

Supporting Information for

SYNTHESIS AND CYTOTOXICITY STUDIES OF SILYL-SUBSTITUTED TITANOCENE DICHLORIDE DERIVATIVES

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Crystallographic Analyses: A single crystal of titanocene **3a** suitable for X-ray diffraction experiments was obtained by the slow diffusion of pentane into saturated solutions of the compound in chloroform, whereas a single crystal of **3b** was obtained by the slow evaporation of chloroform from a saturated solution at 25 °C. X-ray diffraction data for **3a** and **3b** was collected on an Agilent Technologies (former Oxford Diffraction) Super Nova A diffractometer at 100 K. **3a** was measured with Mo-K α (0.71073 Å), **3b** with Cu-K α (1.54184 Å). A complete dataset was collected, assuming that the Friedel pairs are not equivalent. An analytical absorption correction based on the shape of the crystal was performed. The crystal structure was then solved by direct methods (SHELXS-97) and refined by full matrix least squares methods against F² (SHELXL-97). Crystal data, data collection parameters, and results of the analyses are listed in Table 1.

Table 1. Crystal data and structure refinement for **3a** and **3b**.

Identification code	3a	3b
Empirical formula	C ₂₆ H ₃₀ Si ₂ Cl ₂ Ti	C ₂₈ H ₃₄ O ₂ Si ₂ Cl ₂ Ti
Formula weight	517.48	577.53
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	1.54184 Å
Crystal system	Orthorhombic	Monoclinic
Space group	Pbca (#61)	C2/c (#15)
Unit cell dimensions	a = 13.2693(3) Å α = 90°.	a = 27.1091(4) Å α = 90°.
	b = 18.6775(4) Å β = 90°.	b = 6.80307(8) Å β = 101.4316(13)°.
	c = 20.5498(4) Å γ = 90°.	c = 31.1056(4) Å γ = 90°.
Volume	5093.01(19) Å ³	5622.85(13) Å ³
Z	8	8
Density (calculated)	1.350 Mg/m ³	1.364 Mg/m ³
Absorption coefficient	0.652 mm ⁻¹	5.331 mm ⁻¹
F(000)	2160	2416
Crystal size	0.3139 x 0.2082 x 0.1456 mm ³	0.1875 x 0.1285 x 0.0273 mm ³
Theta range for data collection	2.85 to 27.13°.	3.33 to 62.45°.
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 23, -26 ≤ l ≤ 25	-27 ≤ h ≤ 30, -7 ≤ k ≤ 7, -35 ≤ l ≤ 34
Reflections collected	34736	23610
Independent reflections	5585 [R(int) = 0.0385]	4461 [R(int) = 0.0335]
Completeness to theta = 26.43°	99.1 %	99.8 %
Absorption correction	Analytical	Analytical
Max. and min. transmission	0.925 and 0.869	0.862 and 0.495
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data / restraints / parameters	5585 / 0 / 284	4461 / 0 / 322
Goodness-of-fit on F ²	1.035	1.050
Final R indices [I > 2σ(I)]	R1 = 0.0293, wR2 = 0.0637	R1 = 0.0270, wR2 = 0.0690
R indices (all data)	R1 = 0.0415, wR2 = 0.0699	R1 = 0.0331, wR2 = 0.0712
Largest diff. peak and hole	0.371 and -0.348 e.Å ⁻³	0.502 and -0.267 e.Å ⁻³

