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Titanium–Tin Complexes: Synthesis and Structure of $Cp_2Ti(SnPh_3)Cl$

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Our interest in early- and late-transition-metal heterobimetallics arose for two reasons: (i) the potential for applications in catalysis and (ii) the possibility of modeling the strong metal–support interactions seen for heterogeneous catalyst systems comprised of late metals dispersed on Lewis acidic supports. In our initial studies of such systems we have developed synthetic strategies for the preparation of a variety of thiolato- and phosphido-bridged early- and late-transition-metal heterobimetallics.[2-12] Recently, Selegue et al.[13,14] have described a convenient route to unsupported Ti–Fe and Ti–Ru metal–metal-bonded systems. In related work, others have previously described early-transition-metal complexes in which the metal is directly bonded to group 14 elements.[15-36] Of these compounds, only three containing Ti, namely $[Cp_2Ti(\mu\text{-}SiH_2)]_2$,[31] $Cp_2Ti(SiMe_3)Cl$,[15] and $Cp_2Ti(GePh_3)COMe$,[30] have been characterized unequivocally. Similarly, few early-transition-metal complexes that contain a metal–tin bond have been characterized. In an initial report by Kingston and Lappert,[29] the metal–metal-bonded compounds $Cp_2M(SnPh_3)Cl$ (M = Zr, Hf) were described as "difficult to purify" and "unstable in solution". Of the early-transition-metal–tin complexes known, only $(C_6H_5Me)_2Hf(SnMe_3)_2$,[19] $(MeCp)_2Nb(SnCl_3)(CO)$,[32] $Cp_2TaH_2(SnMeCl_2)$,[24] and $Cp_3U(SnPh_3)$[33] have been characterized unequivocally. Although compounds containing Ti–Sn bonds have been described,[34] no such Ti–Sn compounds have been characterized crystallographically to date. Herein, we report an alternative synthesis of the known compound $Cp_2Ti(SnPh_3)Cl$ and its crystal and molecular structure. This represents the first report of a structure containing a Ti–Sn bond.

Table I. Crystallographic Parameters

formula	$C_{28}H_{25}ClTiSn$
cryst color, form	green blocks
a, Å	17.293 (5)
b, Å	10.053 (5)
c, Å	14.231 (5)
α, deg	85.24 (2)
β, deg	92.06 (2)
γ, deg	90.45 (2)
cryst syst	triclinic
space group	$P\bar{1}$
V, $Å^3$	2463 (1)
d(calcd), g cm^{-3}	1.52
Z	4
cryst dimens, mm	0.35 × 0.40 × 0.35
abs coeff, μ, cm^{-1}	13.39
radiation (λ, Å)	Mo Kα (0.71069, graphite monochromator)
temp, °C	24
scan speed, deg min^{-1}	2.0–5.0 ($\theta/2\theta$ scan)
scan range, deg	1.0 below Kα_1 to 1.0 above Kα_2
bdgd/scan time ratio	0.5
data collected	2θ of 4.5–40.0° ($h,\pm k,\pm l$)
total no. of data collected	4882
no. of unique data, $F_o^2 > 3\sigma(F_o^2)$	3687
no. of variables	379 (2 blocks)
R, %[a]	3.67
R_w, %[b]	4.14
max Δ/σ in final cycle	0.002
largest residual electron density, e $Å^{-3}$	0.66
atom associated with residual density	Sn1, Ti1

[a] $R = \sum||F_o| - |F_c|/\sum|F_o||$. [b] $R_w = (\sum w(|F_o| - |F_c|)^2/\sum wF_o^2)^{1/2}$.

Experimental Section

All preparations were done under an atmosphere of dry, O_2-free N_2. Solvents were reagent grade and were distilled from the appropriate drying agents under N_2 and degassed by the freeze–thaw method at least three times prior to use. ^1H NMR spectra were recorded on a Bruker AC-300 spectrometer, using the trace of protonated solvent as the reference. The chemical shifts are reported in ppm relative to $Si(CH_3)_4$ for the ^1H NMR data. Melting points are reported uncorrected.

Preparation of $Cp_2Ti(SnPh_3)Cl$ (1). Ph_2SnCl_2 (2.76 g, 8.0 mmol) in THF (25 mL) was added dropwise to a suspension of lithium (0.4 g, 576 mmol) in 15 mL of THF with stirring.[37] After it was heated at 60 °C for 8 h, the reaction mixture became yellow-brown and was filtered. The clear filtrate was added slowly to a flask charged with 1.25 g (5.0 mmol) of Cp_2TiCl_2. The color of the solution changed to green immediately. After the mixture was stirred overnight at 25 °C, 5 mL of hexane was added slowly. The solution was filtered, and the solvent was removed, yielding a green residue. This solid was extracted with two 75-mL portions of a 2:1 mixture of acetone/hexane. Chromatography on silica with elution by THF afforded a green fraction. Removal of the solvent, followed by crystallization from THF/hexane, yielded a pure green microcrystalline compound: yield 1.17 g (40%); mp 180–182 °C dec (lit.[29] mp 177–180 °C dec). ^1H NMR ($CDCl_3$): δ 7.33 (br m, 15 H), 6.26 (s, 10 H).

X-ray Data Collection and Reduction. Green crystals of **1** were obtained by vapor diffusion of hexane into an acetone solution of **1**. Diffraction experiments were performed on a four-circle Syntex $P2_1$ diffractometer with graphite-monochromatized Mo Kα radiation. The initial orientation matrix was obtained from 15 machine-centered re-

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(1) Current address: Sichuan Institute of Chemical Technology, Dengguan Zigong, Sichuan, China.

(2) Gelmini, L.; Matassa, L. C.; Stephan, D. W. *Inorg. Chem.* **1985**, *24*, 2585.

(3) Gelmini, L.; Stephan, D. W. *Inorg. Chem.* **1986**, *25*, 1222.

(4) Gelmini, L.; Stephan, D. W. *Inorg. Chim. Acta* **1986**, *111*, L17.

(5) Loeb, S. J.; Taylor, H. A.; Gelmini, L.; Stephan, D. W. *Inorg. Chem.* **1986**, *25*, 1977.

(6) White, G. S.; Stephan, D. W. *Inorg. Chem.* **1985**, *24*, 1499.

(7) Wark, T. A.; Stephan, D. W. *Inorg. Chem.* **1987**, *26*, 363.

(8) White, G. S.; Stephan, D. W. *Organometallics* **1987**, *6*, 2169.

(9) Wark, T. A.; White, G. S.; Tse, J. S.; Stephan, D. W., unpublished results.

(10) Gelmini, L.; Stephan, D. W. *Organometallics* **1987**, *6*, 1515.

(11) White, G. S.; Stephan, D. W. *Organometallics* **1988**, *7*, 903.

(12) Gelmini, L.; Stephan, D. W. *Organometallics* **1988**, *7*, 849.

(13) Sartain, W. J.; Selegue, J. P. *J. Am. Chem. Soc.* **1985**, *107*, 5818.

(14) Sartain, W. J.; Selegue, J. P. *Organometallics* **1987**, *6*, 1812.

(15) Rosch, L.; Altman, G.; Erb, W.; Pickardt, J.; Bruncks, N. *J. Organomet. Chem.* **1980**, *197*, 51.

(16) Holtman, M. S.; Schram, E. P. *J. Organomet. Chem.* **1980**, *187*, 147.

(17) Blakeney, A. J.; Gladysz, J. A. *J. Organomet. Chem.* **1980**, *186*, 241.

(18) Cardoso, A. M. *J. Organomet. Chem.* **1980**, *186*, 241.

(19) Cloke, F. G. N.; Cox, K. P.; Green, M. L. H.; Bashkin, J.; Prout, K. *J. Chem. Soc., Chem. Commun.* **1981**, 117.

(20) Curtis, M. D.; Bell, L. G.; Butler, W. M. *Organometallics* **1985**, *4*, 701.

(21) Tilley, T. D. *Organometallics* **1985**, *4*, 1452.

(22) Tilley, T. D. *J. Am. Chem. Soc.* **1985**, *107*, 4084.

(23) Arnold, J.; Tilley, T. D. *J. Am. Chem. Soc.* **1985**, *107*, 6409.

(24) Arhireeva, T. M. *J. Organomet. Chem.* **1986**, *316*, 33.

(25) Arnold, J.; Shina, D. N.; Tilley, T. D.; Arif, A. M. *Organometallics* **1986**, *5*, 2037.

(26) Aitken, C. T. *J. Am. Chem. Soc.* **1986**, *108*, 4059.

(27) Arnold, J.; Tilley, T. D.; Rheingold, A. L. *J. Am. Chem. Soc.* **1986**, *108*, 5355.

(28) Campion, B. K.; Falk, J.; Tilley, T. D. *J. Am. Chem. Soc.* **1987**, *109*, 2049.

(29) Kingston, B. M.; Lappert, M. F. *J. Chem. Soc., Chem. Commun.* **1972**, 69.

(30) Harrod, J. F.; Malek, A.; Rochon, F. D.; Melanson, R. *Organometallics* **1987**, *6*, 2117.

(31) Hencken, G.; Weiss, E. *Chem. Ber.* **1971**, *106*, 1747.

(32) Skripkin, Y. V.; Volkov, O. G.; Pasynskii, A. A.; Anttsystikina, A. S.; Dikaveva, L. M.; Ostrikova, V. N.; Porai-Koskits, M. A.; Devydova, S. L.; Sakharov, S. G. *J. Organomet. Chem.* **1984**, *263*, 345.

(33) Porchia, M.; Casellato, U. *J. Chem. Soc., Chem. Commun.* **1986**, 1034.

(34) Coutts, R. S. P.; Wailes, P. C. *Chem. Commun.* **1968**, 260.

(35) Creemers, H. M. J. C.; Verbeek, F.; Noltes, J. G. *J. Organomet. Chem.* **1968**, *15*, 125.

(36) Cardin, D. J.; Keppie, S. A.; Kingston, B. M.; Lappert, M. F. *Chem. Commun.* **1967**, 1035.

(37) Gilman, H.; Marrs, O. L.; Sim, S. Y. *J. Org. Chem.* **1962**, *27*, 4232.

0020-1669/88/1327-2386$01.50/0

Table II. Positional Parameters[a]

atom	*x*	*y*	*z*	atom	*x*	*y*	*z*
Sn1	2668 (1)	273 (1)	−1060 (1)	Sn2	2310 (1)	−4252 (1)	−6116 (1)
Ti1	2324 (1)	2324 (1)	119 (1)	Ti2	2711 (1)	−1786 (1)	−5378 (1)
Cl1	1724 (1)	3431 (2)	−1205 (1)	Cl2	3283 (1)	−1237 (2)	−6824 (1)
C1	3444 (4)	−1300 (7)	−483 (5)	C2	3610 (4)	−1500 (7)	475 (5)
C3	4140 (5)	−2484 (8)	844 (6)	C4	4484 (5)	−3258 (8)	252 (6)
C5	4345 (5)	−3077 (8)	−700 (6)	C6	3824 (4)	−2115 (7)	−1064 (6)
C11	1701 (4)	−789 (7)	−1679 (5)	C12	1718 (4)	−2174 (7)	−1701 (5)
C13	1083 (5)	−2879 (9)	−2070 (6)	C14	445 (5)	−2202 (9)	−2391 (6)
C15	399 (5)	−882 (9)	−2385 (6)	C16	1029 (5)	−134 (8)	−2027 (5)
C21	3286 (4)	1146 (7)	−2257 (5)	C22	4085 (4)	1054 (7)	−2325 (5)
C23	4459 (5)	1696 (7)	−3077 (5)	C24	4065 (5)	2438 (8)	−3781 (6)
C25	3271 (5)	2560 (8)	−3741 (6)	C26	2889 (4)	1928 (7)	−2976 (5)
C31	3453 (5)	3351 (9)	−498 (6)	C32	3702 (4)	2185 (9)	2 (6)
C33	3528 (5)	2301 (10)	947 (7)	C34	3203 (6)	3538 (10)	1019 (7)
C35	3153 (5)	4212 (9)	118 (7)	C41	1080 (6)	1384 (17)	360 (7)
C42	1607 (10)	453 (11)	754 (11)	C43	1992 (7)	1022 (18)	1475 (10)
C44	1697 (9)	2272 (15)	1544 (8)	C45	1136 (7)	2479 (12)	844 (10)
C51	3292 (4)	4563 (6)	−6431 (4)	C52	3294 (4)	3179 (7)	−6283 (5)
C53	3939 (5)	2426 (8)	−6487 (6)	C54	4580 (5)	3056 (8)	−6855 (6)
C55	4596 (5)	4389 (7)	−7020 (5)	C56	3958 (4)	5154 (7)	−6817 (5)
C61	1572 (4)	4393 (7)	−5287 (5)	C62	1486 (4)	4543 (7)	−4324 (5)
C63	1011 (5)	3674 (8)	−3781 (6)	C64	635 (5)	2678 (8)	−4187 (6)
C65	689 (5)	2508 (8)	−5132 (5)	C66	1167 (4)	3376 (7)	−5666 (5)
C71	1679 (4)	−3967 (6)	2534 (5)	C72	882 (4)	−4112 (7)	2450 (5)
C73	499 (5)	−3881 (8)	1572 (6)	C74	894 (5)	−3496 (8)	796 (6)
C75	1694 (5)	−3343 (8)	853 (6)	C76	2069 (4)	−3581 (7)	1732 (5)
C81	1337 (4)	−1932 (9)	−5388 (9)	C82	1535 (5)	−1104 (10)	−6170 (6)
C83	1882 (5)	21 (8)	−5889 (7)	C84	1938 (5)	−70 (10)	−4936 (7)
C85	1581 (6)	−1271 (13)	−4601 (7)	C91	3430 (6)	−3426 (9)	−4391 (7)
C92	3946 (5)	−2696 (13)	−4914 (6)	C93	3951 (6)	−151 (12)	−4685 (8)
C94	3417 (8)	−1317 (12)	−3996 (8)	C95	3094 (5)	−2874 (14)	−3823 (6)

[a] Multiplied by 10^4.

Table III. Selected Bond Distances and Angles

	Distances (Å)		
Ti1–Sn1	2.843 (1)	Ti1–Cl1	2.324 (2)
Ti1–C31	2.363 (8)	Ti1–C32	2.400 (8)
Ti1–C33	2.353 (9)	Ti1–C34	2.35 (1)
Ti1–C35	2.369 (9)	Ti1–C41	2.37 (1)
Ti1–C42	2.38 (1)	Ti1–C43	2.33 (2)
Ti1–C44	2.33 (1)	Ti1–C45	2.34 (1)
Sn1–C1	2.172 (7)	Sn1–C11	2.176 (7)
Sn1–C21	2.164 (7)		
Ti2–Sn2	2.843 (1)	Ti2–Cl2	2.337 (2)
Ti2–C81	2.380 (8)	Ti2–C82	2.369 (8)
Ti2–C83	2.373 (8)	Ti2–C84	2.33 (1)
Ti2–C85	2.36 (1)	Ti–C91	2.399 (9)
Ti2–C92	2.379 (9)	Ti2–C93	2.36 (1)
Ti2–C94	2.36 (1)	Ti2–C95	2.361 (9)
Sn2–C51	2.164 (6)	Sn2–C61	2.166 (7)
Sn2–C71	2.174 (6)		
	Angles (deg)[a]		
Sn1–Ti1–Cl1	86.8 (1)	Cp3–Ti1–Cp4	132.5 (2)
Ti1–Sn1–C11	117.8 (2)	Ti1–Sn1–C21	108.6 (2)
Ti1–Sn1–C6	117.5 (2)	C1–Cn1–C11	104.1 (3)
C1–Sn1–C21	102.5 (3)	C11–Sn1–C21	104.6 (3)
Sn2–Ti2–Cl2	85.7 (1)	Cp8–Ti2–Cp9	133.1 (2)
Ti2–Sn2–C51	114.2 (2)	Ti2–Sn2–C61	117.5 (2)
Ti2–Sn2–C71	112.1 (2)	C51–Sn2–C61	105.2 (2)
C51–Sn2–C71	103.1 (2)	C61–Sn2–C71	103.2 (2)

[a] Cp3, Cp4, Cp8, and Cp9 refer to the cyclopentadienyl rings numbered C31–C35, C41–C45, C81–C85, and C91–C95, respectively.

flections selected from a rotation photograph. These data were used to determine the crystal system. Partial rotation photographs around each axis were consistent with a triclinic crystal system. Ultimately, 30 high-angle reflections ($22° < 2\theta < 25°$) were used to obtain the final lattice parameters and the orientation matrix. Machine parameters, crystal data, and data collection parameters are summarized in Table I. The observed extinctions were consistent with the space group $P\bar{1}$. $\pm h,\pm k,+l$ data were collected in one shell ($4.5° < 2\theta < 40°$), and three standard reflections were recorded every 197 reflections. Their intensities showed no statistically significant change over the duration of the data collection. The data were processed by using the SHELX-76 program package on the computing facilities at the University of Windsor. A total of 3687 reflections with $F_o^2 > 3\sigma F_o^2$ were used in the refinement. The absorption coefficient was small ($\mu = 13.39$ cm^{-1}), and thus no absorption correction was applied to the data.

Structure Solution and Refinement. Non-hydrogen atomic scattering factors were taken from the literature tabulations.[38,39] The Sn atom position was determined by using the heavy-atom (Patterson) method. The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The initial refinements were carried out by using full-matrix least-squares techniques on F, minimizing the function $\sum w(|F_o| - |F_c|)^2$, where the weight, w, is defined as $4F_o^2/\sigma^2(F_o^2)$ and F_o and F_c are the observed and calculated structure factor amplitudes. In the final cycles of block-diagonal refinement Sn, Ti, Cl, and the cyclopentadienyl carbon atoms were assigned anisotropic temperature factors. The carbon atoms of the phenyl rings were described by isotropic thermal parameters. Hydrogen atom positions were calculated, and the atoms were allowed to ride on the carbon to which they were bonded by assuming a C–H bond length of 0.95 Å. Hydrogen atom temperature factors were fixed at 1.1 times the isotropic temperature factor of the carbon atom to which they are bonded. In all cases the hydrogen atom contributions were calculated but not refined. The final values of R and R_w are given in Table I. The maximum Δ/σ value on any of the parameters in the final cycles of the refinement and the location of the largest peaks in the final difference Fourier map calculation are also given in Table I. The residual electron densities were of no chemical significance. The following data are tabulated: positional parameters (Table II) and selected bond distances and angles (Table III). Thermal parameters (Table S1), hydrogen atom parameters (Table S2), bond distances and angles associated with the cyclopentadienyl and phenyl rings (Table S3), and values of $10|F_o|$ and $10|F_c|$ (Table S4) have been deposited as supplementary material.

Results and Discussion

The known synthetic routes to group 4/group 14 metal–metal bonds include (i) nucleophilic attack of a group 4 halide by

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(38) (a) Cromer, D. T.; Mann, J. B. *Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr.* **1968**, *A24*, 324. (b) Cromer, D. T.; Mann, J. B. *Acta Crystallogr., Sect. A: Cryst. Phys., Diffr., Theor. Gen. Crystallogr.* **1968**, *A24*, 390.

(39) Cromer, D. T.; Waber, J. T. *International Tables for X-ray Crystallography*; Kynoch: Birmingham, England, 1974.

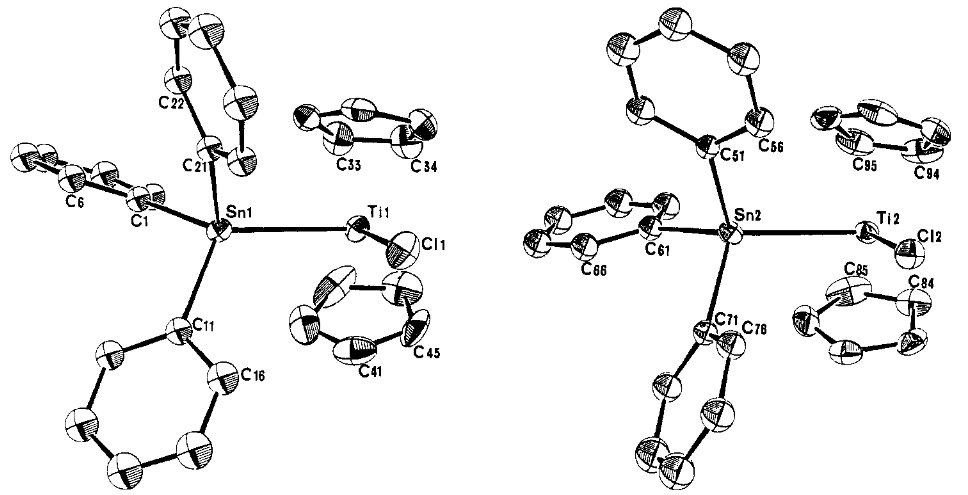

Figure 1. ORTEP drawing of the two crystallographically independent molecules of **2**. Hydrogen atoms are omitted for clarity; 30% thermal ellipsoids are shown.

$(R_3M)_nM'$ (M = Si, Ge, Sn; n = 1, M′ = Li, Na; n = 3, M′ = Al),[15,21,29,34-36] (ii) the reaction of group 4 alkyls with group 14 hydrides,[30] and (iii) oxidative additions of group 14 species $(R_3M)_2$ to low-valent group 4 species.[19] Harrod et al.[30] have recently mentioned unsuccessful attempts to use the second method for the preparation of $Cp_2Ti(SnMe_3)Me$. In addition, to our knowledge, the use of oxidative additions to form Ti–Sn bonds has not been explored. In fact, only the first route has been employed to prepare Ti–Sn-bonded compounds. Coutts and Wailes[34] have reported the use of Ph_3SnLi in the syntheses of the Ti(IV) and Ti(III) compounds $Cp_2Ti(SnPh_3)Cl$ (**1**) and $Cp_2TiSnPh_3$. In a similar manner $Ti(SnPh_3)_4$ and $(MeO)_2Ti(SnPh_3)_2$ were prepared by Creemers et al.[35] from the appropriate titanium halide species. Related Zr and Hf species, $Cp_2M(SnPh_3)Cl$ (M = Zr (**3**), Hf (**4**)), were reported by Kingston and Lappert.[29] In our efforts to study related Ti–Sn metal–metal-bonded species we have found an alternative synthetic route to **1**. While investigating reactions involving the generation of solutions of Ph_2SnLi_2 from Ph_2SnCl_2 and Li, we have found the formation of the dianion is not complete. Reaction of such solutions with Cp_2TiCl_2 led to the formation of a green solid, which was formulated as **1** on the basis of the comparison of the melting point and ^1H NMR data with literature data.[34] Compound **1** is isolated from the reaction mixture in 40% yield by column chromatography on silica. Although the mechanism of formation of this product is not known, it is apparent that the formation of **1** requires the migration of a phenyl group from one Sn species to another, yielding the $SnPh_3$ moiety. Such migrations of substituents have been noted in other reactions of Sn species.[40]

Structure Description. The X-ray crystallographic investigation of **1** revealed that the unit cell is triclinic with two discrete molecules per asymmetric unit. The closest nonbonded distance between discrete molecules is 2.499 Å (H24···H92). An ORTEP drawing of the two independent molecules in the asymmetric unit is shown in Figure 1. The geometries of the two molecules are very similar. The coordination sphere of Ti is pseudotetrahedral in geometry. Two cyclopentadienyl rings are bonded to the Ti atoms. The Ti–C distances are typical.[6-8,11] The Cp–Ti–Cp angles are 132.5 (2) and 133.1 (2)°. These values compare with that of 132 (3)° found in $Cp_2Ti(SiMe_3)Cl$ (**2**).[15] A chlorine atom and the $SnPh_3$ groups complete each of the Ti coordination spheres of **1**. The Ti–Cl distances of 2.324 (2) and 2.337 (2) Å are slightly longer than the Ti–Cl distance seen in **2** (2.31 (1) Å).[15] The Ti–Sn distance is 2.843 (1) Å in both molecules in the asymmetric unit. To our knowledge this represents the first report of a crystallographic study of a compound containing a Ti–Sn bond. The Sn–Ti–Cl angles are 86.8 (1) and 85.7 (1)°, which are comparable to the Si–Ti–Cl angle of 87 (1)° found in **2**.[15] The geometries about the tin atoms in the two independent molecules in the asymmetric unit are similar, both being pseudotetrahedral. Sn–C bond lengths average 2.169 Å, which are typical.[19,24,33,34] The Ti–Sn–C angles range from 108.6 to117.8°, while the C–Sn–C angles fall between 102.5 and 105.2°. This distortion of the geometry about tin may arise from steric interaction between the phenyl and cyclopentadienyl rings. The difference between the crystallographically independent molecules is the helical orientation of the phenyl rings of the $SnPh_3$ group.

The Ti–Sn distance found in **1** (2.843 (1) Å) is longer than the sum of the covalent radii for Ti and Sn (2.77 Å). Similar "long" bonds are seen in other early-transition-metal–tin species (i.e., $Cp_2Nb(CO)SnPh_3$ (2.825 (2) Å),[32] $(MeCp)_2Nb(CO)SnCl_3$ (2.764 (1) Å),[32] and $(C_6H_5Me)_2Hf(SnMe_3)_2$ (2.953 (1) Å)[19]). The length of these bonds has been attributed to a minimization of the steric interactions between the substituents on the tin and the Cp groups. This may also be true in the present compound as the closest approach of the phenyl rings to the cyclopentadienyl rings is 2.660 Å (H32···H22). It is noteworthy that in **2** the Ti–Si distance was found to be 2.67 (1) Å,[15] 0.2 Å longer than the sum of the covalent radii of Ti and Si. In compound **1**, the Ti–Sn distance is 0.07 Å longer than the sum of the covalent radii. The length of the Ti–Sn bond suggests that the bond is inherently weak and thus susceptible to attack. This may account for difficulties in manipulation and the extreme air sensitivity of **1**.

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Supplementary Material Available: Thermal parameters (Table S1), hydrogen atom parameters (Table S2), and bond distances and angles associated with the phenyl and cyclopentadienyl rings (Table S3) (7 pages); values of $10|F_o|$ and $10|F_c|$ (Table S4) (13 pages). Ordering information is given on any current masthead page.

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(40) Wells, W. L. *J. Organomet. Chem.* **1968**, *11*, 271.