

# ORGANOMETALLICS

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**Table S1.**Experimental data for the crystal structure determination of  $\text{Ti}(\text{ebmp})\text{Br}_2$ 

Crystal data:			
Habitus, colour	cuboid, dark red		
Crystal size	0.50 x 0.30 x 0.10 mm		
Crystal system	triclinic		
Space group	P-1, Z= 2		
Unit cell dimensions	$a = 928.8(3)$ pm $\alpha = 101.61(4)^\circ$ $b = 1151.2(4)$ pm $\beta = 104.77(4)^\circ$ $c = 1311.8(8)$ pm $\gamma = 102.80(3)^\circ$ $1.272(1)$ nm <sup>3</sup>		
Volume	$1.272(1)$ nm <sup>3</sup>		
Chemical formula	$\text{C}_{24}\text{H}_{32}\text{Br}_2\text{O}_2\text{Ti}$		
Formula weight	560.22		
F(000)	568		
Density (calculated)	1.462 Mg/m <sup>3</sup>		
Absorption coefficient	$3.493 \text{ mm}^{-1}$		
Data collection:			
Diffractometer type	Enraf Nonius CAD4		
Wavelength	$\text{MoK}_\alpha$ (71.073 pm)		
Temperature	296(2) K		
$\theta$ -range for data collection	3 to 30°		
Index ranges	0= $=h<=13$ , -16= $=k<=15$ , -18= $=l<=17$		
Scan method	Omega-scans		
Data collection software	CAD4		
Cell refinement software	CAD4		
Data reduction software	MolEN (Enraf Nonius, 1990)		
Solution and refinement:			
Reflections collected	7795		
Independent reflections	7372 [ $R_{\text{int}} = 0.0369$ ]		
Observed reflections	3524 [ $I > 2\sigma(I)$ ]		
Reflections used for refinement	7369		
Largest diff. peak and hole	708 and $-674 \cdot 10^{30}$ m <sup>-3</sup>		
Solution	direct methods; difmap; H-atoms: geom.		
Refinement	Full-matrix refinement at $F^2$		
Programs used	SHELXS-86 (Sheldrick, 1990); SHELXL-93 (Sheldrick, 1993) 7369 / 0 / 281		
Data / restraints / parameters			
Weighting scheme	$w = 1/[\sigma^2(F_0^2) + (0.0325P)^2 + 3.2394P];$ $P = (F_0^2 + 2F_c^2)/3$		
Goodness-of-fit on $F^2$	1.170		
Final R indices [I > 2σ(I)]	R1 = 0.0687; wR <sub>2</sub> = 0.1152		
R indices (all data)	R1 = 0.1849; wR <sub>2</sub> = 0.1738		

**Table S2.**

Atomic coordinates and equivalent isotropic displacement parameters ( $\text{pm}^2 \times 10^{-4}$ ) for  $\text{Ti}(\text{ebmp})\text{Br}_2$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$ -tensor.

Atom	x	y	z	$U(\text{eq})$
Ti	1.0656(1)	0.3978(1)	0.1981(1)	0.040(1)
Br(1)	0.8482(1)	0.4755(1)	0.1536(1)	0.076(1)
Br(2)	1.0195(1)	0.2515(1)	0.2978(1)	0.082(1)
O(1)	1.2312(4)	0.5185(3)	0.2816(3)	0.040(1)
O(2)	1.0865(4)	0.3164(3)	0.0777(3)	0.042(1)
C(1)	1.3794(6)	0.5999(5)	0.3249(5)	0.037(1)
C(2)	1.4271(7)	0.6811(5)	0.4295(5)	0.042(1)
C(3)	1.5763(7)	0.7616(5)	0.4630(5)	0.049(2)
C(4)	1.6737(7)	0.7649(6)	0.3988(5)	0.050(2)
C(5)	1.6218(7)	0.6820(5)	0.2968(5)	0.044(1)
C(6)	1.4732(6)	0.5990(5)	0.2566(5)	0.038(1)
C(7)	1.4156(7)	0.5082(5)	0.1447(5)	0.040(1)
C(8)	1.4082(7)	0.3758(5)	0.1472(5)	0.039(1)
C(9)	1.3116(6)	0.2789(5)	0.0416(5)	0.039(1)
C(10)	1.1485(6)	0.2540(5)	0.0071(4)	0.032(1)
C(11)	1.0520(6)	0.1673(5)	-0.0911(5)	0.036(1)
C(12)	1.1281(7)	0.1051(5)	-0.1520(5)	0.043(1)
C(13)	1.2887(7)	0.1249(5)	-0.1201(5)	0.042(1)
C(14)	1.3778(7)	0.2137(5)	-0.0237(5)	0.045(1)
C(15)	1.3263(7)	0.6790(6)	0.5060(5)	0.049(2)
C(16)	1.2926(10)	0.5531(7)	0.5316(6)	0.074(2)
C(17)	1.4081(9)	0.7771(7)	0.6167(6)	0.077(2)
C(18)	1.1730(9)	0.7035(8)	0.4529(6)	0.074(2)
C(19)	1.8330(7)	0.8565(7)	0.4404(6)	0.070(2)
C(20)	0.8747(6)	0.1378(5)	-0.1269(5)	0.044(1)
C(21)	0.7986(8)	0.0432(7)	-0.2394(6)	0.074(2)
C(22)	0.8139(7)	0.0810(7)	-0.0443(6)	0.065(2)
C(23)	0.8239(7)	0.2541(6)	-0.1358(6)	0.056(2)
C(24)	1.3593(7)	0.0477(6)	-0.1882(6)	0.061(2)

**Table S3.**  
Bond lengths [pm] and angles [ $^{\circ}$ ] for Ti(ebmp)Br<sub>2</sub>.

Ti-O(2)	174.7(4)	Ti-O(1)	175.4(4)
Ti-Br(2)	236.3(2)	Ti-Br(1)	237.2(2)
O(1)-C(1)	138.2(6)	O(2)-C(10)	137.6(6)
C(1)-C(2)	139.4(7)	C(1)-C(6)	140.1(7)
C(2)-C(3)	138.8(8)	C(2)-C(15)	153.8(8)
C(3)-C(4)	138.5(9)	C(4)-C(5)	137.3(8)
C(4)-C(19)	150.5(8)	C(5)-C(6)	139.2(7)
C(6)-C(7)	150.6(8)	C(7)-C(8)	151.8(8)
C(8)-C(9)	150.6(8)	C(9)-C(14)	137.4(8)
C(9)-C(10)	141.0(7)	C(10)-C(11)	139.9(7)
C(11)-C(12)	139.1(7)	C(11)-C(20)	153.0(7)
C(12)-C(13)	139.5(8)	C(13)-C(14)	137.9(8)
C(13)-C(24)	150.1(8)	C(15)-C(18)	153.2(9)
C(15)-C(17)	153.5(9)	C(15)-C(16)	153.6(9)
C(20)-C(21)	153.1(9)	C(20)-C(23)	153.1(8)
C(20)-C(22)	153.5(9)		
O(2)-Ti-O(1)	114.3(2)	O(2)-Ti-Br(2)	105.61(14)
O(1)-Ti-Br(2)	107.52(14)	O(2)-Ti-Br(1)	109.40(14)
O(1)-Ti-Br(1)	110.05(14)	Br(2)-Ti-Br(1)	109.80(6)
C(1)-O(1)-Ti	163.5(3)	C(10)-O(2)-Ti	161.0(3)
O(1)-C(1)-C(2)	120.5(5)	O(1)-C(1)-C(6)	116.4(5)
C(2)-C(1)-C(6)	123.1(5)	C(3)-C(2)-C(1)	115.5(5)
C(3)-C(2)-C(15)	121.4(5)	C(1)-C(2)-C(15)	123.0(5)
C(4)-C(3)-C(2)	123.9(5)	C(5)-C(4)-C(3)	118.4(5)
C(5)-C(4)-C(19)	121.0(6)	C(3)-C(4)-C(19)	120.6(6)
C(4)-C(5)-C(6)	121.4(6)	C(5)-C(6)-C(1)	117.8(5)
C(5)-C(6)-C(7)	121.6(5)	C(1)-C(6)-C(7)	120.6(5)
C(6)-C(7)-C(8)	113.7(5)	C(9)-C(8)-C(7)	114.9(5)
C(14)-C(9)-C(10)	118.3(5)	C(14)-C(9)-C(8)	121.9(5)
C(10)-C(9)-C(8)	119.8(5)	O(2)-C(10)-C(11)	120.7(4)
O(2)-C(10)-C(9)	116.4(5)	C(11)-C(10)-C(9)	122.8(5)
C(12)-C(11)-C(10)	115.2(5)	C(12)-C(11)-C(20)	121.9(5)
C(10)-C(11)-C(20)	122.8(5)	C(11)-C(12)-C(13)	124.0(5)
C(14)-C(13)-C(12)	118.1(5)	C(14)-C(13)-C(24)	121.9(5)
C(12)-C(13)-C(24)	120.0(5)	C(9)-C(14)-C(13)	121.6(5)
C(18)-C(15)-C(17)	108.0(6)	C(18)-C(15)-C(16)	109.7(6)
C(17)-C(15)-C(16)	106.5(6)	C(18)-C(15)-C(2)	110.2(5)
C(17)-C(15)-C(2)	112.1(5)	C(16)-C(15)-C(2)	110.3(5)
C(11)-C(20)-C(21)	111.8(5)	C(11)-C(20)-C(23)	111.1(5)
C(21)-C(20)-C(23)	106.9(5)	C(11)-C(20)-C(22)	108.9(5)
C(21)-C(20)-C(22)	107.4(6)	C(23)-C(20)-C(22)	110.7(6)

**Table S4.**

Torsion angles [°] for Ti(ebmp)Br <sub>2</sub>	
Br1-Ti-O1-C1	-126.61(1.08)
Br2-Ti-O1-C1	113.87(1.09)
O2-Ti-O1-C1	-2.91(1.15)
Br1-Ti-O2-C10	169.38(0.92)
Br2-Ti-O2-C10	-72.46(0.97)
O1-Ti-O2-C10	45.35(1.00)
Ti-O1-C1-C2	-171.12(0.86)
Ti-O1-C1-C6	10.23(1.37)
Ti-O2-C10-C9	-23.63(1.20)
Ti-O2-C10-C11	154.45(0.77)
O1-C1-C2-C3	-177.99(0.45)
O1-C1-C2-C15	3.77(0.75)
C6-C1-C2-C3	0.57(0.75)
C6-C1-C2-C15	-177.67(0.48)
O1-C1-C6-C5	178.76(0.44)
O1-C1-C6-C7	-2.35(0.68)
C2-C1-C6-C5	0.15(0.76)
C2-C1-C6-C7	179.04(0.47)
C1-C2-C3-C4	-0.07(0.84)
C15-C2-C3-C4	178.19(0.52)
C1-C2-C15-C16	61.91(0.66)
C1-C2-C15-C17	179.43(0.51)
C1-C2-C15-C18	-60.08(0.70)
C3-C2-C15-C16	-116.22(0.58)
C3-C2-C15-C17	1.30(0.75)
C3-C2-C15-C18	121.79(0.59)
C2-C3-C4-C5	-1.15(0.87)
C2-C3-C4-C19	179.08(0.54)
C3-C4-C5-C6	1.91(0.83)
C19-C4-C5-C6	-178.32(0.52)
C4-C5-C6-C1	-1.42(0.77)
C4-C5-C6-C7	179.70(0.49)
C1-C6-C7-C8	-72.36(0.61)
C5-C6-C7-C8	106.50(0.55)
C6-C7-C8-C9	163.69(0.43)
C7-C8-C9-C10	-71.29(0.61)
C7-C8-C9-C14	109.84(0.55)
C8-C9-C10-O2	-2.83(0.67)
C8-C9-C10-C11	179.14(0.45)
C14-C9-C10-O2	176.09(0.43)
C14-C9-C10-C11	-1.94(0.74)
C8-C9-C14-C13	179.12(0.48)
C10-C9-C14-C13	0.22(0.76)
O2-C10-C11-C12	-176.28(0.42)
O2-C10-C11-C20	0.71(0.71)
C9-C10-C11-C12	1.67(0.70)
C9-C10-C11-C20	178.67(0.46)
C10-C11-C12-C13	0.26(0.72)
C20-C11-C12-C13	-176.78(0.47)
C10-C11-C20-C21	177.70(0.48)
C10-C11-C20-C22	-62.76(0.62)
C10-C11-C20-C23	58.28(0.63)
C12-C11-C20-C21	-5.48(0.69)
C12-C11-C20-C22	114.05(0.53)
C12-C11-C20-C23	-124.90(0.51)
C11-C12-C13-C14	-1.87(0.78)
C11-C12-C13-C24	176.65(0.49)
C12-C13-C14-C9	1.59(0.78)
C24-C13-C14-C9	-176.90(0.50)

**Table S5.**

Anisotropic displacement parameters ( $\text{pm}^2 \times 10^{-4}$ ) for  $\text{Ti}(\text{ebmp})\text{Br}_2$ .  
 The anisotropic displacement factor exponent takes the form:  
 $-2p^2 [ (\text{ha}^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$

Atom	U11	U22	U33	U23	U13	U12
Br1	0.0369(2)	0.0748(4)	0.0981(5)	0.0230(2)	0.0153(3)	0.0004(4)
Br2	0.1165(5)	0.0514(3)	0.0696(4)	0.0014(4)	0.0446(3)	0.0183(3)
Ti	0.0277(4)	0.0370(5)	0.0440(5)	0.0045(3)	0.0161(3)	0.0035(4)
O1	0.027(1)	0.041(2)	0.035(2)	0.003(1)	0.009(1)	0.005(1)
O2	0.027(1)	0.040(2)	0.042(2)	0.005(1)	0.011(1)	0.005(2)
C1	0.032(2)	0.032(2)	0.038(3)	0.007(2)	0.010(2)	0.005(2)
C2	0.040(2)	0.041(3)	0.038(3)	0.016(2)	0.008(2)	0.010(2)
C3	0.043(3)	0.043(3)	0.039(3)	0.004(2)	0.001(2)	-0.001(3)
C4	0.038(3)	0.041(3)	0.050(3)	0.001(2)	0.010(2)	0.008(2)
C5	0.035(2)	0.041(3)	0.050(3)	0.005(2)	0.015(2)	0.011(2)
C6	0.031(2)	0.028(2)	0.038(3)	0.005(2)	0.008(2)	0.006(2)
C7	0.036(2)	0.041(3)	0.038(3)	0.010(2)	0.015(2)	0.010(2)
C8	0.026(2)	0.047(3)	0.038(3)	0.009(2)	0.009(2)	0.007(2)
C9	0.030(2)	0.033(2)	0.039(3)	0.008(2)	0.011(2)	0.009(2)
C10	0.032(2)	0.029(2)	0.040(3)	0.009(2)	0.016(2)	0.013(2)
C11	0.033(2)	0.028(2)	0.037(3)	0.008(2)	0.012(2)	0.009(2)
C12	0.041(3)	0.032(2)	0.035(3)	0.002(2)	0.010(2)	0.003(2)
C13	0.039(2)	0.033(2)	0.048(3)	0.007(2)	0.018(2)	0.004(2)
C14	0.028(2)	0.042(3)	0.048(3)	0.005(2)	0.009(2)	0.007(2)
C15	0.045(3)	0.053(3)	0.033(3)	0.012(2)	0.010(2)	-0.001(3)
C16	0.084(4)	0.078(4)	0.055(3)	0.016(3)	0.037(3)	0.018(3)
C17	0.077(4)	0.084(4)	0.053(4)	0.010(3)	0.025(3)	-0.009(3)
C18	0.067(3)	0.108(5)	0.068(4)	0.038(3)	0.035(3)	0.014(4)
C19	0.045(3)	0.065(4)	0.063(4)	-0.013(3)	0.006(3)	-0.001(3)
C20	0.027(2)	0.039(3)	0.045(3)	0.005(2)	0.004(2)	0.011(2)
C21	0.043(3)	0.071(4)	0.074(4)	0.007(3)	-0.004(3)	-0.009(4)
C22	0.035(3)	0.064(3)	0.085(4)	-0.001(3)	0.016(3)	0.032(3)
C23	0.036(3)	0.057(3)	0.066(4)	0.011(2)	0.001(3)	0.020(3)
C24	0.043(3)	0.057(3)	0.066(4)	0.011(2)	0.014(3)	-0.004(3)

**Table S6.**Hydrogen coordinates and isotropic displacement parameters ( $\text{pm}^2 \times 10^{-4}$ ) for  $\text{Ti}(\text{ebmp})\text{Br}_2$ .

Atom	x	y	z	U(eq)
H3	1.614	0.820	0.536	4.9
H5	1.690	0.681	0.250	4.3
H7a	1.315(5)	0.514(4)	0.107(4)	3.9
H7b	1.486(5)	0.535(4)	0.104(4)	3.9
H8a	1.366(5)	0.360(4)	0.204(4)	3.9
H8b	1.506(5)	0.364(4)	0.161(4)	3.9
H12	1.065	0.043	-0.222	4.1
H14	1.492	0.230	0.000	4.3
H16a	1.236	0.556	0.586	7.3
H16b	1.390	0.535	0.562	7.3
H16c	1.229	0.489	0.464	7.3
H17a	1.507	0.764	0.651	7.8
H17b	1.342	0.770	0.664	7.8
H17c	1.425	0.858	0.603	7.8
H18a	1.124	0.650	0.378	8.0
H18b	1.192	0.791	0.452	8.0
H18c	1.104	0.687	0.497	8.0
H19b	1.885	0.845	0.384	6.8
H19c	1.895	0.845	0.508	6.8
H19a	1.824	0.942	0.455	6.8
H21a	0.818	-0.036	-0.237	7.4
H21b	0.843	0.076	-0.292	7.4
H21c	0.687	0.034	-0.261	7.4
H22b	0.884	0.129	0.029	6.4
H22c	0.817	-0.004	-0.058	6.4
H22a	0.708	0.085	-0.050	6.4
H23b	0.710	0.229	-0.162	5.7
H23a	0.862	0.314	-0.063	5.7
H23c	0.866	0.290	-0.187	5.7
H24c	1.296	0.024	-0.265	6.1
H24a	1.364	-0.027	-0.164	6.1
H24b	1.465	0.096	-0.180	6.1

Hydrogen atoms H7a, H7b, H8a, and H8b were refined in their positions.

**Table S7.**Experimental data of the crystal structure determination of  $\text{Ti}(\text{ebmp})(\text{CH}_2\text{TMS})_2$ 

Crystal data:			
Habitus, colour	prism, yellow		
Crystal size	0.60 x 0.60 x 0.90 mm		
Crystal system	orthorhombic		
Space group	Pbca, Z = 8		
Unit cell dimensions	a = 2470.8(9) pm	$\alpha = 90^\circ$	
	b = 2470.8(5) pm	$\beta = 90^\circ$	
	c = 1152.8(2) pm	$\gamma = 90^\circ$	
Volume	7.038(3) nm <sup>3</sup>		
Chemical formula	$\text{C}_{32}\text{H}_{54}\text{O}_2\text{Si}_2\text{Ti}$		
Formula weight	574.83		
F(000)	2496		
Density (calculated)	1.085 Mg/m <sup>3</sup>		
Absorption coefficient	0.335 mm <sup>-1</sup>		
Data collection:			
Diffractometer type	Enraf Nonius CAD4		
Wavelength	$\text{MoK}_\alpha$ (71.070 pm)		
Temperature	296(2) K		
$\theta$ -range for data collection	3 to 30°		
Index ranges	0 <= h <= 34, 0 <= k <= 34, -16 <= l <= 11		
Scan method	Omega-scans		
Data collection software	CAD4		
Cell refinement software	CAD4		
Data reduction software	MolEN (Enraf Nonius, 1990)		
Solution and refinement:			
Reflections collected	13511		
Independent reflections	10244 [ $R_{\text{int}} = 0.0313$ ]		
Observed reflections	3935 [ $I > 2\sigma(I)$ ]		
Reflections used for refinement	10242		
Largest diff. peak and hole	321 and $-292 \cdot 10^{30}$ m <sup>-3</sup>		
Solution	direct methods; difmap; H-atoms: geom.		
Refinement	Full-matrix refinement at $F^2$		
Programs used	SHELXS-86 (Sheldrick, 1990); SHELXL-93 (Sheldrick, 1993)		
Data / restraints / parameters	10242 / 0 / 487		
Weighting scheme	$w = 1/[\sigma^2(F_0^2) + (0.0088P)^2 + 8.2458P]$ ; $P = (F_0^2 + 2F_c^2) / 3$		
Goodness-of-fit on $F^2$	1.134		
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0772$ ; $wR_2 = 0.0947$		
R indices (all data)	$R_1 = 0.2334$ ; $wR_2 = 0.1506$		

**Table S8.**

Atomic coordinates and equivalent isotropic displacement parameters ( $\text{pm}^2 \times 10^{-4}$ ) for  $\text{Ti}(\text{ebmp})(\text{CH}_2\text{TMS})_2$ .  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$ -tensor.

Atom	x	y	z	$U(\text{eq})$
Ti	0.6401(1)	0.3765(1)	0.3609(1)	0.043(1)
Si(1)	0.5713(1)	0.4386(1)	0.1375(1)	0.053(1)
Si(2)	0.7324(1)	0.2986(1)	0.5083(1)	0.065(1)
O(1)	0.6613(1)	0.4371(1)	0.4317(2)	0.048(1)
O(2)	0.5803(1)	0.3419(1)	0.4061(2)	0.048(1)
C(1)	0.6585(2)	0.4821(2)	0.5011(3)	0.044(1)
C(2)	0.6190(2)	0.4823(2)	0.5881(3)	0.046(1)
C(3)	0.6139(2)	0.5285(2)	0.6553(4)	0.052(1)
C(4)	0.6462(2)	0.5731(2)	0.6389(4)	0.052(1)
C(5)	0.6860(2)	0.5704(2)	0.5552(4)	0.053(1)
C(6)	0.6943(2)	0.5253(2)	0.4840(3)	0.046(1)
C(7)	0.7407(2)	0.5240(2)	0.3954(3)	0.050(1)
C(8)	0.7781(2)	0.4760(2)	0.4231(5)	0.069(2)
C(9)	0.7750(2)	0.5758(2)	0.3988(5)	0.068(2)
C(10)	0.7190(2)	0.5191(3)	0.2705(5)	0.074(2)
C(11)	0.6391(2)	0.6242(2)	0.7111(4)	0.076(1)
C(12)	0.5827(2)	0.4343(2)	0.6056(4)	0.053(1)
C(13)	0.5354(2)	0.4313(2)	0.5191(4)	0.053(1)
C(14)	0.5075(2)	0.3777(2)	0.5143(3)	0.047(1)
C(15)	0.5305(2)	0.3340(2)	0.4553(3)	0.046(1)
C(16)	0.5040(2)	0.2840(2)	0.4445(3)	0.049(1)
C(17)	0.4539(2)	0.2801(2)	0.5004(4)	0.062(1)
C(18)	0.4307(2)	0.3224(2)	0.5623(4)	0.060(1)
C(19)	0.4575(2)	0.3709(2)	0.5670(4)	0.056(1)
C(20)	0.5278(2)	0.2363(2)	0.3767(4)	0.058(1)
C(21)	0.5373(3)	0.2528(2)	0.2490(5)	0.079(2)
C(22)	0.5810(2)	0.2185(2)	0.4315(5)	0.073(2)
C(23)	0.4893(3)	0.1872(2)	0.3756(5)	0.082(2)
C(24)	0.3765(2)	0.3152(3)	0.6225(7)	0.095(2)
C(25)	0.6290(2)	0.3960(2)	0.1876(3)	0.049(1)
C(26)	0.5719(3)	0.5063(2)	0.2077(6)	0.082(2)
C(27)	0.5737(2)	0.4493(2)	-0.0227(5)	0.072(2)
C(28)	0.5064(2)	0.4043(3)	0.1728(5)	0.073(2)
C(29)	0.7043(2)	0.3229(2)	0.3677(4)	0.055(1)
C(30)	0.6917(4)	0.3220(3)	0.6338(6)	0.119(3)
C(31)	0.7329(3)	0.2234(2)	0.5124(6)	0.089(2)
C(32)	0.8028(3)	0.3239(3)	0.5284(8)	0.124(3)

**Table S9.**  
Bond lengths [pm] and angles [ $^{\circ}$ ] for Ti(ebmp)(CH<sub>2</sub>TMS)<sub>2</sub>.

Ti-O(1)	178.4(3)	Ti-O(2)	178.6(3)
Ti-C(29)	206.7(4)	Ti-C(25)	207.3(4)
Si(1)-C(26)	185.8(6)	Si(1)-C(28)	186.1(6)
Si(1)-C(25)	186.3(4)	Si(1)-C(27)	186.7(5)
Si(2)-C(30)	185.4(7)	Si(2)-C(31)	186.0(6)
Si(2)-C(29)	186.3(5)	Si(2)-C(32)	186.3(8)
O(1)-C(1)	137.2(4)	O(2)-C(15)	136.9(4)
C(1)-C(6)	139.9(5)	C(1)-C(2)	140.0(5)
C(2)-C(3)	138.5(5)	C(2)-C(12)	150.0(6)
C(3)-C(4)	137.5(6)	C(4)-C(5)	138.0(6)
C(4)-C(11)	152.0(5)	C(5)-C(6)	139.9(5)
C(6)-C(7)	153.6(5)	C(7)-C(9)	153.7(6)
C(7)-C(8)	153.8(6)	C(7)-C(10)	154.1(6)
C(12)-C(13)	153.7(6)	C(13)-C(14)	149.6(6)
C(14)-C(19)	138.6(5)	C(14)-C(15)	139.7(5)
C(15)-C(16)	140.3(5)	C(16)-C(17)	140.0(6)
C(16)-C(20)	153.1(6)	C(17)-C(18)	138.9(6)
C(18)-C(19)	137.0(6)	C(18)-C(24)	151.8(7)
C(20)-C(22)	152.4(7)	C(20)-C(23)	154.0(6)
C(20)-C(21)	154.5(7)		
O(1)-Ti-O(2)	120.77(12)	O(1)-Ti-C(29)	107.2(2)
O(2)-Ti-C(29)	108.5(2)	O(1)-Ti-C(25)	106.5(2)
O(2)-Ti-C(25)	106.5(2)	C(29)-Ti-C(25)	106.7(2)
C(26)-Si(1)-C(28)	108.8(3)	C(26)-Si(1)-C(25)	111.5(2)
C(28)-Si(1)-C(25)	109.6(2)	C(26)-Si(1)-C(27)	107.6(3)
C(28)-Si(1)-C(27)	108.0(3)	C(25)-Si(1)-C(27)	111.3(2)
C(30)-Si(2)-C(31)	107.2(4)	C(30)-Si(2)-C(29)	112.1(3)
C(31)-Si(2)-C(29)	110.3(3)	C(30)-Si(2)-C(32)	107.8(4)
C(31)-Si(2)-C(32)	109.0(3)	C(29)-Si(2)-C(32)	110.4(3)
C(1)-O(1)-Ti	158.9(3)	C(15)-O(2)-Ti	158.9(3)
O(1)-C(1)-C(6)	120.3(4)	O(1)-C(1)-C(2)	117.0(4)
C(6)-C(1)-C(2)	122.7(4)	C(3)-C(2)-C(1)	117.8(4)
C(3)-C(2)-C(12)	121.4(4)	C(1)-C(2)-C(12)	120.8(4)
C(4)-C(3)-C(2)	122.1(4)	C(3)-C(4)-C(5)	118.1(4)
C(3)-C(4)-C(11)	121.6(4)	C(5)-C(4)-C(11)	120.3(4)
C(4)-C(5)-C(6)	123.6(4)	C(5)-C(6)-C(1)	115.6(4)
C(5)-C(6)-C(7)	121.0(4)	C(1)-C(6)-C(7)	123.3(4)
C(6)-C(7)-C(9)	112.2(4)	C(6)-C(7)-C(8)	109.1(4)
C(9)-C(7)-C(8)	107.8(4)	C(6)-C(7)-C(10)	111.4(4)
C(9)-C(7)-C(10)	106.4(4)	C(8)-C(7)-C(10)	110.0(4)
C(2)-C(12)-C(13)	113.9(4)	C(14)-C(13)-C(12)	114.7(4)
C(19)-C(14)-C(15)	118.8(4)	C(19)-C(14)-C(13)	120.2(4)
C(15)-C(14)-C(13)	121.0(4)	O(2)-C(15)-C(14)	117.2(4)
O(2)-C(15)-C(16)	120.4(4)	C(14)-C(15)-C(16)	122.3(4)
C(17)-C(16)-C(15)	115.5(4)	C(17)-C(16)-C(20)	121.4(4)
C(15)-C(16)-C(20)	123.0(4)	C(18)-C(17)-C(16)	123.4(4)
C(19)-C(18)-C(17)	118.6(4)	C(19)-C(18)-C(24)	120.7(5)
C(17)-C(18)-C(24)	120.7(5)	C(18)-C(19)-C(14)	121.3(4)
C(22)-C(20)-C(16)	109.9(4)	C(22)-C(20)-C(23)	107.9(4)
C(16)-C(20)-C(23)	112.0(4)	C(22)-C(20)-C(21)	109.9(5)
C(16)-C(20)-C(21)	110.0(4)	C(23)-C(20)-C(21)	107.1(4)
Si(1)-C(25)-Ti	122.1(2)	Si(2)-C(29)-Ti	121.7(2)

**Table S10.**  
Torsion angles [°] for Ti(ebmp)(CH<sub>2</sub>TMS)<sub>2</sub>.

O2-Ti-O1-C1	-14.4(7)	C29-Ti-O1-C1	-139.1(7)
C25-Ti-O1-C1	106.9(7)	O1-Ti-O2-C15	23.2(7)
C29-Ti-O2-C15	147.3(7)	C25-Ti-O2-C15	-98.2(7)
Ti-O1-C1-C6	-158.8(5)	Ti-O1-C1-C2	21.6(9)
O1-C1-C2-C3	-177.0(3)	C6-C1-C2-C3	3.4(6)
O1-C1-C2-C12	1.6(6)	C6-C1-C2-C12	-178.0(4)
C1-C2-C3-C4	-0.2(6)	C12-C2-C3-C4	-178.8(4)
C2-C3-C4-C5	-2.3(7)	C2-C3-C4-C11	178.3(4)
C3-C4-C5-C6	1.9(7)	C11-C4-C5-C6	-178.8(4)
C4-C5-C6-C1	1.1(6)	C4-C5-C6-C7	-177.8(4)
O1-C1-C6-C5	176.6(3)	C2-C1-C6-C5	-3.8(6)
O1-C1-C6-C7	-4.6(6)	C2-C1-C6-C7	175.0(4)
C5-C6-C7-C9	1.3(6)	C1-C6-C7-C9	-177.5(4)
C5-C6-C7-C8	120.6(4)	C1-C6-C7-C8	-58.1(5)
C5-C6-C7-C10	-117.8(5)		
C1-C6-C7-C10	63.4(5)		
C3-C2-C12-C13	99.0(5)		
C1-C2-C12-C13	-79.5(5)		
C2-C12-C13-C14	164.9(4)		
C12-C13-C14-C19	103.9(5)		
C12-C13-C14-C15	-77.3(5)		
Ti-O2-C15-C14	-4.6(9)		
Ti-O2-C15-C16	174.5(5)		
C19-C14-C15-O2	-178.9(3)		
C13-C14-C15-O2	2.3(5)		
C19-C14-C15-C16	2.0(6)		
C13-C14-C15-C16	-176.8(4)		
O2-C15-C16-C17	178.7(3)		
C14-C15-C16-C17	-2.3(6)		
O2-C15-C16-C20	-1.2(6)		
C14-C15-C16-C20	177.8(4)		
C15-C16-C17-C18	0.5(6)		
C20-C16-C17-C18	-179.6(4)		
C16-C17-C18-C19	1.5(7)		
C16-C17-C18-C24	-179.1(5)		
C17-C18-C19-C14	-1.9(7)		
C24-C18-C19-C14	178.7(5)		
C15-C14-C19-C18	0.2(6)		
C13-C14-C19-C18	179.0(4)		
C17-C16-C20-C22	-117.9(5)		
C15-C16-C20-C22	62.0(5)		
C17-C16-C20-C23	2.1(6)		
C15-C16-C20-C23	-178.1(4)		
C17-C16-C20-C21	121.0(5)		
C15-C16-C20-C21	-59.1(6)		
C26-Si1-C25-Ti	-59.0(4)		
C28-Si1-C25-Ti	-61.5(3)		
C27-Si1-C25-Ti	-179.2(3)		
O1-Ti-C25-Si1	-71.4(3)		
O2-Ti-C25-Si1	58.6(3)		
C29-Ti-C25-Si1	174.3(3)		
C30-Si2-C29-Ti	-6.2(5)		
C31-Si2-C29-Ti	-125.6(3)		
C32-Si2-C29-Ti	-113.9(4)		
O1-Ti-C29-Si2	61.2(3)		
O2-Ti-C29-Si2	-70.7(3)		
C25-Ti-C29-Si2	174.9(3)		

**Table S11.**Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{Ti}(\text{ebmp})(\text{CH}_2\text{TMS})_2$ .

The anisotropic displacement factor exponent takes the form:

$$-2P^2 [ (ha^*)^2 U_{11} + \dots + 2 h k a^* b^* U_{12} ]$$

Atom	U11	U22	U33	U23	U13	U12
Ti	51(1)	42(1)	37(1)	-2(1)	1(1)	2(1)
Si(1)	56(1)	57(1)	47(1)	0(1)	-4(1)	6(1)
Si(2)	73(1)	58(1)	65(1)	3(1)	-9(1)	18(1)
O(1)	59(2)	45(2)	40(2)	-4(1)	3(1)	-1(1)
O(2)	53(2)	47(2)	44(2)	0(1)	6(1)	-3(1)
C(1)	49(2)	43(2)	40(2)	-4(2)	-5(2)	5(2)
C(2)	51(2)	47(2)	39(2)	-5(2)	-1(2)	3(2)
C(3)	51(3)	59(3)	46(3)	-9(2)	8(2)	4(2)
C(4)	54(3)	50(2)	53(2)	-10(2)	-4(2)	3(2)
C(5)	58(3)	43(3)	57(3)	-3(2)	-5(2)	-3(2)
C(6)	50(3)	45(2)	44(2)	0(2)	-2(2)	3(2)
C(7)	58(3)	50(3)	42(2)	-1(2)	1(2)	-9(2)
C(8)	65(4)	67(3)	74(4)	0(3)	12(3)	8(3)
C(9)	69(4)	68(3)	67(4)	0(3)	4(3)	-17(3)
C(10)	78(4)	95(4)	49(3)	0(3)	-2(3)	-21(3)
C(11)	82(3)	59(3)	87(3)	-28(3)	6(3)	2(3)
C(12)	62(3)	50(3)	47(3)	-3(2)	9(2)	-5(2)
C(13)	56(3)	47(3)	58(3)	-1(2)	0(2)	4(2)
C(14)	44(2)	52(2)	46(2)	6(2)	-9(2)	-3(2)
C(15)	52(3)	48(2)	38(2)	8(2)	-8(2)	-1(2)
C(16)	55(3)	50(3)	42(2)	6(2)	-6(2)	-3(2)
C(17)	63(3)	63(3)	59(3)	8(3)	-17(3)	-11(3)
C(18)	42(3)	77(3)	60(3)	8(3)	-10(2)	-4(3)
C(19)	41(2)	67(3)	60(3)	-3(3)	-3(2)	-1(2)
C(20)	78(3)	47(3)	49(3)	-3(2)	-9(3)	-9(2)
C(21)	128(5)	67(3)	43(3)	-8(3)	-4(3)	-12(4)
C(22)	85(4)	58(3)	75(4)	-1(3)	-6(4)	7(3)
C(23)	109(5)	60(3)	78(4)	-3(3)	-9(4)	-24(3)
C(24)	58(4)	111(6)	115(6)	-7(4)	9(4)	-19(4)
C(25)	56(3)	52(3)	39(2)	1(2)	0(2)	1(2)
C(26)	95(5)	61(3)	88(4)	-13(3)	-20(4)	16(3)
C(27)	67(3)	88(4)	61(3)	16(3)	-2(3)	8(3)
C(28)	62(3)	88(4)	68(4)	3(3)	6(3)	6(3)
C(29)	61(3)	53(3)	53(3)	-6(2)	3(3)	9(2)
C(30)	160(7)	140(6)	57(4)	6(5)	1(5)	68(6)
C(31)	90(5)	67(3)	111(5)	14(4)	-4(4)	14(3)
C(32)	112(6)	105(5)	154(9)	32(6)	-56(6)	-13(5)

**Table S12.**  
Hydrogen coordinates and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $\text{Ti}(\text{ebmp})(\text{CH}_2\text{TMS})_2$ .

Atom	x	y	z	U(eq)
H(3)	5865(15)	5284(15)	7153(33)	63
H(5)	7073(16)	5996(16)	5462(35)	63
H(8A)	7588(20)	4406(20)	4175(44)	103
H(8B)	7938(20)	4828(21)	4967(44)	103
H(8C)	8061(20)	4746(20)	3670(44)	103
H(9A)	8033(20)	5717(20)	3430(42)	102
H(9B)	7937(20)	5797(19)	4756(44)	102
H(9C)	7536(19)	6098(19)	3815(43)	102
H(10A)	6963(20)	4875(20)	2608(46)	111
H(10B)	7503(21)	5143(21)	2208(44)	111
H(10C)	6974(21)	5507(20)	2572(48)	111
H(11A)	6651(2)	6507(2)	6872(4)	114
H(11B)	6444(2)	6157(2)	7916(4)	114
H(11C)	6032(2)	6382(2)	7001(4)	114
H(11D)	6101(2)	6190(2)	7654(4)	114
H(11E)	6308(2)	6540(2)	6610(4)	114
H(11F)	6720(2)	6316(2)	7525(4)	114
H(12A)	6037(15)	3991(15)	6012(33)	64
H(12B)	5687(16)	4342(16)	6777(34)	64
H(13A)	5098(15)	4602(15)	5380(34)	64
H(13B)	5482(16)	4391(16)	4460(35)	64
H(17)	4363(16)	2460(18)	4966(37)	74
H(19)	4415(16)	4026(16)	6065(34)	67
H(21A)	5016(21)	2657(21)	2163(47)	119
H(21B)	5637(22)	2802(22)	2467(50)	119
H(21C)	5486(22)	2237(22)	2054(47)	119
H(22A)	5756(22)	2060(21)	5052(46)	109
H(22B)	5955(20)	1890(20)	3919(46)	109
H(22C)	6095(19)	2485(21)	4368(43)	109
H(23A)	5062(22)	1593(22)	3303(48)	124
H(23B)	4531(21)	1954(22)	3384(49)	124
H(23C)	4824(22)	1729(22)	4551(49)	124
H(24A)	3505(24)	3066(26)	5691(55)	142
H(24B)	3717(26)	3409(25)	6732(56)	142
H(24C)	3749(26)	2822(23)	6575(56)	142
H(25A)	6243(14)	3588(15)	1505(32)	59
H(25B)	6644(15)	4144(14)	1640(32)	59
H(26A)	5804(24)	5085(23)	2838(49)	122
H(26B)	5376(22)	5224(22)	2005(49)	122
H(26C)	5980(22)	5299(22)	1737(50)	122
H(27A)	6043(21)	4708(21)	-468(45)	108
H(27B)	5412(20)	4714(20)	-461(43)	108
H(27C)	5770(22)	4169(21)	-549(47)	108
H(28A)	4754(20)	4255(19)	1333(44)	109
H(28B)	4992(22)	4011(21)	2461(48)	109
H(28C)	5062(21)	3692(21)	1447(46)	109
H(29A)	7325(16)	3415(16)	3270(33)	66
H(29B)	6924(17)	2960(16)	3239(34)	66
H(30A)	6989(28)	3621(27)	6302(65)	178
H(30B)	7021(31)	3115(30)	6938(60)	178
H(30C)	6551(28)	3090(30)	6301(71)	178
H(31A)	6959(23)	2077(23)	5153(52)	134
H(31B)	7521(24)	2095(24)	4414(51)	134
H(31C)	7529(25)	2114(24)	5729(51)	134
H(32A)	8033(29)	3636(28)	5326(65)	186
H(32B)	8160(32)	3075(31)	5888(66)	186
H(32C)	8216(35)	3131(37)	4733(74)	186