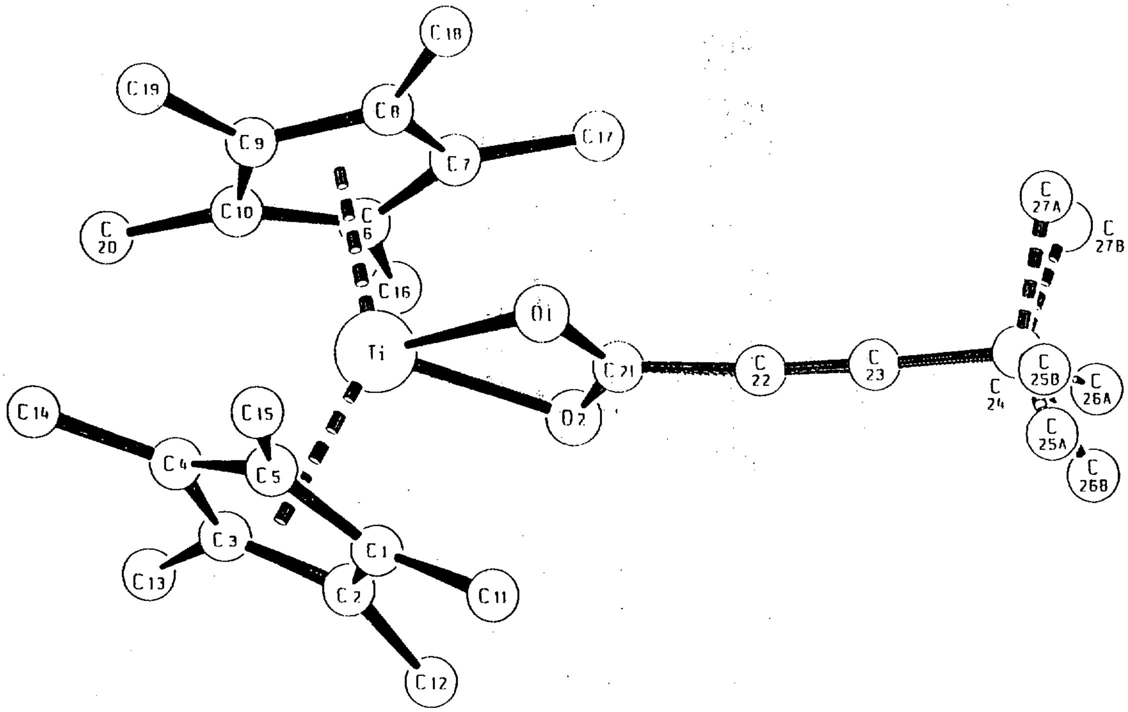

C18
C19
C8
C17
C9
C7
C10
C6
C20
C16
Ti
O1
C21
C22
C23
C27A
C27B
C24
C25B
C26A
C25A
C26B
O2
C14
C15
C4
C5
C3
C1
C13
C2
C11
C12

SCHAKAL

Table 1. Crystal data and structure refinement for 7.

Identification code	736
Empirical formula	C27 H39 O2 Ti
Formula weight	443.48
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a= 10.192(2) A alpha= 90 deg. b= 9.713(2) A beta= 110.14(3) deg. c= 14.011(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	1302.2(5) A^3
Z	2
Density (calculated)	1.131 Mg/m^3
Absorption coefficient	0.347 mm^-1
F(000)	478
Crystal colour	green
Crystal description	prism
Crystal size	0.5 x 0.4 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	2.13 to 24.29 deg.
Index ranges	-11<=h<=11, -11<=k<=11, -15<=l<=16
Reflections collected	7039
Independent reflections	4121 [R(int) = 0.0328]

Reflections unique	4121
Reflections observed	3499
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	4121 / 1 / 269
Final R indices [I>2sigma(I)]	R1 = 0.0436, wR2 = 0.1080
R indices (all data)	R1 = 0.0547, wR2 = 0.1131
Goodness-of-fit on F^2(all)	1.027
Goodness-of-fit on F^2(obs)	1.070
Shift/esd(max)	0.040
Shift/esd(mean)	0.003
Absolute structure parameter	0.00(3)
Weighting scheme	

calc w=1/[\s^2^(Fo^2^)+(0.0728P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.311 and -0.246 e.A^-3
Diff. density rms	0.045
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 7. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti	-7657(1)	-2(1)	-2038(1)	32(1)
O(1)	-6723(3)	-410(2)	-3193(2)	48(1)
O(2)	-6092(3)	-1626(3)	-1801(2)	46(1)
C(1)	-5663(4)	1464(4)	-1477(3)	48(1)
C(2)	-5784(4)	886(4)	-599(3)	54(1)
C(3)	-7028(5)	1367(4)	-499(3)	52(1)
C(4)	-7677(4)	2249(4)	-1321(3)	47(1)
C(5)	-6843(4)	2299(4)	-1945(3)	43(1)
C(6)	-9250(4)	-1666(4)	-1842(3)	44(1)
C(7)	-9079(4)	-1929(4)	-2780(3)	48(1)
C(8)	-9648(4)	-842(5)	-3432(3)	54(1)
C(9)	-10177(3)	132(5)	-2909(3)	57(1)
C(10)	-9950(3)	-393(4)	-1927(3)	47(1)
C(11)	-4423(5)	1338(6)	-1835(5)	90(2)
C(12)	-4734(5)	-24(7)	148(3)	100(2)
C(13)	-7418(7)	1155(7)	449(3)	102(2)
C(14)	-8881(5)	3216(5)	-1410(5)	79(2)
C(15)	-7098(6)	3170(5)	-2873(3)	78(2)
C(16)	-8839(6)	-2608(5)	-937(4)	77(1)
C(17)	-8536(6)	-3268(4)	-3053(4)	81(2)
C(18)	-9735(6)	-724(7)	-4524(3)	101(2)
C(19)	-11063(5)	1348(6)	-3409(5)	102(2)
C(20)	-10631(5)	113(7)	-1184(4)	88(2)
C(21)	-6028(4)	-1382(4)	-2664(3)	45(1)
C(22)	-5120(4)	-2223(5)	-3052(3)	57(1)
C(23)	-4475(4)	-2941(4)	-3399(3)	53(1)
C(24)	-3701(4)	-3836(4)	-3876(3)	55(1)
C(25A)	-2531(13)	-2989(13)	-4037(10)	90(4)
C(26A)	-3207(12)	-5083(16)	-3298(8)	96(3)
C(27A)	-4751(12)	-4248(13)	-4983(9)	94(3)
C(25B)	-3072(15)	-2967(14)	-4499(11)	98(4)
C(26B)	-2392(12)	-4488(14)	-3007(9)	100(4)
C(27B)	-4599(13)	-4920(18)	-4449(10)	118(4)

Table 3. Bond lengths [A] and angles [deg] for 7.

Ti-O(1)	2.178(2)
Ti-O(2)	2.185(3)
Ti-C(5)	2.372(4)
Ti-C(6)	2.373(4)
Ti-C(7)	2.376(4)
Ti-C(1)	2.382(4)
Ti-C(4)	2.409(4)
Ti-C(2)	2.409(4)
Ti-C(8)	2.423(4)
Ti-C(3)	2.424(4)
Ti-C(10)	2.425(3)
Ti-C(9)	2.438(3)
O(1)-C(21)	1.257(4)
O(2)-C(21)	1.256(4)
C(1)-C(2)	1.396(6)
C(1)-C(5)	1.410(5)
C(1)-C(11)	1.518(6)
C(2)-C(3)	1.402(6)
C(2)-C(12)	1.500(6)
C(3)-C(4)	1.404(6)
C(3)-C(13)	1.526(6)
C(4)-C(5)	1.415(5)
C(4)-C(14)	1.516(6)
C(5)-C(15)	1.498(5)
C(6)-C(10)	1.411(5)
C(6)-C(7)	1.408(5)
C(6)-C(16)	1.502(6)
C(7)-C(8)	1.386(6)
C(7)-C(17)	1.514(6)
C(8)-C(9)	1.413(6)
C(8)-C(18)	1.507(6)
C(9)-C(10)	1.410(5)
C(9)-C(19)	1.505(6)
C(10)-C(20)	1.518(5)
C(21)-C(22)	1.471(5)
C(22)-C(23)	1.173(5)
C(23)-C(24)	1.478(5)
C(24)-C(27B)	1.44(2)
C(24)-C(26A)	1.448(14)
C(24)-C(25B)	1.507(13)
C(24)-C(25A)	1.528(13)
C(24)-C(27A)	1.603(12)
C(24)-C(26B)	1.596(11)
O(1)-Ti-O(2)	59.94(9)
O(1)-Ti-C(5)	88.76(11)
O(2)-Ti-C(5)	116.66(13)
O(1)-Ti-C(6)	116.98(11)
O(2)-Ti-C(6)	89.04(12)
C(5)-Ti-C(6)	151.12(13)
O(1)-Ti-C(7)	83.60(12)
O(2)-Ti-C(7)	78.54(13)
C(5)-Ti-C(7)	156.26(13)
C(6)-Ti-C(7)	34.48(13)
O(1)-Ti-C(1)	79.20(13)
O(2)-Ti-C(1)	83.49(12)
C(5)-Ti-C(1)	34.51(13)
C(6)-Ti-C(1)	155.34(14)
C(7)-Ti-C(1)	159.68(13)
O(1)-Ti-C(4)	122.96(11)
O(2)-Ti-C(4)	134.59(12)

C(6)-Ti-C(4)	117.71(13)
C(7)-Ti-C(4)	143.66(14)
C(1)-Ti-C(4)	56.55(14)
O(1)-Ti-C(2)	105.33(13)
O(2)-Ti-C(2)	78.74(12)
C(5)-Ti-C(2)	56.98(13)
C(6)-Ti-C(2)	121.55(14)
C(7)-Ti-C(2)	146.76(14)
C(1)-Ti-C(2)	33.9(2)
C(4)-Ti-C(2)	56.21(13)
O(1)-Ti-C(8)	78.39(12)
O(2)-Ti-C(8)	104.15(13)
C(5)-Ti-C(8)	122.81(14)
C(6)-Ti-C(8)	56.45(13)
C(7)-Ti-C(8)	33.55(14)
C(1)-Ti-C(8)	148.2(2)
C(4)-Ti-C(8)	121.12(14)
C(2)-Ti-C(8)	176.2(2)
O(1)-Ti-C(3)	135.35(12)
O(2)-Ti-C(3)	107.74(12)
C(5)-Ti-C(3)	56.88(13)
C(6)-Ti-C(3)	104.63(13)
C(7)-Ti-C(3)	139.10(14)
C(1)-Ti-C(3)	56.23(14)
C(4)-Ti-C(3)	33.77(14)
C(2)-Ti-C(3)	33.72(14)
C(8)-Ti-C(3)	142.5(2)
O(1)-Ti-C(10)	134.16(11)
O(2)-Ti-C(10)	123.08(12)
C(5)-Ti-C(10)	118.08(13)
C(6)-Ti-C(10)	34.19(12)
C(7)-Ti-C(10)	56.53(13)
C(1)-Ti-C(10)	143.50(13)
C(4)-Ti-C(10)	88.19(12)
C(2)-Ti-C(10)	120.37(14)
C(8)-Ti-C(10)	55.99(13)
C(3)-Ti-C(10)	89.68(13)
O(1)-Ti-C(9)	107.01(13)
O(2)-Ti-C(9)	134.63(14)
C(5)-Ti-C(9)	105.4(2)
C(6)-Ti-C(9)	56.60(14)
C(7)-Ti-C(9)	56.3(2)
C(1)-Ti-C(9)	139.9(2)
C(4)-Ti-C(9)	90.1(2)
C(2)-Ti-C(9)	142.6(2)
C(8)-Ti-C(9)	33.79(14)
C(3)-Ti-C(9)	109.0(2)
C(10)-Ti-C(9)	33.70(13)
C(21)-O(1)-Ti	90.0(2)
C(21)-O(2)-Ti	89.7(2)
C(2)-C(1)-C(5)	108.7(4)
C(2)-C(1)-C(11)	126.6(4)
C(5)-C(1)-C(11)	124.5(4)
C(2)-C(1)-Ti	74.1(2)
C(5)-C(1)-Ti	72.3(2)
C(11)-C(1)-Ti	123.8(3)
C(1)-C(2)-C(3)	108.1(3)
C(1)-C(2)-C(12)	126.4(4)
C(3)-C(2)-C(12)	125.4(4)
C(1)-C(2)-Ti	72.0(2)
C(3)-C(2)-Ti	73.7(2)
C(12)-C(2)-Ti	122.8(3)
C(4)-C(3)-C(2)	108.0(3)
C(4)-C(3)-C(13)	127.2(5)

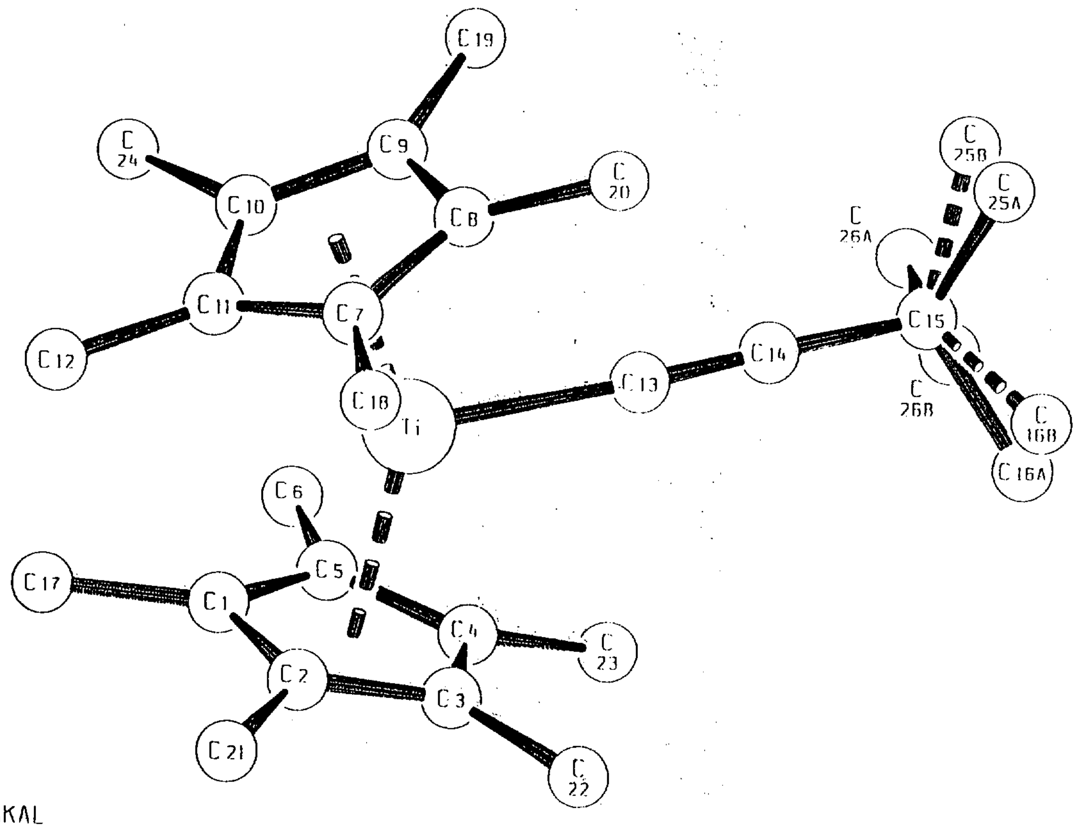
C(2)-C(3)-Ti	72.5(2)
C(13)-C(3)-Ti	129.2(3)
C(3)-C(4)-C(5)	108.3(3)
C(3)-C(4)-C(14)	125.8(4)
C(5)-C(4)-C(14)	124.7(4)
C(3)-C(4)-Ti	73.7(2)
C(5)-C(4)-Ti	71.3(2)
C(14)-C(4)-Ti	130.6(3)
C(4)-C(5)-C(1)	106.9(3)
C(4)-C(5)-C(15)	126.5(4)
C(1)-C(5)-C(15)	126.4(4)
C(4)-C(5)-Ti	74.2(2)
C(1)-C(5)-Ti	73.2(2)
C(15)-C(5)-Ti	122.1(3)
C(10)-C(6)-C(7)	107.5(3)
C(10)-C(6)-C(16)	126.2(4)
C(7)-C(6)-C(16)	126.1(4)
C(10)-C(6)-Ti	74.9(2)
C(7)-C(6)-Ti	72.9(2)
C(16)-C(6)-Ti	120.6(3)
C(8)-C(7)-C(6)	108.6(3)
C(8)-C(7)-C(17)	126.5(4)
C(6)-C(7)-C(17)	124.4(4)
C(8)-C(7)-Ti	75.1(2)
C(6)-C(7)-Ti	72.6(2)
C(17)-C(7)-Ti	124.5(3)
C(7)-C(8)-C(9)	108.4(3)
C(7)-C(8)-C(18)	126.3(5)
C(9)-C(8)-C(18)	125.2(4)
C(7)-C(8)-Ti	71.4(2)
C(9)-C(8)-Ti	73.7(2)
C(18)-C(8)-Ti	122.2(3)
C(8)-C(9)-C(10)	107.4(4)
C(8)-C(9)-C(19)	124.0(4)
C(10)-C(9)-C(19)	127.5(5)
C(8)-C(9)-Ti	72.5(2)
C(10)-C(9)-Ti	72.6(2)
C(19)-C(9)-Ti	129.4(3)
C(6)-C(10)-C(9)	107.9(3)
C(6)-C(10)-C(20)	124.2(4)
C(9)-C(10)-C(20)	126.3(4)
C(6)-C(10)-Ti	70.9(2)
C(9)-C(10)-Ti	73.7(2)
C(20)-C(10)-Ti	132.2(3)
O(1)-C(21)-O(2)	120.3(3)
O(1)-C(21)-C(22)	119.8(3)
O(2)-C(21)-C(22)	119.9(4)
O(1)-C(21)-Ti	60.0(2)
O(2)-C(21)-Ti	60.3(2)
C(22)-C(21)-Ti	177.8(3)
C(23)-C(22)-C(21)	175.5(5)
C(22)-C(23)-C(24)	177.8(5)
C(27B)-C(24)-C(23)	110.2(6)
C(26A)-C(24)-C(23)	112.1(5)
C(27B)-C(24)-C(25B)	113.6(8)
C(23)-C(24)-C(25B)	109.4(6)
C(26A)-C(24)-C(25A)	113.2(7)
C(23)-C(24)-C(25A)	108.4(6)
C(26A)-C(24)-C(27A)	108.7(7)
C(23)-C(24)-C(27A)	107.6(5)
C(25A)-C(24)-C(27A)	106.6(7)
C(27B)-C(24)-C(26B)	109.8(8)
C(23)-C(24)-C(26B)	109.0(5)
C(25B)-C(24)-C(26B)	104.6(7)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 7.
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	33(1)	31(1)	31(1)	-2(1)	12(1)	2(1)
O(1)	55(1)	54(2)	43(1)	2(1)	26(1)	7(1)
O(2)	51(2)	50(2)	41(1)	0(1)	20(1)	14(1)
C(1)	39(2)	43(2)	60(3)	-8(2)	15(2)	-7(2)
C(2)	54(2)	45(2)	47(2)	-6(2)	-4(2)	-4(2)
C(3)	71(3)	50(2)	37(2)	-12(2)	21(2)	-14(2)
C(4)	50(2)	39(2)	55(2)	-13(2)	22(2)	0(2)
C(5)	50(2)	35(2)	47(2)	-5(2)	18(2)	-4(2)
C(6)	46(2)	42(2)	52(2)	4(2)	26(2)	-6(2)
C(7)	46(2)	42(2)	57(2)	-11(2)	18(2)	-13(2)
C(8)	47(2)	65(3)	39(2)	-2(2)	3(2)	-18(2)
C(9)	34(2)	47(2)	72(2)	8(2)	-1(2)	-4(2)
C(10)	32(2)	49(3)	64(2)	-9(2)	23(2)	-2(2)
C(11)	50(3)	83(4)	155(5)	-24(4)	58(3)	-17(3)
C(12)	102(3)	77(3)	72(3)	5(4)	-33(2)	9(4)
C(13)	139(5)	128(5)	48(3)	-28(3)	44(3)	-45(4)
C(14)	72(3)	52(3)	117(4)	-18(3)	38(3)	11(2)
C(15)	112(4)	52(3)	71(3)	16(2)	33(3)	-3(3)
C(16)	91(4)	67(3)	80(3)	25(3)	38(3)	-4(3)
C(17)	95(4)	53(3)	106(4)	-33(3)	51(3)	-20(3)
C(18)	100(4)	150(5)	35(2)	-8(3)	-1(2)	-39(4)
C(19)	60(3)	73(4)	143(5)	32(4)	-5(3)	14(3)
C(20)	74(3)	82(3)	133(4)	-23(4)	70(3)	-5(3)
C(21)	46(2)	45(2)	48(2)	-8(2)	20(2)	2(2)
C(22)	56(2)	65(3)	57(2)	-11(2)	27(2)	8(2)
C(23)	51(2)	57(2)	61(2)	-9(2)	30(2)	6(2)
C(24)	55(2)	57(2)	62(2)	-14(2)	31(2)	8(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 7.

	x	y	z	U(eq)
H(11A)	-4613(5)	1833(6)	-2462(5)	136
H(11B)	-4263(5)	385(6)	-1941(5)	136
H(11C)	-3608(5)	1718(6)	-1330(5)	136
H(12A)	-5074(5)	-279(7)	683(3)	150
H(12B)	-3865(5)	461(7)	431(3)	150
H(12C)	-4590(5)	-838(7)	-193(3)	150
H(13A)	-6797(7)	493(7)	886(3)	153
H(13B)	-8361(7)	824(7)	254(3)	153
H(13C)	-7341(7)	2014(7)	803(3)	153
H(14A)	-9133(5)	3703(5)	-2044(5)	118
H(14B)	-8603(5)	3863(5)	-858(5)	118
H(14C)	-9668(5)	2695(5)	-1384(5)	118
H(15A)	-6375(6)	3006(5)	-3154(3)	117
H(15B)	-7095(6)	4124(5)	-2693(3)	117
H(15C)	-7989(6)	2938(5)	-3368(3)	117
H(16A)	-8374(6)	-3403(5)	-1075(4)	115
H(16B)	-9660(6)	-2892(5)	-801(4)	115
H(16C)	-8220(6)	-2132(5)	-356(4)	115
H(17A)	-8201(6)	-3843(4)	-2460(4)	121
H(17B)	-7785(6)	-3080(4)	-3300(4)	121
H(17C)	-9276(6)	-3732(4)	-3570(4)	121
H(18A)	-10173(6)	131(7)	-4802(3)	152
H(18B)	-10275(6)	-1475(7)	-4909(3)	152
H(18C)	-8810(6)	-754(7)	-4559(3)	152
H(19A)	-11303(5)	1864(6)	-2908(5)	154
H(19B)	-11901(5)	1030(6)	-3924(5)	154
H(19C)	-10551(5)	1925(6)	-3713(5)	154
H(20A)	-11043(5)	1000(7)	-1396(4)	131
H(20B)	-9938(5)	183(7)	-518(4)	131
H(20C)	-11343(5)	-526(7)	-1169(4)	131
H(25A)	-2919(13)	-2179(13)	-4423(10)	135
H(25B)	-2069(13)	-3531(13)	-4399(10)	135
H(25C)	-1870(13)	-2726(13)	-3389(10)	135
H(26A)	-2711(12)	-5633(16)	-3631(8)	145
H(26B)	-3989(12)	-5594(16)	-3251(8)	145
H(26C)	-2593(12)	-4849(16)	-2627(8)	145
H(27A)	-5084(12)	-3429(13)	-5375(9)	141
H(27B)	-5528(12)	-4750(13)	-4919(9)	141
H(27C)	-4270(12)	-4813(13)	-5319(9)	141
H(25D)	-2483(15)	-2273(14)	-4074(11)	147
H(25E)	-3804(15)	-2533(14)	-5041(11)	147
H(25F)	-2526(15)	-3539(14)	-4778(11)	147
H(26D)	-1803(12)	-3763(14)	-2624(9)	150
H(26E)	-1871(12)	-5054(14)	-3311(9)	150
H(26F)	-2713(12)	-5039(14)	-2562(9)	150
H(27D)	-4087(13)	-5491(18)	-4756(10)	177
H(27E)	-5386(13)	-4522(18)	-4969(10)	177
H(27F)	-4920(13)	-5466(18)	-4002(10)	177


C19
C24
C9
C20
C10
C8
C25B
C25A
C26A
C11
C7
C15
C14
C12
C13
C18
Ti
C26B
C16B
C16A
C6
C17
C5
C1
C4
C23
C2
C3
C21
C22

SCHAKAL

Table 1. Crystal data and structure refinement for 5.

Identification code	840
Empirical formula	C26 H39 Ti
Formula weight	399.47
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a= 14.556(3) A alpha= 90 deg. b= 12.015(2) A beta= 108.45(3) deg. c= 14.685(3) A gamma= 90 deg.
Temperature for cell	200(2)
Number of reflecions for cell	4800
Theta for cell determination	4 to 20 deg
Volume	2436.3(8) A^3
Z	4
Density (calculated)	1.089 Mg/m^3
Absorption coefficient	0.358 mm^-1
F(000)	868
Crystal colour	brown
Crystal description	prism
Crystal size	0.3 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	2.24 to 24.31 deg.
Index ranges	-16<=h<=15, -13<=k<=13, 0<=l<=16
Reflections collected	7157
[illegible]	3734 [R(int) = 0.1019]

Reflections unique	3734
Reflections observed	1743
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	3733 / 6 / 241
Final R indices [I>2sigma(I)]	R1 = 0.0658, wR2 = 0.1458
R indices (all data)	R1 = 0.1320, wR2 = 0.1671
Goodness-of-fit on F^2(all)	0.824
Goodness-of-fit on F^2(obs)	1.099
Shift/esd(max)	0.000
Shift/esd(mean)	0.000
Weighting scheme	

calc w=1/[\s^2^(Fo^2^)+(0.0632P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3

Largest diff. peak and hole	0.373 and -0.318 e.A^-3
Diff. density rms	0.064
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 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3637(4)	1720(5)	5947(4)	62(2)
C(2)	2640(4)	1860(4)	5389(4)	59(2)
C(3)	2312(3)	824(5)	4980(4)	55(1)
C(4)	3078(4)	61(4)	5268(4)	55(1)
C(5)	3882(3)	600(6)	5896(4)	60(2)
C(17)	4344(5)	2654(6)	6384(5)	124(3)
C(21)	2088(5)	2928(5)	5153(5)	108(3)
C(22)	1296(4)	563(6)	4311(4)	94(2)
C(23)	3074(5)	-1094(5)	4876(5)	96(2)
C(6)	4882(4)	89(7)	6341(5)	117(3)
C(7)	1800(3)	1580(4)	7503(4)	47(1)
C(8)	1873(3)	477(4)	7835(3)	44(1)
C(9)	2873(3)	247(4)	8315(4)	49(1)
C(10)	3397(3)	1202(5)	8263(4)	54(1)
C(11)	2747(4)	2049(4)	7786(4)	53(1)
C(12)	2958(4)	3268(4)	7777(4)	79(2)
C(13)	2213(4)	-1067(5)	6470(4)	62(2)
C(14)	1996(4)	-2037(5)	6388(4)	51(1)
C(15)	1760(3)	-3233(4)	6272(3)	54(1)
C(18)	870(4)	2194(5)	7021(4)	72(2)
C(19)	3266(4)	-829(5)	8799(4)	75(2)
C(20)	1044(3)	-284(4)	7781(4)	61(2)
C(24)	4483(3)	1344(6)	8772(4)	92(2)
C(16A)	1264(7)	-3505(8)	5204(6)	78(3)
C(25A)	1145(7)	-3590(8)	6903(7)	69(3)
C(26A)	2743(6)	-3836(8)	6604(9)	78(3)
C(16B)	778(11)	-3369(18)	5481(14)	136(8)
C(25B)	1693(13)	-3750(14)	7208(10)	90(6)
C(26B)	2507(13)	-3921(15)	5970(17)	123(8)
Ti	2690(1)	599(1)	6663(1)	42(1)

C(3)-C(4)-Ti	72.5(3)
C(23)-C(4)-Ti	127.4(4)
C(4)-C(5)-C(1)	107.9(5)
C(4)-C(5)-C(6)	125.6(6)
C(1)-C(5)-C(6)	126.1(6)
C(4)-C(5)-Ti	74.0(3)
C(1)-C(5)-Ti	74.7(3)
C(6)-C(5)-Ti	123.0(4)
C(8)-C(7)-C(11)	108.3(4)
C(8)-C(7)-C(18)	125.6(4)
C(11)-C(7)-C(18)	125.8(5)
C(8)-C(7)-Ti	73.6(3)
C(11)-C(7)-Ti	73.2(3)
C(18)-C(7)-Ti	123.8(4)
C(7)-C(8)-C(9)	107.8(4)
C(7)-C(8)-C(20)	126.0(4)
C(9)-C(8)-C(20)	125.9(5)
C(7)-C(8)-Ti	72.0(3)
C(9)-C(8)-Ti	72.9(3)
C(20)-C(8)-Ti	125.3(3)
C(10)-C(9)-C(8)	107.7(4)
C(10)-C(9)-C(19)	127.0(5)
C(8)-C(9)-C(19)	125.3(5)
C(10)-C(9)-Ti	71.7(3)
C(8)-C(9)-Ti	72.3(3)
C(19)-C(9)-Ti	122.4(4)
C(9)-C(10)-C(11)	109.1(4)
C(9)-C(10)-C(24)	124.4(5)
C(11)-C(10)-C(24)	126.0(5)
C(9)-C(10)-Ti	74.2(3)
C(11)-C(10)-Ti	73.4(3)
C(24)-C(10)-Ti	125.3(4)
C(10)-C(11)-C(7)	107.0(4)
C(10)-C(11)-C(12)	126.9(5)
C(7)-C(11)-C(12)	124.6(5)
C(10)-C(11)-Ti	71.9(3)
C(7)-C(11)-Ti	72.0(3)
C(12)-C(11)-Ti	132.2(4)
C(14)-C(13)-Ti	176.1(5)
C(13)-C(14)-C(15)	177.8(5)
C(14)-C(15)-C(25A)	111.1(5)
C(14)-C(15)-C(26B)	113.4(8)
C(14)-C(15)-C(16B)	108.5(9)
C(26B)-C(15)-C(16B)	107.3(13)
C(14)-C(15)-C(25B)	111.6(7)
C(26B)-C(15)-C(25B)	106.9(11)
C(16B)-C(15)-C(25B)	108.9(12)
C(14)-C(15)-C(16A)	110.0(5)
C(25A)-C(15)-C(16A)	112.3(6)
C(14)-C(15)-C(26A)	105.3(5)
C(25A)-C(15)-C(26A)	109.8(6)
C(16A)-C(15)-C(26A)	108.2(7)
C(13)-Ti-C(5)	101.5(2)
C(13)-Ti-C(10)	116.5(2)
C(5)-Ti-C(10)	108.8(2)
C(13)-Ti-C(7)	109.3(2)
C(5)-Ti-C(7)	149.2(2)
C(10)-Ti-C(7)	57.7(2)
C(13)-Ti-C(3)	90.6(2)
C(5)-Ti-C(3)	57.5(2)
C(10)-Ti-C(3)	152.4(2)
C(7)-Ti-C(3)	120.1(2)
C(13)-Ti-C(4)	77.6(2)
C(5)-Ti-C(4)	34.4(2)

Table 3. Bond lengths [A] and angles [deg] for 5.

C(1)-C(5)	1.400(8)
C(1)-C(2)	1.433(7)
C(1)-C(17)	1.520(7)
C(1)-Ti	2.395(5)
C(2)-C(3)	1.398(7)
C(2)-C(21)	1.495(7)
C(2)-Ti	2.391(5)
C(3)-C(4)	1.402(7)
C(3)-C(22)	1.527(7)
C(3)-Ti	2.371(5)
C(4)-C(5)	1.398(7)
C(4)-C(23)	1.502(7)
C(4)-Ti	2.379(5)
C(5)-C(6)	1.523(7)
C(5)-Ti	2.348(5)
C(7)-C(8)	1.405(6)
C(7)-C(11)	1.423(6)
C(7)-C(18)	1.507(6)
C(7)-Ti	2.367(5)
C(8)-C(9)	1.429(6)
C(8)-C(20)	1.496(6)
C(8)-Ti	2.387(5)
C(9)-C(10)	1.393(6)
C(9)-C(19)	1.499(7)
C(9)-Ti	2.394(5)
C(10)-C(11)	1.415(7)
C(10)-C(24)	1.529(6)
C(10)-Ti	2.362(5)
C(11)-C(12)	1.497(7)
C(11)-Ti	2.383(5)
C(13)-C(14)	1.204(6)
C(13)-Ti	2.108(6)
C(14)-C(15)	1.474(7)
C(15)-C(25A)	1.539(6)
C(15)-C(26B)	1.539(11)
C(15)-C(16B)	1.539(11)
C(15)-C(25B)	1.539(11)
C(15)-C(16A)	1.539(6)
C(15)-C(26A)	1.539(6)
C(5)-C(1)-C(2)	108.1(5)
C(5)-C(1)-C(17)	125.7(6)
C(2)-C(1)-C(17)	125.6(6)
C(5)-C(1)-Ti	71.0(3)
C(2)-C(1)-Ti	72.4(3)
C(17)-C(1)-Ti	129.5(4)
C(3)-C(2)-C(1)	106.7(5)
C(3)-C(2)-C(21)	125.4(6)
C(1)-C(2)-C(21)	127.3(6)
C(3)-C(2)-Ti	72.1(3)
C(1)-C(2)-Ti	72.7(3)
C(21)-C(2)-Ti	127.3(4)
C(2)-C(3)-C(4)	108.8(5)
C(2)-C(3)-C(22)	126.1(5)
C(4)-C(3)-C(22)	125.1(6)
C(2)-C(3)-Ti	73.7(3)
C(4)-C(3)-Ti	73.1(3)
C(22)-C(3)-Ti	120.3(4)
C(5)-C(4)-C(3)	108.4(5)
C(5)-C(4)-C(23)	125.6(6)

C(3)-Ti-C(4)	34.3(2)
C(13)-Ti-C(11)	136.5(2)
C(5)-Ti-C(11)	117.5(2)
C(10)-Ti-C(11)	34.7(2)
C(7)-Ti-C(11)	34.9(2)
C(3)-Ti-C(11)	125.7(2)
C(4)-Ti-C(11)	146.0(2)
C(13)-Ti-C(8)	79.6(2)
C(5)-Ti-C(8)	163.4(2)
C(10)-Ti-C(8)	57.3(2)
C(7)-Ti-C(8)	34.4(2)
C(3)-Ti-C(8)	139.0(2)
C(4)-Ti-C(8)	155.8(2)
C(11)-Ti-C(8)	57.4(2)
C(13)-Ti-C(2)	124.7(2)
C(5)-Ti-C(2)	57.9(2)
C(10)-Ti-C(2)	118.7(2)
C(7)-Ti-C(2)	101.9(2)
C(3)-Ti-C(2)	34.2(2)
C(4)-Ti-C(2)	57.0(2)
C(11)-Ti-C(2)	93.7(2)
C(8)-Ti-C(2)	134.8(2)
C(13)-Ti-C(9)	83.9(2)
C(5)-Ti-C(9)	128.6(2)
C(10)-Ti-C(9)	34.1(2)
C(7)-Ti-C(9)	57.5(2)
C(3)-Ti-C(9)	172.5(2)
C(4)-Ti-C(9)	147.6(2)
C(11)-Ti-C(9)	57.2(2)
C(8)-Ti-C(9)	34.8(2)
C(2)-Ti-C(9)	150.6(2)
C(13)-Ti-C(1)	133.3(2)
C(5)-Ti-C(1)	34.3(2)
C(10)-Ti-C(1)	97.7(2)
C(7)-Ti-C(1)	115.8(2)
C(3)-Ti-C(1)	56.9(2)
C(4)-Ti-C(1)	56.6(2)
C(11)-Ti-C(1)	89.6(2)
C(8)-Ti-C(1)	147.0(2)
C(2)-Ti-C(1)	34.9(2)
C(9)-Ti-C(1)	130.5(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 5.
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)	63(4)	87(5)	36(4)	1(3)	14(3)	-30(4)
C(2)	80(4)	52(4)	48(4)	11(3)	27(3)	4(3)
C(3)	48(3)	75(4)	39(3)	5(3)	10(2)	-7(3)
C(4)	68(4)	58(4)	50(4)	-2(3)	34(3)	-5(3)
C(5)	43(3)	92(5)	51(4)	18(4)	22(3)	-2(4)
C(17)	138(6)	153(7)	96(6)	-28(5)	57(5)	-94(6)
C(21)	168(7)	82(5)	77(6)	37(4)	46(5)	35(5)
C(22)	67(4)	153(6)	48(4)	-1(4)	-4(3)	-19(4)
C(23)	139(6)	80(5)	104(6)	-13(4)	86(5)	-9(4)
C(6)	47(4)	216(9)	89(6)	35(5)	24(3)	37(4)
C(7)	44(3)	53(3)	42(3)	0(3)	10(2)	3(3)
C(8)	34(3)	62(4)	36(3)	0(3)	12(2)	0(3)
C(9)	43(3)	65(4)	41(3)	8(3)	15(2)	6(3)
C(10)	38(3)	86(4)	35(4)	-6(3)	6(2)	-6(3)
C(11)	51(3)	64(4)	44(4)	-8(3)	13(2)	-14(3)
C(12)	95(5)	70(4)	80(5)	-20(3)	37(4)	-26(4)
C(13)	86(4)	62(4)	51(4)	4(3)	39(3)	-3(3)
C(14)	60(3)	48(4)	51(4)	0(3)	26(3)	4(3)
C(15)	51(3)	58(4)	53(4)	3(3)	17(3)	0(3)
C(18)	58(4)	77(4)	81(5)	13(3)	21(3)	21(3)
C(19)	76(4)	98(5)	51(4)	25(3)	22(3)	28(3)
C(20)	50(3)	76(4)	64(4)	-1(3)	28(3)	-3(3)
C(24)	41(3)	165(7)	54(5)	-3(4)	-5(3)	-22(4)
Ti	36(1)	52(1)	36(1)	3(1)	9(1)	-3(1)

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

	x	y	z	U(eq)
H(17A)	3989(5)	3357(6)	6329(5)	187
H(17B)	4820(5)	2716(6)	6041(5)	187
H(17C)	4677(5)	2492(6)	7062(5)	187
H(21A)	2475(5)	3532(5)	5536(5)	161
H(21B)	1479(5)	2858(5)	5299(5)	161
H(21C)	1949(5)	3093(5)	4469(5)	161
H(22A)	1258(4)	-225(6)	4128(4)	141
H(22B)	1156(4)	1026(6)	3733(4)	141
H(22C)	821(4)	719(6)	4641(4)	141
H(23A)	2422(5)	-1275(5)	4454(5)	145
H(23B)	3266(5)	-1628(5)	5408(5)	145
H(23C)	3532(5)	-1133(5)	4511(5)	145
H(6A)	5315(4)	640(7)	6753(5)	175
H(6B)	5142(4)	-141(7)	5831(5)	175
H(6C)	4831(4)	-561(7)	6726(5)	175
H(12A)	2376(4)	3660(4)	7389(4)	119
H(12B)	3482(4)	3385(4)	7500(4)	119
H(12C)	3156(4)	3555(4)	8435(4)	119
H(18A)	1019(4)	2950(5)	6860(4)	108
H(18B)	481(4)	2230(5)	7456(4)	108
H(18C)	506(4)	1801(5)	6433(4)	108
H(19A)	2734(4)	-1356(5)	8722(4)	112
H(19B)	3593(4)	-695(5)	9484(4)	112
H(19C)	3730(4)	-1138(5)	8507(4)	112
H(20A)	1293(3)	-1006(4)	8063(4)	92
H(20B)	652(3)	-387(4)	7109(4)	92
H(20C)	643(3)	44(4)	8137(4)	92
H(24A)	4687(3)	2083(6)	8629(4)	137
H(24B)	4840(3)	773(6)	8547(4)	137
H(24C)	4617(3)	1268(6)	9467(4)	137
H(16A)	1110(7)	-4300(8)	5133(6)	116
H(16B)	1701(7)	-3316(8)	4838(6)	116
H(16C)	666(7)	-3071(8)	4962(6)	116
H(25A)	999(7)	-4386(8)	6812(7)	104
H(25B)	539(7)	-3165(8)	6719(7)	104
H(25C)	1505(7)	-3445(8)	7578(7)	104
H(26A)	2638(6)	-4642(8)	6545(9)	116
H(26B)	3084(6)	-3647(8)	7276(9)	116
H(26C)	3134(6)	-3603(8)	6203(9)	116
H(16D)	611(11)	-4161(18)	5396(14)	204
H(16E)	820(11)	-3063(18)	4877(14)	204
H(16F)	277(11)	-2972(18)	5667(14)	204
H(25D)	1536(13)	-4543(14)	7106(10)	135
H(25E)	1185(13)	-3373(14)	7398(10)	135
H(25F)	2316(13)	-3665(14)	7716(10)	135
H(26D)	2311(13)	-4705(15)	5905(17)	184
H(26E)	3144(13)	-3851(15)	6458(17)	184
H(26F)	2542(13)	-3646(15)	5353(17)	184