)	3927(6)	111(2)
C(20)	6945(4)	-710(3)	1108(4)	82(2)
C(21)	4275(4)	194(4)	2561(4)	88(2)
C(22)	5265(6)	1595(4)	328(4)	95(2)
C(23)	3605(3)	3582(3)	2862(3)	54(1)
C(24)	7222(4)	4393(4)	-366(3)	60(1)
C(25)	8914(3)	1731(3)	-72(3)	53(1)
C(26)	6881(4)	2828(4)	4831(3)	73(1)
C(27)	4742(4)	5928(3)	2266(3)	64(1)
C(28)	10280(3)	1629(3)	1603(3)	51(1)
C(29)	9708(3)	4212(4)	2163(3)	57(1)
C(30)	6659(4)	5565(4)	3636(4)	70(1)
Si(1)	9663(1)	-1822(1)	3972(1)	42(1)
Si(2)	5746(1)	714(1)	1494(1)	38(1)
Ti	6984(1)	3156(1)	2219(1)	24(1)

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Table 13. Bond lengths [A] and angles [deg] for **3**.

C(1)-C(2)	1.311(4)
C(1)-Si(2)	1.856(3)
C(1)-Ti	2.123(3)
C(2)-C(3)	1.401(4)
C(2)-Ti	2.085(3)
C(3)-C(4)	1.215(4)
C(4)-Si(1)	1.819(3)
C(5)-C(9)	1.407(4)
C(5)-C(6)	1.410(4)
C(5)-C(23)	1.512(4)
C(5)-Ti	2.402(3)
C(6)-C(7)	1.409(4)
C(6)-C(27)	1.525(4)
C(6)-Ti	2.383(3)
C(7)-C(8)	1.427(5)
C(7)-C(30)	1.507(4)
C(7)-Ti	2.426(3)
C(8)-C(9)	1.409(4)
C(8)-C(26)	1.511(4)
C(8)-Ti	2.410(3)
C(9)-C(10)	1.502(4)
C(9)-Ti	2.454(3)
C(11)-C(12)	1.415(4)
C(11)-C(15)	1.417(4)
C(11)-C(24)	1.506(4)
C(11)-Ti	2.404(3)
C(12)-C(13)	1.400(4)
C(12)-C(25)	1.504(4)
C(12)-Ti	2.442(3)
C(13)-C(14)	1.404(4)
C(13)-C(28)	1.507(4)
C(13)-Ti	2.411(3)
C(14)-C(15)	1.418(4)
C(14)-C(29)	1.518(4)
C(14)-Ti	2.408(3)
C(15)-C(16)	1.509(4)
C(15)-Ti	2.435(3)
C(17)-Si(1)	1.857(4)
C(18)-Si(1)	1.856(4)
C(19)-Si(1)	1.847(4)
C(20)-Si(2)	1.860(4)
C(21)-Si(2)	1.861(4)
C(22)-Si(2)	1.867(4)
C(2)-C(1)-Si(2)	130.0(2)
C(2)-C(1)-Ti	70.3(2)
Si(2)-C(1)-Ti	159.7(2)
C(1)-C(2)-C(3)	141.9(3)
C(1)-C(2)-Ti	73.4(2)
C(3)-C(2)-Ti	144.6(2)
C(4)-C(3)-C(2)	174.7(3)
C(3)-C(4)-Si(1)	171.7(3)
C(9)-C(5)-C(6)	108.3(3)
C(9)-C(5)-C(23)	126.7(3)
C(6)-C(5)-C(23)	124.7(3)
C(9)-C(5)-Ti	75.2(2)

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C(6)-C(5)-Ti	72.1(2)
C(23)-C(5)-Ti	123.2(2)
C(7)-C(6)-C(5)	108.5(3)
C(7)-C(6)-C(27)	127.9(3)
C(5)-C(6)-C(27)	122.9(3)
C(7)-C(6)-Ti	74.6(2)
C(5)-C(6)-Ti	73.6(2)
C(27)-C(6)-Ti	125.5(2)
C(6)-C(7)-C(8)	107.0(3)
C(6)-C(7)-C(30)	127.3(3)
C(8)-C(7)-C(30)	124.3(3)
C(6)-C(7)-Ti	71.3(2)
C(8)-C(7)-Ti	72.2(2)
C(30)-C(7)-Ti	132.2(2)
C(9)-C(8)-C(7)	108.3(3)
C(9)-C(8)-C(26)	124.7(3)
C(7)-C(8)-C(26)	126.7(3)
C(9)-C(8)-Ti	74.9(2)
C(7)-C(8)-Ti	73.4(2)
C(26)-C(8)-Ti	122.5(2)
C(5)-C(9)-C(8)	107.7(3)
C(5)-C(9)-C(10)	126.2(3)
C(8)-C(9)-C(10)	125.9(3)
C(5)-C(9)-Ti	71.1(2)
C(8)-C(9)-Ti	71.5(2)
C(10)-C(9)-Ti	126.0(2)
C(12)-C(11)-C(15)	107.8(2)
C(12)-C(11)-C(24)	125.7(3)
C(15)-C(11)-C(24)	126.4(3)
C(12)-C(11)-Ti	74.5(2)
C(15)-C(11)-Ti	74.2(2)
C(24)-C(11)-Ti	120.4(2)
C(13)-C(12)-C(11)	108.4(3)
C(13)-C(12)-C(25)	125.6(3)
C(11)-C(12)-C(25)	125.9(3)
C(13)-C(12)-Ti	72.0(2)
C(11)-C(12)-Ti	71.6(2)
C(25)-C(12)-Ti	125.3(2)
C(14)-C(13)-C(12)	107.9(2)
C(14)-C(13)-C(28)	124.3(3)
C(12)-C(13)-C(28)	127.2(3)
C(14)-C(13)-Ti	73.0(2)
C(12)-C(13)-Ti	74.4(2)
C(28)-C(13)-Ti	125.5(2)
C(13)-C(14)-C(15)	108.7(3)
C(13)-C(14)-C(29)	123.3(3)
C(15)-C(14)-C(29)	126.9(3)
C(13)-C(14)-Ti	73.2(2)
C(15)-C(14)-Ti	74.0(2)
C(29)-C(14)-Ti	128.2(2)
C(14)-C(15)-C(11)	107.1(2)
C(14)-C(15)-C(16)	126.0(3)
C(11)-C(15)-C(16)	125.5(3)
C(14)-C(15)-Ti	72.0(2)
C(11)-C(15)-Ti	71.8(2)
C(16)-C(15)-Ti	131.8(2)
C(4)-Si(1)-C(19)	110.1(2)
C(4)-Si(1)-C(17)	107.2(2)
C(19)-Si(1)-C(17)	110.7(3)
C(4)-Si(1)-C(18)	109.1(2)

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C(19)-Si(1)-C(18)	109.5(3)
C(17)-Si(1)-C(18)	110.1(2)
C(21)-Si(2)-C(1)	112.2(2)
C(21)-Si(2)-C(20)	104.8(2)
C(1)-Si(2)-C(20)	109.6(2)
C(21)-Si(2)-C(22)	108.7(2)
C(1)-Si(2)-C(22)	111.4(2)
C(20)-Si(2)-C(22)	109.9(3)
C(2)-Ti-C(1)	36.30(10)
C(2)-Ti-C(6)	133.29(10)
C(1)-Ti-C(6)	117.44(10)
C(2)-Ti-C(5)	100.34(10)
C(1)-Ti-C(5)	85.18(10)
C(6)-Ti-C(5)	34.27(10)
C(2)-Ti-C(11)	115.00(11)
C(1)-Ti-C(11)	98.18(11)
C(6)-Ti-C(11)	104.90(10)
C(5)-Ti-C(11)	123.83(10)
C(2)-Ti-C(8)	93.27(12)
C(1)-Ti-C(8)	111.76(11)
C(6)-Ti-C(8)	56.81(11)
C(5)-Ti-C(8)	56.40(10)
C(11)-Ti-C(8)	149.56(11)
C(2)-Ti-C(14)	112.69(10)
C(1)-Ti-C(14)	131.81(10)
C(6)-Ti-C(14)	109.06(10)
C(5)-Ti-C(14)	142.77(10)
C(11)-Ti-C(14)	56.55(10)
C(8)-Ti-C(14)	103.45(11)
C(2)-Ti-C(13)	82.14(10)
C(1)-Ti-C(13)	98.28(10)
C(6)-Ti-C(13)	142.67(10)
C(5)-Ti-C(13)	176.45(10)
C(11)-Ti-C(13)	56.62(10)
C(8)-Ti-C(13)	121.14(10)
C(14)-Ti-C(13)	33.87(10)
C(2)-Ti-C(7)	127.59(11)
C(1)-Ti-C(7)	137.96(10)
C(6)-Ti-C(7)	34.05(11)
C(5)-Ti-C(7)	56.55(10)
C(11)-Ti-C(7)	116.61(11)
C(8)-Ti-C(7)	34.33(11)
C(14)-Ti-C(7)	88.76(10)
C(13)-Ti-C(7)	119.92(10)
C(2)-Ti-C(15)	137.10(10)
C(1)-Ti-C(15)	131.87(11)
C(6)-Ti-C(15)	89.60(10)
C(5)-Ti-C(15)	121.56(10)
C(11)-Ti-C(15)	34.04(11)
C(8)-Ti-C(15)	116.37(12)
C(14)-Ti-C(15)	34.04(10)
C(13)-Ti-C(15)	56.47(9)
C(7)-Ti-C(15)	86.86(11)
C(2)-Ti-C(12)	83.74(10)
C(1)-Ti-C(12)	80.19(10)
C(6)-Ti-C(12)	138.85(10)
C(5)-Ti-C(12)	148.89(10)
C(11)-Ti-C(12)	33.95(9)
C(8)-Ti-C(12)	154.67(10)
C(14)-Ti-C(12)	55.73(10)

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C(13)-Ti-C(12)	33.54(10)
C(7)-Ti-C(12)	141.67(10)
C(15)-Ti-C(12)	55.97(10)
C(2)-Ti-C(9)	78.68(11)
C(1)-Ti-C(9)	82.55(11)
C(6)-Ti-C(9)	56.33(10)
C(5)-Ti-C(9)	33.67(10)
C(11)-Ti-C(9)	157.49(9)
C(8)-Ti-C(9)	33.66(10)
C(14)-Ti-C(9)	137.08(11)
C(13)-Ti-C(9)	145.77(10)
C(7)-Ti-C(9)	56.20(10)
C(15)-Ti-C(9)	142.36(10)
C(12)-Ti-C(9)	161.67(10)

Symmetry transformations used to generate equivalent atoms:

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Table 14. 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(1)	25(1)	29(1)	27(2)	-5(1)	-4(1)	-4(1)
C(2)	22(1)	29(1)	30(2)	-3(1)	-4(1)	-4(1)
C(3)	27(1)	31(2)	38(2)	-1(1)	-9(1)	-7(1)
C(4)	33(2)	42(2)	50(2)	3(2)	-15(1)	-4(1)
C(5)	22(1)	43(2)	32(2)	-10(1)	-5(1)	0(1)
C(6)	33(2)	33(2)	34(2)	-11(1)	-3(1)	5(1)
C(7)	32(2)	51(2)	36(2)	-25(1)	5(1)	-11(1)
C(8)	27(1)	69(2)	24(2)	-18(1)	-5(1)	4(1)
C(9)	30(1)	41(2)	25(2)	-5(1)	0(1)	-3(1)
C(10)	51(2)	53(2)	39(2)	4(2)	2(2)	-9(2)
C(11)	30(1)	43(2)	25(2)	5(1)	-5(1)	-9(1)
C(12)	28(1)	34(2)	24(2)	-7(1)	4(1)	-9(1)
C(13)	21(1)	39(2)	28(2)	-2(1)	0(1)	-7(1)
C(14)	29(1)	47(2)	26(2)	-6(1)	1(1)	-18(1)
C(15)	33(2)	27(1)	35(2)	-1(1)	4(1)	-7(1)
C(16)	59(2)	36(2)	62(3)	-4(2)	7(2)	-13(2)
C(17)	39(2)	99(3)	53(3)	-21(2)	-19(2)	15(2)
C(18)	50(2)	109(3)	54(3)	-6(2)	-20(2)	-15(2)
C(19)	150(5)	39(2)	180(6)	-8(3)	-109(5)	-5(3)
C(20)	65(3)	57(2)	140(5)	-53(3)	-35(3)	-5(2)
C(21)	70(3)	107(4)	97(4)	-37(3)	1(2)	-60(3)
C(22)	152(5)	74(3)	115(4)	6(3)	-104(4)	-39(3)
C(23)	29(2)	68(2)	66(3)	-21(2)	-19(2)	1(2)
C(24)	55(2)	77(2)	41(2)	13(2)	-23(2)	-14(2)
C(25)	51(2)	57(2)	46(2)	-25(2)	-1(2)	-14(2)
C(26)	47(2)	132(4)	38(2)	-21(2)	-21(2)	2(2)
C(27)	51(2)	40(2)	74(3)	-2(2)	-11(2)	11(2)
C(28)	28(2)	54(2)	57(2)	3(2)	-10(2)	-3(1)
C(29)	43(2)	84(3)	53(3)	-25(2)	-8(2)	-26(2)
C(30)	50(2)	92(3)	73(3)	-55(2)	6(2)	-26(2)
Si(1)	39(1)	36(1)	57(1)	-5(1)	-29(1)	2(1)
Si(2)	38(1)	34(1)	47(1)	-8(1)	-18(1)	-9(1)
Ti	21(1)	25(1)	22(1)	-4(1)	-5(1)	-3(1)

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Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(10A)	5299(3)	1322(3)	4996(3)	83
H(10B)	4920(3)	1192(3)	4045(3)	83
H(10C)	3868(3)	1870(3)	4983(3)	83
H(16A)	7392(4)	6343(3)	413(3)	92
H(16B)	8769(4)	6312(3)	466(3)	92
H(16C)	7531(4)	6287(3)	1520(3)	92
H(17A)	11985(3)	-2188(4)	3355(3)	100
H(17B)	11437(3)	-787(4)	3146(3)	100
H(17C)	11498(3)	-1640(4)	2382(3)	100
H(18A)	9945(4)	-2290(4)	5649(3)	108
H(18B)	8453(4)	-1761(4)	5810(3)	108
H(18C)	9456(4)	-884(4)	5399(3)	108
H(19A)	10070(6)	-3957(4)	4196(6)	166
H(19B)	9625(6)	-3421(4)	3200(6)	166
H(19C)	8575(6)	-3442(4)	4362(6)	166
H(20A)	7736(4)	-509(3)	555(4)	123
H(20B)	6568(4)	-1174(3)	849(4)	123
H(20C)	7149(4)	-1180(3)	1722(4)	123
H(21A)	3929(4)	-271(4)	2275(4)	132
H(21B)	3615(4)	888(4)	2811(4)	132
H(21C)	4524(4)	-304(4)	3146(4)	132
H(22A)	6017(6)	1869(4)	-228(4)	143
H(22B)	4582(6)	2285(4)	552(4)	143
H(22C)	4949(6)	1084(4)	61(4)	143
H(23A)	3434(3)	4278(3)	2355(3)	81
H(23B)	2815(3)	3524(3)	3475(3)	81
H(23C)	3886(3)	2859(3)	2535(3)	81
H(24A)	6830(4)	5237(4)	-329(3)	89
H(24B)	6542(4)	3932(4)	-148(3)	89
H(24C)	7790(4)	4296(4)	-1089(3)	89
H(25A)	8402(3)	1998(3)	-534(3)	79
H(25B)	8625(3)	1041(3)	433(3)	79
H(25C)	9828(3)	1506(3)	-494(3)	79
H(26A)	7445(4)	3350(4)	4783(3)	109
H(26B)	7406(4)	2057(4)	4631(3)	109
H(26C)	6277(4)	2709(4)	5553(3)	109
H(27A)	4155(4)	5770(3)	1979(3)	96
H(27B)	5481(4)	6195(3)	1688(3)	96
H(27C)	4285(4)	6549(3)	2715(3)	96
H(28A)	10318(3)	925(3)	1325(3)	77
H(28B)	9992(3)	1461(3)	2372(3)	77
H(28C)	11139(3)	1828(3)	1328(3)	77
H(29A)	9362(3)	5050(4)	2259(3)	86
H(29B)	10639(3)	4100(4)	1774(3)	86
H(29C)	9547(3)	3710(4)	2851(3)	86
H(30A)	7224(4)	5196(4)	4048(4)	105
H(30B)	5954(4)	6161(4)	4010(4)	105
H(30C)	7158(4)	5951(4)	2950(4)	105

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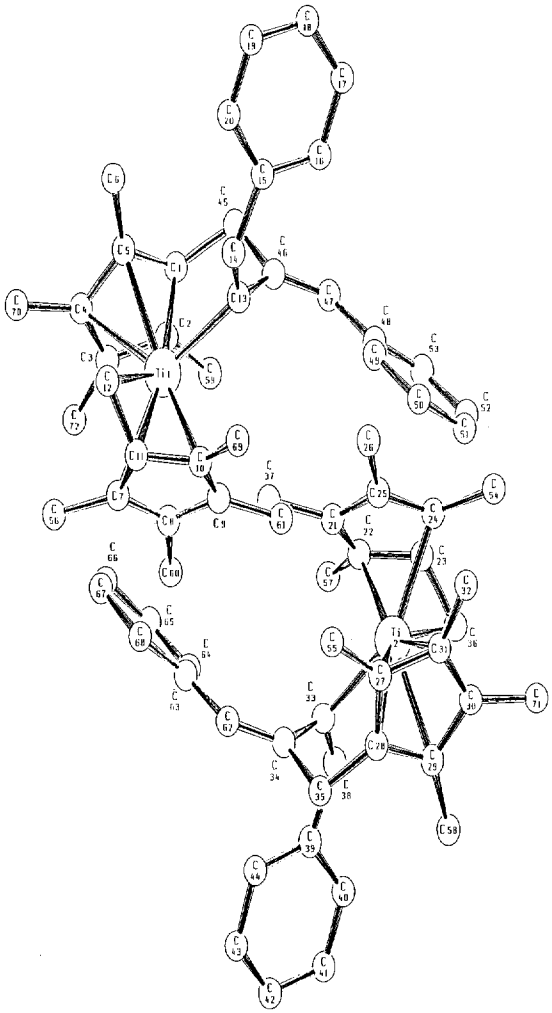


Figure 4: Molecular structure of **4**

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Table 16. Crystal data and structure refinement for **4**.

Identification code	201
Empirical formula	C36 H40 Ti
Formula weight	520.58
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a= 26.632(5) A alpha= 90 deg. b= 8.931(2) A beta= 109.16(3) deg. c= 25.953(5) A gamma= 90 deg.
Temperature for cell	293(2)
Number for reflecions for cell	5000
Theta for cell determination	4 to 20 deg
Volume	5831(2) A^3
Z	8
Density (calculated)	1.186 Mg/m^3
Absorption coefficient	0.315 mm^-1
F(000)	2224
Crystal colour	green
Crystal description	prism
Crystal size	0.4 x 0.3 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	1.59 to 21.05 deg.

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Index ranges	0<=h<=26, -8<=k<=8, -26<=l<=24
Reflections collected	11175
Independent reflections	6155 [R(int) = 0.0412]
Reflections unique	6155
Reflections observed	3793
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	6155 / 0 / 667
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1023
R indices (all data)	R1 = 0.0831, wR2 = 0.1108
Goodness-for-fit on F^2(all)	0.861
Goodness-for-fit on F^2(obs)	1.051
Shift/esd(max)	-0.002
Shift/esd(mean)	0.000

Weighting scheme

calc w=1/[\s^2^(Fo^2^)+(0.0557P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.244 and -0.248 e.A^-3
Diff. density rms	0.047
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

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Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**. U(eq) is defined as one third for the trace for the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	9250(2)	4378(5)	10750(2)	36(1)
C(2)	9014(2)	4357(5)	11166(2)	42(1)
C(3)	9307(2)	3338(5)	11570(2)	43(1)
C(4)	9707(2)	2692(5)	11397(2)	45(1)
C(5)	9671(2)	3339(5)	10887(2)	39(1)
C(6)	10043(2)	3031(6)	10568(2)	58(2)
C(7)	8618(2)	167(5)	11219(2)	43(1)
C(8)	8175(2)	1113(5)	11112(2)	41(1)
C(9)	7924(2)	1195(5)	10535(2)	42(1)
C(10)	8197(2)	274(5)	10283(2)	36(1)
C(11)	8657(2)	-331(5)	10704(2)	41(1)
C(12)	9175(2)	-322(5)	10640(2)	53(1)
C(13)	8669(2)	2897(5)	9861(2)	33(1)
C(14)	8887(2)	2264(5)	9526(2)	39(1)
C(15)	9031(2)	2976(5)	9072(2)	38(1)
C(16)	8737(2)	4068(5)	8727(2)	49(1)
C(17)	8914(2)	4721(6)	8329(2)	55(2)
C(18)	9393(2)	4293(6)	8281(2)	54(1)
C(19)	9685(2)	3198(6)	8611(2)	56(1)
C(20)	9510(2)	2537(5)	9003(2)	47(1)
C(21)	7141(2)	8350(5)	11526(2)	36(1)
C(22)	6820(2)	9316(5)	11707(2)	35(1)
C(23)	6386(2)	9807(5)	11241(2)	40(1)
C(24)	6484(2)	9229(5)	10764(2)	41(1)
C(25)	6940(2)	8311(5)	10943(2)	40(1)
C(26)	7219(2)	7573(6)	10587(2)	62(2)
C(27)	6098(2)	5063(5)	10887(2)	41(1)
C(28)	5819(2)	5077(5)	11264(2)	37(1)
C(29)	5384(2)	6079(5)	11072(2)	38(1)
C(30)	5387(2)	6639(5)	10562(2)	47(1)
C(31)	5819(2)	6011(6)	10445(2)	48(1)
C(32)	5904(2)	6041(6)	9893(2)	78(2)
C(33)	6325(2)	6771(5)	12129(2)	34(1)
C(34)	6472(2)	5179(5)	12185(2)	34(1)
C(35)	6006(2)	4285(5)	11809(2)	45(1)
C(36)	5853(2)	9831(5)	11251(2)	51(1)
C(37)	7653(2)	7636(6)	11861(2)	57(1)
C(38)	6064(2)	7458(5)	12424(2)	41(1)
C(39)	5890(2)	6873(5)	12874(2)	38(1)
C(40)	5453(2)	7510(6)	12965(2)	57(1)
C(41)	5261(2)	6976(7)	13363(2)	71(2)
C(42)	5503(2)	5793(7)	13683(2)	67(2)
C(43)	5932(2)	5151(6)	13605(2)	66(2)
C(44)	6129(2)	5676(6)	13207(2)	55(1)
C(45)	9039(2)	5297(5)	10234(2)	48(1)
C(46)	8548(2)	4500(5)	9859(2)	35(1)
C(47)	8087(2)	5262(5)	9634(2)	41(1)
C(48)	7567(2)	4756(5)	9264(2)	39(1)
C(49)	7492(2)	3443(6)	8961(2)	50(1)
C(50)	6993(2)	3023(6)	8619(2)	64(2)
C(51)	6562(2)	3910(8)	8564(2)	75(2)

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C(52)	6623(2)	5236(8)	8850(2)	73(2)
C(53)	7125(2)	5656(6)	9191(2)	56(2)
C(54)	6176(2)	9677(6)	10180(2)	61(2)
C(55)	6561(2)	4061(5)	10916(2)	62(2)
C(56)	8968(2)	-404(6)	11770(2)	64(2)
C(57)	6942(2)	9895(5)	12283(2)	53(1)
C(58)	4979(2)	6430(6)	11341(2)	59(2)
C(59)	8572(2)	5376(6)	11198(2)	65(2)
C(60)	7944(2)	1780(6)	11523(2)	66(2)
C(61)	7417(2)	2012(6)	10252(2)	66(2)
C(62)	6943(2)	4503(5)	12443(2)	41(1)
C(63)	7440(2)	5141(5)	12808(2)	38(1)
C(64)	7460(2)	6434(6)	13110(2)	45(1)
C(65)	7946(2)	7023(6)	13436(2)	59(2)
C(66)	8409(2)	6305(8)	13471(2)	69(2)
C(67)	8398(2)	5010(8)	13187(2)	70(2)
C(68)	7915(2)	4409(6)	12862(2)	57(2)
C(69)	8021(2)	-184(5)	9690(2)	56(2)
C(70)	10150(2)	1663(6)	11720(2)	71(2)
C(71)	4954(2)	7589(6)	10180(2)	75(2)
C(72)	9280(2)	3230(6)	12145(2)	75(2)
Ti(1)	8858(1)	2001(1)	10712(1)	32(1)
Ti(2)	6196(1)	7495(1)	11274(1)	33(1)

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Table 18. Bond lengths [A] and angles [deg] for **4**.

C(1)-C(5)	1.407(6)
C(1)-C(2)	1.416(6)
C(1)-C(45)	1.513(6)
C(1)-Ti(1)	2.354(4)
C(2)-C(3)	1.414(6)
C(2)-C(59)	1.513(6)
C(2)-Ti(1)	2.381(4)
C(3)-C(4)	1.408(6)
C(3)-C(72)	1.521(6)
C(3)-Ti(1)	2.463(4)
C(4)-C(5)	1.418(6)
C(4)-C(70)	1.513(6)
C(4)-Ti(1)	2.454(4)
C(5)-C(6)	1.510(6)
C(5)-Ti(1)	2.383(4)
C(7)-C(8)	1.405(6)
C(7)-C(11)	1.444(6)
C(7)-C(56)	1.516(6)
C(7)-Ti(1)	2.317(4)
C(8)-C(9)	1.429(6)
C(8)-C(60)	1.514(6)
C(8)-Ti(1)	2.501(4)
C(9)-C(10)	1.394(6)
C(9)-C(61)	1.498(6)
C(9)-Ti(1)	2.481(4)
C(10)-C(11)	1.452(6)
C(10)-C(69)	1.509(6)
C(10)-Ti(1)	2.329(4)
C(11)-C(12)	1.444(6)
C(11)-Ti(1)	2.148(4)
C(12)-Ti(1)	2.271(5)
C(13)-C(14)	1.322(6)
C(13)-C(46)	1.467(6)
C(13)-Ti(1)	2.246(4)
C(14)-C(15)	1.494(6)
C(15)-C(16)	1.381(6)
C(15)-C(20)	1.400(6)
C(16)-C(17)	1.396(6)
C(17)-C(18)	1.377(6)
C(18)-C(19)	1.362(7)
C(19)-C(20)	1.384(6)
C(21)-C(22)	1.401(6)
C(21)-C(25)	1.431(6)
C(21)-C(37)	1.497(6)
C(21)-Ti(2)	2.503(4)
C(22)-C(23)	1.440(6)
C(22)-C(57)	1.515(6)
C(22)-Ti(2)	2.332(4)
C(23)-C(36)	1.429(6)
C(23)-C(24)	1.442(6)
C(23)-Ti(2)	2.135(4)
C(24)-C(25)	1.411(6)
C(24)-C(54)	1.520(6)
C(24)-Ti(2)	2.326(4)
C(25)-C(26)	1.515(6)
C(25)-Ti(2)	2.511(4)

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C(27)-C(28)	1.409(6)
C(27)-C(31)	1.424(6)
C(27)-C(55)	1.505(6)
C(27)-Ti(2)	2.371(4)
C(28)-C(29)	1.418(6)
C(28)-C(35)	1.512(6)
C(28)-Ti(2)	2.377(4)
C(29)-C(30)	1.419(6)
C(29)-C(58)	1.499(6)
C(29)-Ti(2)	2.410(4)
C(30)-C(31)	1.398(6)
C(30)-C(71)	1.512(6)
C(30)-Ti(2)	2.456(5)
C(31)-C(32)	1.521(7)
C(31)-Ti(2)	2.446(5)
C(33)-C(38)	1.341(6)
C(33)-C(34)	1.469(6)
C(33)-Ti(2)	2.226(4)
C(34)-C(62)	1.355(6)
C(34)-C(35)	1.528(6)
C(36)-Ti(2)	2.272(5)
C(38)-C(39)	1.485(6)
C(39)-C(40)	1.382(6)
C(39)-C(44)	1.390(6)
C(40)-C(41)	1.380(7)
C(41)-C(42)	1.367(7)
C(42)-C(43)	1.350(7)
C(43)-C(44)	1.385(6)
C(45)-C(46)	1.525(6)
C(46)-C(47)	1.357(6)
C(47)-C(48)	1.474(6)
C(48)-C(53)	1.387(6)
C(48)-C(49)	1.390(6)
C(49)-C(50)	1.386(6)
C(50)-C(51)	1.363(7)
C(51)-C(52)	1.378(8)
C(52)-C(53)	1.390(7)
C(62)-C(63)	1.468(6)
C(63)-C(68)	1.391(6)
C(63)-C(64)	1.387(6)
C(64)-C(65)	1.395(6)
C(65)-C(66)	1.366(7)
C(66)-C(67)	1.366(7)
C(67)-C(68)	1.393(7)

C(5)-C(1)-C(2)	108.3(4)
C(5)-C(1)-C(45)	127.9(4)
C(2)-C(1)-C(45)	123.6(4)
C(5)-C(1)-Ti(1)	73.8(3)
C(2)-C(1)-Ti(1)	73.6(3)
C(45)-C(1)-Ti(1)	114.9(3)
C(1)-C(2)-C(3)	107.4(4)
C(1)-C(2)-C(59)	125.6(5)
C(3)-C(2)-C(59)	126.6(5)
C(1)-C(2)-Ti(1)	71.6(3)
C(3)-C(2)-Ti(1)	76.3(3)
C(59)-C(2)-Ti(1)	123.1(3)
C(4)-C(3)-C(2)	108.6(4)
C(4)-C(3)-C(72)	124.8(5)
C(2)-C(3)-C(72)	125.2(5)