

Reaction between InCl_3 and $\text{Li}(\text{C}_5\text{H}_5)$ in Et_2O by using the Literature

Procedure.⁸ Three independent reactions with purified reagents and carefully controlled the reaction conditions were investigated. The reagent $\text{Li}(\text{C}_5\text{H}_5)$ was freshly prepared, isolated and purified. The benzene mixture was heated with an oil bath in order to carefully control temperature. Even with these precautions, experimental observations were consistent with thermal decomposition of $\text{In}(\text{C}_5\text{H}_5)_3$. The percent carbon and hydrogen for each of the three products was low. Second, the chemical shift of resonance for the cyclopentadienide protons was variable but the chemical shift was always lower than that of analytically pure $\text{In}(\text{C}_5\text{H}_5)_3$. Lastly, the insoluble material from the preparative reaction changed color from yellow to brownish orange as the benzene was heated. **Reaction 1.** Reagents: 4.30 g (19.4 mmol) of InCl_3 , 4.32 g (60.0 mmol) of $\text{Li}(\text{C}_5\text{H}_5)$. Product: Bright yellow powder, 4.63 g (14.9 mmol if pure $\text{In}(\text{C}_5\text{H}_5)_3$, 76.8 % based on InCl_3). Properties: Mp: 152 – 164 °C (dec., color change to orange). ^1H NMR (THF-d_8): δ 5.862 (s). Anal. Calcd. for $\text{C}_{15}\text{H}_{15}\text{In}$: C, 58.10; H, 4.88; In, 37.03. Found C, 47.25; H, 4.22. Solubility: Soluble in THF. No appreciable solubility in Et_2O , C_6H_6 , C_5H_{12} or CHCl_3 . **Reaction 2.** Reagents: 2.22 g (10.0 mmol) of InCl_3 , 2.25 g (31.2 mmol) of $\text{Li}(\text{C}_5\text{H}_5)$. Product: Bright yellow powder, 1.92 g (6.19 mmol if pure $\text{In}(\text{C}_5\text{H}_5)_3$, 61.9 % based on InCl_3). Properties: Mp: 136 – 170 °C (dec., color change to orange). ^1H NMR (THF-d_8): δ 5.963 (s). Anal. Found C, 54.60; H, 4.47. **Reaction 3.** Reagents: 2.21 g (10.0 mmol) of InCl_3 , 2.28 g (31.6 mmol) of $\text{Li}(\text{C}_5\text{H}_5)$. Product: Bright yellow powder, 1.83 g (5.90 mmol if pure $\text{In}(\text{C}_5\text{H}_5)_3$, 59.0% based on InCl_3). Properties: Mp: 150 – 169 °C (dec., color change to orange). ^1H NMR (THF-d_8): δ 5.786 (s). Anal. Found C, 54.18; H, 4.85; In, 33.56.

Solubility and Stability of $\text{In}(\text{C}_5\text{H}_5)_3$ in C_6D_6 . Pure $\text{In}(\text{C}_5\text{H}_5)_3$ was placed in a small vessel with an attached NMR tube and then carefully dried d_6 -benzene was added by vacuum distillation. The sample was then heated in an oil bath at 70 °C for 1 h and then allowed to cool to room temperature. A bright yellow solution above a small amount of a yellow solid was present. A portion of the solution was then carefully decanted into the NMR tube. The NMR tube and vessel were cooled with liquid nitrogen in order to flame-seal the NMR tube. After the NMR tube was warmed to room temperature, a yellow precipitate was present. The mixture was reheated to 70 °C for another hour but complete dissolution of the solid did not occur. The tube was cooled to room temperature

and an NMR spectrum was recorded. The sample was reheated at 60 °C for various times and NMR spectra were recorded.

Another sample of $\text{In}(\text{C}_5\text{H}_5)_3$ was placed in a second small vessel with an attached NMR tube so that a standard solution that had received no external heating could be prepared. This mixture was stirred at room temperature without heating for 2 h. A yellow precipitate was observed beneath the colorless liquid phase. The liquid was then carefully decanted into the NMR tubes and then the tube was flame sealed. **Unheated sample:** ^1H NMR (C_6D_6): δ 7.15 (s, $\text{C}_6\text{D}_5\text{H}$ -impurity, 4H), 6.14 (s, C_5H_5 , 1H). **Heated sample:** ^1H NMR (C_6D_6 , Initial spectrum): δ 7.15 (s, $\text{C}_6\text{D}_5\text{H}$ -impurity, 1.67 H), 6.12 (s, C_5H_5 , 5.00 H), 6.49 (m, 0.17 H, C_5H_6), 6.30 (m, 0.25 H, C_5H_6), 3.39 (s, 0.07 H), 2.99 (s, 0.06 H), 2.69 (m, 0.22 H, C_5H_6), 1.28 (m, 0.45 H) 0.83 (m, 0.15 H), 0.30 (m, 0.06 H). Spectrum after heating sample in NMR tube at 60 °C for 48 h: δ 7.15 (s, $\text{C}_6\text{D}_5\text{H}$ -impurity, 4.59 H) 6.04 (s, C_5H_5 , 5.00 H), 6.49 (m, 0.91 H), 6.30 (m, 0.95 H), 3.39 (s, 0.19 H), 2.99 (s, 1.08 H), 2.69 (m, 1.03 H), 2.15 (br, 1.76 H) 1.38 (br, 0.69 H), 0.86 (m, 0.02 H), 0.30 (br, 0.02 H). Spectrum after heating sample in NMR tube at 60 °C for 72 h: 7.15 (s, $\text{C}_6\text{D}_5\text{H}$ -impurity, 6.98 H) 5.96 (s, C_5H_5 , 5.00 H), 6.49 (m, 1.02 H), 6.30 (m, 1.15 H), 5.55 (br, 0.91 H), 3.57 (s, 0.29 H), 3.11 (br, 2.25 H), 2.69 (m, 1.67 H), 2.15 (br, 3.31 H) 1.42 (br, 1.24 H), 0.30 (br, 0.01 H).

Variable Temperature NMR Spectral Data for THF Solutions of

Heteroleptic Organoindium(III) Cyclopentadienide Derivatives: $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$: ^1H NMR (THF-d_8 , $T = -30$ °C): 6.02 (s, C_5H_5 , 5.00H), -0.53 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$ and InMe_3 , 5.71H), -1.22 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 0.18H). (-40 °C): 5.99 (s, C_5H_5 , 5.00H), -0.53 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 4.42H), -0.56 (s, InMe_3 , 0.68H), -1.27 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 0.14H). (-60 °C): 5.99 (s, C_5H_5 , 5.00H), -0.53 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 4.68H), -0.55 (s, InMe_3 , 0.69H), -1.35 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 0.11 H). (-80 °C): 5.96 (s, C_5H_5 , 5.00H), -0.53 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 5.14H), -0.56 (s, InMe_3 , 0.58H), -1.53 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 0.11H). (-90 °C): 5.97 (s, C_5H_5 , 5.00H), -0.53 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 4.95H), -0.56 (s, InMe_3 , 0.85H), -1.64 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 0.17H). **$(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$:** ^1H NMR (THF-d_8 , $T = 0$ °C): δ 6.08 (s, C_5H_5 , 4.17H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.65H), 0.58 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.50H), 0.83 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.27H), 1.11 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.74H), 0.81 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.60H). (-20 °C): 6.04 (s, C_5H_5 , 0.44H), 6.08 (s, C_5H_5 , 4.30H), 0.98 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.31H), 0.55 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.44H), 0.83 (s,

$(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.27H), 1.01 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.61H), 0.80 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.59H). (-30 °C): 6.07 (s, C_5H_5 , 0.84 H), 6.08 (s, C_5H_5 , 3.94H), 0.98 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.21H), 0.54 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.56H), 0.84 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.34H), 1.01 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.54H), 0.79 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.60H). (-40 °C): 6.07 (s, C_5H_5 , 0.69H), 6.08 (s, C_5H_5 , 3.91H), 0.98 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.15H), 0.53 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.50H), 0.84 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.47H), 1.01 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.72H), 0.79 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.57H). (-50 °C): ^1H NMR: (THF- d_8 , δ) 6.07 (s, C_5H_5 , 0.68H), 6.08 (s, C_5H_5 , 4.12H), 0.98 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.28H), 0.52 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.42H), 0.84 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.58H), 1.00 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.37H), 0.78 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.58H). (-60 °C): 6.07 (s, C_5H_5 , 1.11H), 6.08 (s, C_5H_5 , 3.92H), 0.98 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 15.60H), 0.51 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 3.38H), 0.84 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 0.37H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 2.04H), 0.77 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.57H). **$\text{MeIn}(\text{C}_5\text{H}_5)_2$** : ^1H NMR (THF- d_8 , -15 °C): 5.95 (s, C_5H_5 , 9.90 H), -0.32 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 1.56H), -1.19 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.56H). (-30 °C): 5.93 (br, C_5H_5 , 9.90H), -0.28 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 1.75H), 1.23 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.48H); (-40 °C): 5.85 (br, C_5H_5 , 10.00H), -0.21 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 1.79H), -1.28 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.20H); (-60 °C): 6.06 (s, C_5H_5 , 4.39H), 5.72 (s, C_5H_5 , 5.50H), -0.13 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 1.94H), -1.38 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.16H); (-70 °C): 6.03 (s, C_5H_5 , 5.00H), 5.71 (s, C_5H_5 , 4.93H), -0.12 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 1.85H), -1.40 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.23H); (-80 °C): 6.02 (s, C_5H_5 , 4.59H), 5.71 (s, C_5H_5 , 5.15H), -0.03 (s, $\text{Me}_2\text{In}(\text{C}_5\text{H}_5)$, 2.15H), -1.49 (s, $\text{MeIn}(\text{C}_5\text{H}_5)_2$, 1.10H). **$(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$** : ^1H NMR (THF- d_8 , T = 0 °C): δ 6.03 (s, C_5H_5 , 10.70H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.87H), 0.59 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.18H), 0.83 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 7.46H), 0.34 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.72H), 1.10 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.09H). (-20 °C): 6.04 (s, C_5H_5 , 11.03H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.82H), 0.57 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.17H), 0.84 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 7.23H), 0.31 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.68H), 1.10 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.07H). (-30 °C): 6.04 (s, C_5H_5 , 10.90H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.80H), 0.56 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.15H), 0.84 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 7.44H), 0.30 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.70H), 1.10 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.09H). (-40 °C): 5.95 (s, C_5H_5 , 3.12H), 6.05 (s, C_5H_5 , 8.53H), 0.99 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.78H), 0.56 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.03H), 0.84 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 6.91H), 0.27 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.59H), 1.10 (s,

$(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.06H). (-50 °C): 5.94 (s, C_5H_5 , 2.78H), 6.05 (s, C_5H_5 , 8.45H), 1.00 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.74H), 0.54 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.01H), 0.84 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 7.35H), 0.25 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.60H), 1.10 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.05H). (-60 °C): 5.93 (s, C_5H_5 , 2.61H), 6.05 (s, C_5H_5 , 8.41H), 1.00 (s, $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$, 0.58H), 0.85 (s, $\text{Me}_3\text{CCH}_2\text{In}(\text{C}_5\text{H}_5)_2$, 7.56H), 0.24 (s, $(\text{Me}_3\text{CCH}_2)\text{In}(\text{C}_5\text{H}_5)_2$, 1.63H), 1.10 (s, $(\text{Me}_3\text{CCH}_2)_3\text{In}$, 0.20H).

Table 1. Atomic coordinates (10^4) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{In}(\text{C}_5\text{H}_5)_3$.

Atom	x	y	z	U(eq)
In(1)	8979(1)	2403(1)	3795(1)	9(1)
C(1)	10030(4)	1709(4)	4549(2)	14(1)
C(2)	10285(4)	3044(4)	4808(2)	12(1)
C(3)	11581(4)	3459(4)	4685(2)	13(1)
C(4)	12212(4)	2396(5)	4369(2)	21(1)
C(5)	11321(4)	1330(4)	4292(2)	18(1)
C(6)	7596(4)	533(4)	3467(2)	10(1)
C(7)	7085(4)	115(4)	3980(2)	10(1)
C(8)	7836(4)	-1052(4)	4158(2)	10(1)
C(9)	8821(4)	-1353(4)	3741(2)	13(1)
C(10)	8669(4)	-430(4)	3327(2)	14(1)
C(11)	9838(4)	3369(4)	3048(2)	11(1)
C(12)	10624(4)	2235(4)	2790(2)	13(1)
C(13)	11971(4)	2498(4)	2849(2)	15(1)
C(14)	12137(4)	3817(4)	3118(2)	15(1)
C(15)	10879(4)	4345(4)	3233(2)	13(1)

Table 2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{In}(\text{C}_5\text{H}_5)_3$.

Atom	U11	U22	U33	U23	U13	U12
In(1)	8(1)	8(1)	11(1)	0(1)	-1(1)	0(1)
C(1)	12(2)	15(2)	14(2)	5(2)	-5(2)	-3(2)
C(2)	17(2)	13(2)	6(2)	2(2)	-2(2)	5(2)
C(3)	14(2)	13(2)	10(2)	3(2)	-2(2)	-4(2)
C(4)	9(2)	41(3)	13(2)	7(2)	2(2)	2(2)
C(5)	23(3)	18(2)	12(2)	-3(2)	-11(2)	10(2)
C(6)	12(2)	6(2)	11(2)	0(2)	-5(2)	-2(2)
C(7)	3(2)	14(2)	11(2)	-5(2)	1(2)	-3(2)
C(8)	9(2)	9(2)	13(2)	2(2)	-1(2)	-7(2)
C(9)	5(2)	9(2)	26(2)	0(2)	-2(2)	-1(2)
C(10)	14(2)	13(2)	16(2)	-4(2)	6(2)	-7(2)
C(11)	6(2)	12(2)	13(2)	6(2)	3(2)	0(2)
C(12)	17(2)	10(2)	12(2)	0(2)	4(2)	-2(2)
C(13)	15(2)	14(2)	15(2)	8(2)	2(2)	3(2)
C(14)	9(2)	22(2)	13(2)	3(2)	0(2)	-3(2)
C(15)	19(2)	10(2)	9(2)	2(2)	1(2)	-1(2)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for $\text{In}(\text{C}_5\text{H}_5)_3$.

$\text{In}(1)-\text{C}(11)$	2.229(4)	$\text{C}(6)-\text{In}(1)-\text{C}(8)\#1$	99.4(1)
$\text{In}(1)-\text{C}(1)$	2.229(4)	$\text{C}(2)-\text{C}(1)-\text{C}(5)$	105.2(3)
$\text{In}(1)-\text{C}(6)$	2.389(4)	$\text{C}(2)-\text{C}(1)-\text{In}(1)$	100.7(2)
$\text{In}(1)-\text{C}(8)\#1$	2.482(4)	$\text{C}(5)-\text{C}(1)-\text{In}(1)$	96.4(3)
$\text{C}(1)-\text{C}(2)$	1.453(6)	$\text{C}(3)-\text{C}(2)-\text{C}(1)$	108.5(4)
$\text{C}(1)-\text{C}(5)$	1.461(6)	$\text{C}(2)-\text{C}(3)-\text{C}(4)$	108.6(4)
$\text{C}(2)-\text{C}(3)$	1.366(6)	$\text{C}(5)-\text{C}(4)-\text{C}(3)$	109.6(4)
$\text{C}(3)-\text{C}(4)$	1.423(6)	$\text{C}(4)-\text{C}(5)-\text{C}(1)$	108.0(4)
$\text{C}(4)-\text{C}(5)$	1.358(6)	$\text{C}(7)-\text{C}(6)-\text{C}(10)$	106.9(3)
$\text{C}(6)-\text{C}(7)$	1.419(6)	$\text{C}(7)-\text{C}(6)-\text{In}(1)$	96.3(2)
$\text{C}(6)-\text{C}(10)$	1.442(5)	$\text{C}(10)-\text{C}(6)-\text{In}(1)$	98.5(2)
$\text{C}(7)-\text{C}(8)$	1.408(5)	$\text{C}(8)-\text{C}(7)-\text{C}(6)$	108.6(3)
$\text{C}(8)-\text{C}(9)$	1.441(5)	$\text{C}(7)-\text{C}(8)-\text{C}(9)$	106.6(3)
$\text{C}(8)-\text{In}(1)\#2$	2.482(4)	$\text{C}(7)-\text{C}(8)-\text{In}(1)\#2$	89.2(2)
$\text{C}(9)-\text{C}(10)$	1.360(5)	$\text{C}(9)-\text{C}(8)-\text{In}(1)\#2$	95.9(2)
$\text{C}(11)-\text{C}(15)$	1.458(5)	$\text{C}(10)-\text{C}(9)-\text{C}(8)$	109.5(4)
$\text{C}(11)-\text{C}(12)$	1.476(5)	$\text{C}(9)-\text{C}(10)-\text{C}(6)$	108.4(4)
$\text{C}(12)-\text{C}(13)$	1.352(6)	$\text{C}(15)-\text{C}(11)-\text{C}(12)$	104.0(3)
$\text{C}(13)-\text{C}(14)$	1.438(5)	$\text{C}(15)-\text{C}(11)-\text{In}(1)$	105.7(3)
$\text{C}(14)-\text{C}(15)$	1.363(6)	$\text{C}(12)-\text{C}(11)-\text{In}(1)$	104.4(2)
$\text{C}(11)-\text{In}(1)-\text{C}(1)$	129.9(2)	$\text{C}(13)-\text{C}(12)-\text{C}(11)$	109.1(4)
$\text{C}(11)-\text{In}(1)-\text{C}(6)$	104.2(1)	$\text{C}(12)-\text{C}(13)-\text{C}(14)$	108.8(4)
$\text{C}(1)-\text{In}(1)-\text{C}(6)$	108.8(1)	$\text{C}(15)-\text{C}(14)-\text{C}(13)$	108.7(4)
$\text{C}(11)-\text{In}(1)-\text{C}(8)\#1$	108.8(1)	$\text{C}(14)-\text{C}(15)-\text{C}(11)$	109.2(3)
$\text{C}(1)-\text{In}(1)-\text{C}(8)\#1$	102.0(1)		

Symmetry transformations used to generate equivalent atoms:

#1 $-x+3/2, y+1/2, z$; #2 $-x+3/2, y-1/2, z$.**Table 4.** Hydrogen coordinates (10^4) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{In}(\text{C}_5\text{H}_5)_3$.

Atom	x	y	z	U(eq)
H(1)	9460(40)	1140(40)	4638(17)	16
H(2)	9660(40)	3550(40)	5021(16)	15
H(3)	11800(40)	4260(40)	4776(16)	15
H(4)	13010(50)	2480(40)	4276(17)	25
H(5)	11460(40)	580(50)	4117(18)	21
H(6)	7170(40)	1100(40)	3236(15)	12
H(7)	6480(40)	390(40)	4170(16)	11
H(8)	7790(40)	-1380(40)	4514(15)	12
H(9)	9460(50)	-1990(50)	3789(14)	16
H(10)	9100(40)	-450(40)	2997(17)	17
H(11)	9090(40)	3630(40)	2903(16)	13
H(12)	10300(40)	1450(40)	2628(16)	15
H(13)	12710(40)	1890(40)	2695(15)	18
H(14)	12930(40)	4220(40)	3230(16)	18
H(15)	10640(40)	5180(40)	3410(16)	15

Table 5. Atomic coordinates (10^4) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{In}(\text{C}_5\text{H}_5)_3\text{PPh}_3$.

Atom	x	y	z	U(eq)
In(1)	9417(1)	5992(1)	2410(1)	12(1)
P(1)	11491(1)	6989(1)	2559(1)	11(1)
C(1)	8314(2)	5942(1)	1027(1)	19(1)
C(2)	7048(2)	5782(2)	1085(1)	26(1)
C(3)	6422(2)	6563(2)	995(1)	33(1)
C(4)	7212(2)	7229(2)	846(1)	30(1)
C(5)	8345(2)	6868(1)	841(1)	22(1)
C(6)	8400(2)	6711(1)	3193(1)	22(1)
C(7)	7683(2)	5962(1)	3303(1)	27(1)
C(8)	8308(2)	5590(1)	4068(1)	26(1)
C(9)	9399(2)	6103(1)	4477(1)	24(1)
C(10)	9454(2)	6793(1)	3968(1)	22(1)
C(11)	10290(2)	4697(1)	2944(1)	18(1)
C(12)	9194(2)	4129(1)	2621(1)	20(1)
C(13)	9248(2)	3756(1)	1890(1)	22(1)
C(14)	10380(2)	4049(1)	1736(1)	21(1)
C(15)	11034(2)	4591(1)	2376(1)	19(1)
C(16)	11211(1)	8120(1)	2771(1)	13(1)
C(17)	11615(2)	8457(1)	3582(1)	17(1)
C(18)	11324(2)	9312(1)	3731(1)	21(1)
C(19)	10649(2)	9842(1)	3067(1)	21(1)
C(20)	10239(2)	9507(1)	2258(1)	21(1)
C(21)	10504(2)	8651(1)	2108(1)	18(1)
C(22)	11990(1)	7020(1)	1631(1)	13(1)
C(23)	11665(2)	6331(1)	1056(1)	15(1)
C(24)	12092(2)	6328(1)	362(1)	18(1)
C(25)	12842(2)	7004(1)	238(1)	19(1)
C(26)	13164(2)	7691(1)	804(1)	19(1)
C(27)	12738(2)	7704(1)	1498(1)	16(1)
C(28)	12891(2)	6657(1)	3418(1)	13(1)
C(29)	12717(2)	6239(1)	4114(1)	16(1)
C(30)	13771(2)	6002(1)	4789(1)	20(1)
C(31)	14999(2)	6179(1)	4776(1)	18(1)
C(32)	15174(2)	6592(1)	4085(1)	18(1)
C(33)	14127(2)	6826(1)	3407(1)	16(1)

Table 6. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

Atom	U11	U22	U33	U23	U13	U12
In(1)	11(1)	14(1)	11(1)	0(1)	3(1)	1(1)
P(1)	12(1)	12(1)	10(1)	0(1)	3(1)	0(1)
C(1)	16(1)	23(1)	15(1)	-2(1)	1(1)	0(1)
C(2)	17(1)	38(1)	20(1)	3(1)	0(1)	-7(1)
C(3)	16(1)	56(1)	24(1)	7(1)	3(1)	8(1)
C(4)	32(1)	33(1)	22(1)	6(1)	3(1)	14(1)
C(5)	22(1)	26(1)	14(1)	2(1)	2(1)	0(1)
C(6)	21(1)	26(1)	21(1)	1(1)	11(1)	6(1)

C(7)	17(1)	40(1)	27(1)	-6(1)	12(1)	-3(1)
C(8)	26(1)	30(1)	31(1)	1(1)	20(1)	-1(1)
C(9)	23(1)	34(1)	18(1)	-1(1)	12(1)	5(1)
C(10)	22(1)	25(1)	23(1)	-7(1)	11(1)	1(1)
C(11)	23(1)	14(1)	16(1)	1(1)	3(1)	0(1)
C(12)	22(1)	18(1)	22(1)	2(1)	8(1)	-3(1)
C(13)	25(1)	18(1)	20(1)	-1(1)	3(1)	-2(1)
C(14)	25(1)	18(1)	21(1)	3(1)	9(1)	6(1)
C(15)	17(1)	16(1)	25(1)	6(1)	5(1)	3(1)
C(16)	12(1)	13(1)	13(1)	-1(1)	4(1)	0(1)
C(17)	19(1)	17(1)	13(1)	-1(1)	3(1)	0(1)
C(18)	25(1)	21(1)	17(1)	-6(1)	6(1)	0(1)
C(19)	23(1)	15(1)	24(1)	-4(1)	6(1)	4(1)
C(20)	23(1)	17(1)	20(1)	2(1)	2(1)	7(1)
C(21)	20(1)	18(1)	13(1)	0(1)	2(1)	4(1)
C(22)	13(1)	14(1)	11(1)	1(1)	4(1)	2(1)
C(23)	17(1)	14(1)	15(1)	0(1)	5(1)	-2(1)
C(24)	22(1)	18(1)	14(1)	-3(1)	5(1)	1(1)
C(25)	18(1)	26(1)	13(1)	2(1)	7(1)	2(1)
C(26)	18(1)	23(1)	16(1)	2(1)	6(1)	-5(1)
C(27)	18(1)	16(1)	14(1)	-1(1)	4(1)	-3(1)
C(28)	15(1)	10(1)	11(1)	-1(1)	1(1)	1(1)
C(29)	15(1)	18(1)	14(1)	0(1)	3(1)	-1(1)
C(30)	21(1)	21(1)	14(1)	2(1)	2(1)	0(1)
C(31)	17(1)	18(1)	16(1)	-1(1)	-1(1)	3(1)
C(32)	13(1)	19(1)	19(1)	-3(1)	3(1)	1(1)
C(33)	15(1)	16(1)	16(1)	1(1)	5(1)	1(1)

Table 7. Bond lengths [Å] and angles [°] for $\text{In}(\text{C}_5\text{H}_5)_3\text{PPh}_3$.

In(1)-C(1)	2.256(2)	C(13)-C(14)	1.429(3)
In(1)-C(11)	2.263(2)	C(14)-C(15)	1.369(3)
In(1)-C(6)	2.270(2)	C(16)-C(17)	1.392(2)
In(1)-P(1)	2.6992(4)	C(16)-C(21)	1.399(2)
P(1)-C(22)	1.814(2)	C(17)-C(18)	1.390(2)
P(1)-C(16)	1.816(2)	C(18)-C(19)	1.390(3)
P(1)-C(28)	1.821(2)	C(19)-C(20)	1.387(3)
C(1)-C(5)	1.455(3)	C(20)-C(21)	1.385(2)
C(1)-C(2)	1.456(3)	C(22)-C(27)	1.396(2)
C(2)-C(3)	1.367(3)	C(22)-C(23)	1.397(2)
C(3)-C(4)	1.417(3)	C(23)-C(24)	1.392(2)
C(4)-C(5)	1.372(3)	C(24)-C(25)	1.383(2)
C(6)-C(7)	1.439(3)	C(25)-C(26)	1.386(2)
C(6)-C(10)	1.451(3)	C(26)-C(27)	1.391(2)
C(7)-C(8)	1.375(3)	C(28)-C(33)	1.397(2)
C(8)-C(9)	1.420(3)	C(28)-C(29)	1.400(2)
C(9)-C(10)	1.372(3)	C(29)-C(30)	1.391(2)
C(11)-C(12)	1.449(2)	C(30)-C(31)	1.392(3)
C(11)-C(15)	1.454(3)	C(31)-C(32)	1.389(2)
C(12)-C(13)	1.372(3)	C(32)-C(33)	1.388(2)
C(1)-In(1)-C(11)	113.68(6)	C(1)-In(1)-P(1)	106.22(5)
C(1)-In(1)-C(6)	114.09(7)	C(11)-In(1)-P(1)	102.53(5)
C(11)-In(1)-C(6)	115.02(7)	C(6)-In(1)-P(1)	103.57(5)

C(22)-P(1)-C(16)	105.10(7)	C(14)-C(15)-C(11)	108.4(2)
C(22)-P(1)-C(28)	105.93(7)	C(17)-C(16)-C(21)	119.3(2)
C(16)-P(1)-C(28)	105.46(7)	C(17)-C(16)-P(1)	121.6(1)
C(22)-P(1)-In(1)	114.63(5)	C(21)-C(16)-P(1)	119.0(1)
C(16)-P(1)-In(1)	111.46(5)	C(18)-C(17)-C(16)	120.3(3)
C(28)-P(1)-In(1)	113.48(5)	C(19)-C(18)-C(17)	120.1(2)
C(5)-C(1)-C(2)	105.6(2)	C(20)-C(19)-C(18)	119.7(2)
C(5)-C(1)-In(1)	98.5(1)	C(21)-C(20)-C(19)	120.4(2)
C(2)-C(1)-In(1)	98.8(1)	C(20)-C(21)-C(16)	120.2(2)
C(3)-C(2)-C(1)	108.0(2)	C(27)-C(22)-C(23)	119.4(1)
C(2)-C(3)-C(4)	109.3(2)	C(27)-C(22)-P(1)	121.0(1)
C(5)-C(4)-C(3)	109.1(2)	C(23)-C(22)-P(1)	119.5(1)
C(4)-C(5)-C(1)	107.9(2)	C(24)-C(23)-C(22)	120.1(2)
C(7)-C(6)-C(10)	105.8(2)	C(25)-C(24)-C(23)	120.2(2)
C(7)-C(6)-In(1)	94.7(1)	C(24)-C(25)-C(26)	120.1(2)
C(10)-C(6)-In(1)	99.1(1)	C(25)-C(26)-C(27)	120.3(2)
C(8)-C(7)-C(6)	108.5(28)	C(26)-C(27)-C(22)	120.0(2)
C(7)-C(8)-C(9)	108.7(2)	C(33)-C(28)-C(29)	119.4(1)
C(10)-C(9)-C(8)	108.9(2)	C(33)-C(28)-P(1)	121.8(1)
C(9)-C(10)-C(6)	108.1(2)	C(29)-C(28)-P(1)	118.8(1)
C(12)-C(11)-C(15)	105.5(2)	C(30)-C(29)-C(28)	119.9(2)
C(12)-C(11)-In(1)	100.2(1)	C(29)-C(30)-C(31)	120.3(2)
C(15)-C(11)-In(1)	95.5(1)	C(32)-C(31)-C(30)	119.9(2)
C(13)-C(12)-C(11)	108.4(2)	C(33)-C(32)-C(31)	120.2(2)
C(12)-C(13)-C(14)	108.8(2)	C(32)-C(33)-C(28)	120.3(2)
C(15)-C(14)-C(13)	108.7(2)		

Table 8. Hydrogen coordinates (10^4) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{In}(\text{C}_5\text{H}_5)_3\text{PPh}_3$

Atom	x	y	z	U(eq)
H(1A)	8790(20)	5509(14)	811(13)	23
H(2A)	6750(20)	5190(16)	1159(14)	32
H(3A)	5560(20)	6678(17)	1036(15)	39
H(4A)	7000(20)	7803(17)	783(15)	36
H(5A)	9010(20)	7144(15)	776(14)	26
H(6A)	8110(20)	7155(15)	2884(14)	26
H(7A)	6980(20)	5784(15)	2914(16)	32
H(8A)	8120(20)	5120(16)	4259(15)	32
H(9A)	10000(20)	5979(14)	5002(16)	29
H(10A)	10030(20)	7271(15)	4078(14)	26
H(11A)	10643(19)	4817(14)	3531(13)	22
H(12A)	8570(20)	4072(13)	2891(14)	24
H(13A)	8640(20)	3326(15)	1537(14)	26
H(14A)	10610(20)	3924(14)	1285(15)	25
H(15A)	11880(20)	4836(14)	2468(13)	23
H(17A)	12100(19)	8085(14)	4053(13)	20
H(18A)	11590(20)	9495(14)	4279(14)	25
H(19A)	10480(20)	10404(15)	3178(14)	26
H(20A)	9760(20)	9887(14)	1794(13)	26
H(21A)	10200(20)	8430(14)	1545(13)	21
H(23A)	11190(20)	5845(13)	1154(13)	18
H(24A)	11910(20)	5849(13)	-14(14)	22

H(25A)	13142 (19)	7017 (14)	-197 (13)	22
H(26A)	13670 (20)	8157 (14)	715 (13)	23
H(27A)	12956 (19)	8162 (14)	1876 (13)	20
H(29A)	11870 (20)	6155 (13)	4136 (14)	19
H(30A)	13610 (20)	5731 (14)	5226 (14)	23
H(31A)	15730 (20)	6033 (13)	5244 (14)	22
H(32A)	15960 (20)	6693 (14)	4063 (13)	21
H(33A)	14263 (19)	7151 (13)	2986 (13)	19

Table 9. Atomic coordinates (10^4) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) at 90.0(1)K for $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$.

Atom	x	y	z	U (eq)
In(1)	7626 (1)	4130 (1)	4517 (1)	12 (1)
In(2)	2626 (1)	4169 (1)	2968 (1)	12 (1)
In(3)	2043 (1)	9200 (1)	456 (1)	12 (1)
In(4)	7067 (1)	9259 (1)	2034 (1)	11 (1)
C(1)	5732 (5)	4751 (3)	3826 (2)	22 (1)
C(2)	5467 (4)	4036 (4)	3397 (2)	21 (1)
C(3)	4476 (5)	3481 (3)	3680 (3)	18 (1)
C(4)	4143 (5)	3838 (3)	4293 (2)	22 (1)
C(5)	4876 (5)	4619 (3)	4369 (2)	28 (1)
C(6)	736 (5)	3564 (4)	3688 (2)	21 (1)
C(7)	-98 (5)	3665 (3)	3122 (2)	24 (1)
C(8)	-851 (5)	4444 (3)	3196 (2)	21 (1)
C(9)	-537 (5)	4829 (3)	3808 (2)	17 (1)
C(10)	450 (4)	4277 (3)	4103 (2)	16 (1)
C(11)	7891 (5)	5223 (4)	5198 (2)	32 (1)
C(12)	7527 (6)	5194 (4)	5902 (3)	21 (1)
C(13)	7765 (7)	6079 (5)	6246 (4)	51 (2)
C(14)	8519 (7)	4506 (4)	6236 (3)	49 (2)
C(15)	6114 (6)	4846 (4)	6033 (3)	44 (2)
C(16)	7627 (5)	2730 (4)	4295 (2)	14 (1)
C(17)	7765 (4)	2057 (4)	4837 (3)	13 (1)
C(18)	6537 (6)	2143 (4)	5296 (3)	27 (1)
C(19)	9113 (5)	2197 (4)	5204 (3)	25 (1)
C(20)	7781 (4)	1107 (4)	4557 (3)	21 (1)
C(21)	2622 (5)	5574 (3)	3201 (2)	13 (1)
C(22)	2681 (5)	6262 (4)	2649 (3)	15 (1)
C(23)	2588 (6)	7201 (4)	2948 (3)	21 (1)
C(24)	4061 (5)	6183 (4)	2302 (3)	23 (1)
C(25)	1480 (6)	6132 (4)	2194 (3)	28 (1)
C(26)	2838 (4)	3058 (3)	2291 (2)	16 (1)
C(27)	2532 (6)	3181 (4)	1564 (3)	19 (1)
C(28)	1076 (5)	3484 (3)	1455 (2)	26 (1)
C(29)	3560 (5)	3829 (3)	1267 (2)	29 (1)
C(30)	2720 (5)	2253 (4)	1238 (3)	28 (1)
C(31)	4095 (5)	9955 (3)	971 (2)	16 (1)
C(32)	5035 (4)	9275 (3)	826 (2)	16 (1)
C(33)	5096 (5)	8689 (3)	1348 (2)	17 (1)
C(34)	4134 (4)	9005 (3)	1824 (2)	19 (1)
C(35)	3554 (4)	9789 (3)	1598 (2)	19 (1)
C(36)	9109 (5)	8505 (3)	1526 (2)	18 (1)
C(37)	8569 (4)	8693 (3)	894 (2)	19 (1)
C(38)	9147 (4)	9479 (3)	679 (2)	16 (1)
C(39)	10113 (5)	9791 (4)	1151 (3)	18 (1)
C(40)	10064 (4)	9183 (3)	1674 (2)	17 (1)
C(41)	1613 (4)	10177 (3)	-297 (2)	19 (1)
C(42)	2511 (6)	10326 (3)	-891 (2)	17 (1)
C(43)	3993 (5)	10516 (4)	-694 (2)	34 (1)
C(44)	2487 (6)	9519 (3)	-1322 (2)	30 (1)
C(45)	1948 (7)	11125 (5)	-1277 (3)	35 (1)
C(46)	2112 (4)	7817 (4)	700 (2)	12 (1)

C(47)	2364 (5)	7150 (4)	155 (3)	14 (1)
C(48)	1189 (5)	7192 (4)	-326 (2)	18 (1)
C(49)	2440 (5)	6200 (4)	437 (3)	19 (1)
C(50)	3732 (5)	7355 (3)	-186 (3)	18 (1)
C(51)	7103 (4)	10662 (3)	1791 (3)	12 (1)
C(52)	7290 (5)	11325 (4)	2354 (3)	15 (1)
C(53)	6146 (5)	11181 (4)	2844 (2)	20 (1)
C(54)	8687 (5)	11213 (3)	2662 (3)	19 (1)
C(55)	7170 (4)	12280 (4)	2087 (3)	18 (1)
C(56)	6624 (4)	8278 (3)	2779 (2)	23 (1)
C(57)	7550 (6)	8093 (4)	3364 (3)	20 (1)
C(58)	8971 (5)	7819 (4)	3162 (2)	40 (1)
C(59)	6936 (8)	7328 (5)	3758 (4)	52 (2)
C(60)	7639 (5)	8932 (4)	3793 (3)	37 (1)

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) at 90.0(1)K
 $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$.

Atom	U11	U22	U33	U23	U13	U12
In(1)	10 (1)	12 (1)	13 (1)	-1 (1)	0 (1)	0 (1)
In(2)	9 (1)	12 (1)	14 (1)	0 (1)	1 (1)	1 (1)
In(3)	10 (1)	11 (1)	14 (1)	0 (1)	1 (1)	1 (1)
In(4)	11 (1)	11 (1)	13 (1)	1 (1)	0 (1)	0 (1)
C(1)	16 (2)	13 (2)	37 (3)	6 (2)	-7 (2)	1 (2)
C(2)	16 (2)	24 (3)	23 (2)	10 (2)	0 (2)	4 (2)
C(3)	12 (2)	16 (2)	26 (3)	5 (2)	-4 (2)	0 (2)
C(4)	9 (2)	41 (3)	17 (2)	7 (2)	-1 (2)	2 (2)
C(5)	27 (3)	32 (3)	25 (2)	-12 (2)	-13 (2)	14 (2)
C(6)	13 (2)	21 (3)	29 (3)	0 (2)	6 (2)	-1 (2)
C(7)	20 (2)	26 (2)	25 (2)	-9 (2)	8 (2)	-14 (2)
C(8)	17 (2)	31 (3)	16 (2)	5 (2)	1 (2)	-7 (2)
C(9)	14 (2)	15 (2)	22 (2)	-1 (2)	6 (2)	2 (2)
C(10)	13 (2)	16 (2)	18 (2)	0 (2)	1 (1)	-9 (2)
C(11)	33 (3)	35 (3)	28 (3)	-17 (2)	9 (2)	-15 (2)
C(12)	20 (2)	21 (2)	21 (3)	-3 (2)	-2 (2)	2 (2)
C(13)	69 (5)	40 (4)	45 (4)	-10 (3)	6 (3)	-7 (3)
C(14)	66 (4)	44 (3)	38 (3)	-9 (3)	-11 (3)	14 (3)
C(15)	40 (3)	56 (4)	37 (3)	-22 (3)	15 (3)	-21 (3)
C(16)	16 (2)	15 (2)	12 (2)	1 (2)	2 (2)	-2 (2)
C(17)	9 (3)	15 (3)	16 (3)	0 (2)	-1 (2)	1 (1)
C(18)	33 (3)	23 (3)	24 (3)	7 (2)	9 (2)	-5 (2)
C(19)	32 (3)	23 (3)	19 (3)	1 (2)	-14 (2)	6 (2)
C(20)	22 (3)	14 (3)	25 (3)	1 (2)	-1 (2)	-2 (2)
C(21)	11 (2)	12 (2)	17 (2)	0 (2)	5 (2)	1 (2)
C(22)	20 (3)	11 (2)	14 (2)	1 (2)	-1 (2)	-3 (2)
C(23)	30 (2)	12 (2)	20 (2)	0 (2)	2 (2)	-1 (2)
C(24)	30 (3)	15 (2)	23 (3)	-4 (2)	9 (2)	-3 (2)
C(25)	31 (3)	24 (3)	28 (3)	6 (2)	-10 (2)	-5 (2)
C(26)	12 (2)	15 (2)	20 (2)	-3 (2)	1 (2)	4 (2)
C(27)	15 (2)	22 (2)	22 (3)	-9 (2)	0 (2)	-2 (2)
C(28)	23 (2)	30 (2)	26 (2)	-8 (2)	-7 (2)	0 (2)

C(29)	28(2)	29(3)	31(2)	-1(2)	8(2)	-7(2)
C(30)	33(3)	22(3)	29(3)	-11(2)	4(2)	1(2)
C(31)	17(2)	10(2)	20(2)	0(2)	-9(2)	-2(2)
C(32)	12(2)	18(2)	18(2)	-1(2)	-3(1)	-4(2)
C(33)	12(2)	14(2)	25(2)	-3(2)	-7(2)	-3(2)
C(34)	11(2)	24(3)	22(2)	6(2)	-1(2)	-5(2)
C(35)	10(2)	22(2)	25(2)	-6(2)	-4(2)	1(2)
C(36)	14(2)	17(2)	23(2)	3(2)	8(2)	5(2)
C(37)	14(2)	22(2)	20(2)	-2(2)	3(2)	-1(2)
C(38)	13(2)	19(2)	17(2)	6(2)	1(2)	7(2)
C(39)	16(2)	11(2)	26(3)	1(2)	7(2)	1(2)
C(40)	11(2)	19(2)	20(2)	-2(2)	4(1)	0(2)
C(41)	20(2)	19(2)	17(2)	5(2)	1(2)	-3(2)
C(42)	22(2)	17(2)	12(2)	1(2)	-3(2)	-3(2)
C(43)	30(3)	50(3)	22(2)	2(2)	2(2)	-16(2)
C(44)	54(3)	16(2)	18(2)	0(2)	-5(2)	3(2)
C(45)	45(3)	29(3)	30(3)	11(3)	7(3)	8(3)
C(46)	15(2)	13(2)	10(2)	-1(2)	-1(1)	2(1)
C(47)	11(2)	13(2)	16(2)	-3(2)	-1(2)	-1(2)
C(48)	17(2)	20(2)	16(2)	-4(2)	-6(2)	-1(2)
C(49)	17(2)	15(2)	26(3)	-2(2)	-1(2)	-1(2)
C(50)	19(2)	12(2)	24(2)	1(2)	7(2)	4(2)
C(51)	13(2)	7(2)	17(2)	1(2)	1(1)	0(1)
C(52)	22(3)	10(2)	11(2)	-3(2)	2(2)	-2(2)
C(53)	23(2)	18(2)	18(2)	0(2)	4(2)	-1(2)
C(54)	22(2)	13(2)	22(2)	-1(2)	-4(2)	0(2)
C(55)	25(3)	12(2)	17(3)	-1(2)	-1(2)	-2(2)
C(56)	17(2)	34(3)	18(2)	12(2)	-4(2)	-10(2)
C(57)	15(2)	25(3)	20(3)	12(2)	-6(2)	-3(2)
C(58)	30(3)	68(4)	22(2)	6(2)	-3(2)	22(3)
C(59)	66(4)	53(5)	37(4)	36(4)	-22(3)	-30(4)
C(60)	40(3)	42(3)	28(2)	-5(2)	-13(2)	9(2)

Table 11. Bond lengths [Å] and angles [°] at 90.0(1)K for (Me₃CCH₂)₂In(C₅H₅).

In(1)-C(16)	2.148(5)	C(1)-C(2)	1.418(7)
In(1)-C(11)	2.180(5)	C(1)-C(5)	1.417(7)
In(1)-C(1)	2.517(5)	C(2)-C(3)	1.404(7)
In(1)-C(9)#1	2.543(5)	C(3)-C(4)	1.419(7)
In(2)-C(21)	2.160(5)	C(4)-C(5)	1.380(7)
In(2)-C(26)	2.190(4)	C(6)-C(10)	1.401(6)
In(2)-C(6)	2.539(5)	C(6)-C(7)	1.436(7)
In(2)-C(3)	2.550(5)	C(7)-C(8)	1.388(7)
In(3)-C(46)	2.135(5)	C(8)-C(9)	1.429(6)
In(3)-C(41)	2.183(4)	C(9)-C(10)	1.408(6)
In(3)-C(39)#2	2.530(5)	C(9)-In(1)#2	2.543(5)
In(3)-C(31)	2.534(4)	C(11)-C(12)	1.505(7)
In(4)-C(51)	2.162(5)	C(12)-C(15)	1.497(8)
In(4)-C(56)	2.179(4)	C(12)-C(13)	1.523(9)
In(4)-C(36)	2.519(4)	C(12)-C(14)	1.575(8)
In(4)-C(33)	2.539(5)	C(16)-C(17)	1.519(7)

C(17)-C(19)	1.532(7)	C(51)-In(4)-C(36)	109.0(2)
C(17)-C(18)	1.535(7)	C(56)-In(4)-C(36)	98.7(2)
C(17)-C(20)	1.539(8)	C(51)-In(4)-C(33)	102.1(2)
C(21)-C(22)	1.544(7)	C(56)-In(4)-C(33)	91.2(2)
C(22)-C(25)	1.517(7)	C(36)-In(4)-C(33)	102.1(2)
C(22)-C(24)	1.530(7)	C(2)-C(1)-C(5)	106.7(4)
C(22)-C(23)	1.541(8)	C(2)-C(1)-In(1)	102.3(3)
C(26)-C(27)	1.551(7)	C(5)-C(1)-In(1)	85.7(3)
C(27)-C(28)	1.507(7)	C(3)-C(2)-C(1)	108.1(4)
C(27)-C(29)	1.526(7)	C(2)-C(3)-C(4)	108.0(5)
C(27)-C(30)	1.558(8)	C(2)-C(3)-In(2)	90.2(3)
C(31)-C(32)	1.403(6)	C(4)-C(3)-In(2)	101.9(3)
C(31)-C(35)	1.426(6)	C(5)-C(4)-C(3)	107.7(4)
C(32)-C(33)	1.397(6)	C(4)-C(5)-C(1)	109.4(4)
C(33)-C(34)	1.443(6)	C(10)-C(6)-C(7)	108.2(4)
C(34)-C(35)	1.386(6)	C(10)-C(6)-In(2)	103.6(3)
C(36)-C(40)	1.411(7)	C(7)-C(6)-In(2)	83.7(3)
C(36)-C(37)	1.442(6)	C(8)-C(7)-C(6)	107.2(4)
C(37)-C(38)	1.380(6)	C(7)-C(8)-C(9)	109.0(4)
C(38)-C(39)	1.438(7)	C(10)-C(9)-C(8)	107.2(4)
C(39)-C(40)	1.418(7)	C(10)-C(9)-In(1)#2	89.2(3)
C(39)-In(3)#1	2.530(5)	C(8)-C(9)-In(1)#2	101.5(3)
C(41)-C(42)	1.529(7)	C(6)-C(10)-C(9)	108.4(4)
C(42)-C(44)	1.506(7)	C(12)-C(11)-In(1)	125.6(4)
C(42)-C(43)	1.527(7)	C(15)-C(12)-C(11)	113.8(5)
C(42)-C(45)	1.542(8)	C(15)-C(12)-C(13)	111.0(5)
C(46)-C(47)	1.530(7)	C(11)-C(12)-C(13)	113.3(5)
C(47)-C(48)	1.521(7)	C(15)-C(12)-C(14)	104.8(5)
C(47)-C(49)	1.541(8)	C(11)-C(12)-C(14)	107.6(5)
C(47)-C(50)	1.540(7)	C(13)-C(12)-C(14)	105.7(5)
C(51)-C(52)	1.546(7)	C(17)-C(16)-In(1)	119.3(4)
C(52)-C(54)	1.513(7)	C(16)-C(17)-C(19)	110.8(4)
C(52)-C(53)	1.525(7)	C(16)-C(17)-C(18)	109.6(4)
C(52)-C(55)	1.540(8)	C(19)-C(17)-C(18)	110.3(4)
C(56)-C(57)	1.538(7)	C(16)-C(17)-C(20)	109.6(5)
C(57)-C(58)	1.503(8)	C(19)-C(17)-C(20)	107.8(4)
C(57)-C(59)	1.531(8)	C(18)-C(17)-C(20)	108.7(4)
C(57)-C(60)	1.544(8)	C(22)-C(21)-In(2)	119.0(4)
C(16)-In(1)-C(11)	150.9(2)	C(25)-C(22)-C(24)	112.0(5)
C(16)-In(1)-C(1)	103.8(2)	C(25)-C(22)-C(23)	108.9(5)
C(11)-In(1)-C(1)	100.3(2)	C(24)-C(22)-C(23)	108.2(4)
C(16)-In(1)-C(9)#1	106.1(2)	C(25)-C(22)-C(21)	110.4(4)
C(11)-In(1)-C(9)#1	89.0(2)	C(24)-C(22)-C(21)	109.3(4)
C(1)-In(1)-C(9)#1	91.9(2)	C(23)-C(22)-C(21)	108.0(4)
C(21)-In(2)-C(26)	152.3(2)	C(27)-C(26)-In(2)	121.1(3)
C(21)-In(2)-C(6)	102.4(2)	C(28)-C(27)-C(29)	111.3(5)
C(26)-In(2)-C(6)	100.1(2)	C(28)-C(27)-C(26)	111.3(4)
C(21)-In(2)-C(3)	105.4(2)	C(29)-C(27)-C(26)	110.1(4)
C(26)-In(2)-C(3)	89.9(2)	C(28)-C(27)-C(30)	108.3(4)
C(6)-In(2)-C(3)	91.5(2)	C(29)-C(27)-C(30)	108.4(4)
C(46)-In(3)-C(41)	145.8(2)	C(26)-C(27)-C(30)	107.2(5)
C(46)-In(3)-C(39)#2	103.1(2)	C(32)-C(31)-C(35)	108.1(4)
C(41)-In(3)-C(39)#2	91.8(2)	C(32)-C(31)-In(3)	95.7(3)
C(46)-In(3)-C(31)	107.98(16)	C(35)-C(31)-In(3)	91.0(3)
C(41)-In(3)-C(31)	98.9(2)	C(33)-C(32)-C(31)	108.6(4)
C(39)#2-In(3)-C(31)	100.8(2)	C(32)-C(33)-C(34)	107.3(4)
C(51)-In(4)-C(56)	145.6(2)	C(32)-C(33)-In(4)	104.8(3)

C(34)-C(33)-In(4)	89.7(3)	C(48)-C(47)-C(46)	109.8(4)
C(35)-C(34)-C(33)	108.1(4)	C(48)-C(47)-C(49)	108.9(5)
C(34)-C(35)-C(31)	107.9(4)	C(46)-C(47)-C(49)	109.3(5)
C(40)-C(36)-C(37)	107.4(4)	C(48)-C(47)-C(50)	109.8(4)
C(40)-C(36)-In(4)	96.1(3)	C(46)-C(47)-C(50)	110.4(4)
C(37)-C(36)-In(4)	90.4(3)	C(49)-C(47)-C(50)	108.5(4)
C(38)-C(37)-C(36)	108.3(4)	C(52)-C(51)-In(4)	116.8(4)
C(37)-C(38)-C(39)	108.8(4)	C(54)-C(52)-C(53)	111.1(4)
C(40)-C(39)-C(38)	107.0(4)	C(54)-C(52)-C(55)	108.9(4)
C(40)-C(39)-In(3)#1	103.7(3)	C(53)-C(52)-C(55)	108.5(4)
C(38)-C(39)-In(3)#1	89.0(3)	C(54)-C(52)-C(51)	110.8(4)
C(36)-C(40)-C(39)	108.5(4)	C(53)-C(52)-C(51)	109.2(4)
C(42)-C(41)-In(3)	124.5(3)	C(55)-C(52)-C(51)	108.4(4)
C(44)-C(42)-C(43)	108.9(5)	C(57)-C(56)-In(4)	124.5(3)
C(44)-C(42)-C(41)	110.7(4)	C(58)-C(57)-C(59)	107.7(5)
C(43)-C(42)-C(41)	110.6(4)	C(58)-C(57)-C(56)	111.7(4)
C(44)-C(42)-C(45)	108.0(5)	C(59)-C(57)-C(56)	109.2(5)
C(43)-C(42)-C(45)	109.3(5)	C(58)-C(57)-C(60)	109.4(5)
C(41)-C(42)-C(45)	109.3(5)	C(59)-C(57)-C(60)	108.8(5)
C(47)-C(46)-In(3)	117.6(4)	C(56)-C(57)-C(60)	110.1(4)

Symmetry transformations used to generate equivalent atoms:

#1 $x+1, y, z$; #2 $x-1, y, z$.

Table 12. Hydrogen coordinates (10^4) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $(\text{Me}_3\text{CCH}_2)_2\text{In}(\text{C}_5\text{H}_5)$

Atom	x	y	z	U(eq)
H(1A)	6230(40)	5270(19)	3650(19)	26
H(2A)	5887	3948	2989	25
H(3A)	4170(50)	2879(15)	3530(20)	22
H(4A)	3525	3585	4597	27
H(5A)	4817	5007	4729	33
H(6A)	1170(40)	2969(15)	3649(19)	25
H(7A)	-128	3271	2764	28
H(8A)	-1474	4683	2890	26
H(9A)	-830(50)	5430(15)	3960(20)	21
H(10A)	853	4371	4513	19
H(11A)	8876	5386	5179	38
H(11B)	7380	5735	5016	38
H(13A)	7191	6541	6049	77
H(13B)	8734	6247	6208	77
H(13C)	7523	6016	6701	77
H(14A)	8218	3897	6137	74
H(14B)	8500	4597	6703	74
H(14C)	9456	4594	6076	74
H(15A)	5433	5252	5846	67
H(15B)	5969	4805	6499	67
H(15C)	6013	4253	5839	67
H(16A)	6762	2597	4064	17

H(16B)	8388	2621	3988	17
H(18A)	6604	2707	5533	40
H(18B)	6541	1644	5600	40
H(18C)	5682	2134	5047	40
H(19A)	9102	2783	5412	37
H(19B)	9885	2164	4903	37
H(19C)	9212	1731	5532	37
H(20A)	6951	1012	4299	31
H(20B)	7806	672	4909	31
H(20C)	8594	1031	4285	31
H(21A)	1783	5696	3455	16
H(21B)	3416	5688	3487	16
H(23A)	2519	7647	2605	31
H(23B)	3413	7316	3206	31
H(23C)	1775	7236	3224	31
H(24A)	4124	6644	1969	34
H(24B)	4134	5593	2102	34
H(24C)	4809	6262	2612	34
H(25A)	1492	6600	1865	41
H(25B)	618	6166	2437	41
H(25C)	1552	5547	1987	41
H(26A)	3794	2839	2327	19
H(26B)	2236	2572	2448	19
H(28A)	923	3577	993	39
H(28B)	917	4045	1686	39
H(28C)	440	3028	1614	39
H(29A)	3450	3832	798	44
H(29B)	4496	3642	1376	44
H(29C)	3395	4431	1435	44
H(30A)	2551	2308	775	42
H(30B)	2068	1827	1424	42
H(30C)	3659	2041	1310	42
H(31A)	3980(50)	10513(16)	715(17)	19
H(32A)	5545	9223	438	19
H(33A)	5480(50)	8072(14)	1400(20)	20
H(34A)	3934	8725	2223	23
H(35A)	2911	10152	1821	23
H(36A)	9050(50)	7903(14)	1729(18)	21
H(37A)	7927	8337	665	23
H(38A)	8941	9768	283	20
H(39A)	10550(40)	10377(17)	1258(19)	21
H(40A)	10586	9225	2059	20
H(41A)	682	10037	-460	23
H(41B)	1544	10762	-79	23
H(43A)	4546	10629	-1080	51
H(43B)	4366	9999	-464	51
H(43C)	4020	11040	-413	51
H(44A)	1538	9391	-1450	44
H(44B)	2866	9005	-1091	44
H(44C)	3040	9636	-1707	44
H(45A)	977	11024	-1376	52
H(45B)	2467	11187	-1678	52
H(45C)	2042	11671	-1021	52
H(46A)	2843	7733	1025	15
H(46B)	1230	7660	908	15
H(48A)	1209	7767	-550	27
H(48B)	313	7127	-99	27

H(48C)	1288	6708	-640	27
H(49A)	3153	6178	770	29
H(49B)	2664	5776	94	29
H(49C)	1551	6042	627	29
H(50A)	3656	7922	-418	27
H(50B)	3943	6876	-492	27
H(50C)	4469	7397	134	27
H(51A)	7857	10762	1480	15
H(51B)	6232	10809	1569	15
H(53A)	6242	11614	3195	29
H(53B)	6207	10575	3019	29
H(53C)	5253	11262	2635	29
H(54A)	8773	11625	3026	28
H(54B)	9403	11344	2344	28
H(54C)	8790	10598	2815	28
H(55A)	7291	12710	2438	27
H(55B)	6262	12362	1892	27
H(55C)	7881	12377	1761	27
H(56A)	5710	8436	2954	28
H(56B)	6511	7700	2555	28
H(58A)	9524	7691	3545	60
H(58B)	9399	8303	2917	60
H(58C)	8916	7283	2893	60
H(59A)	7596	7139	4086	78
H(59B)	6729	6825	3472	78
H(59C)	6089	7531	3966	78
H(60A)	8297	8827	4142	55
H(60B)	6733	9060	3977	55
H(60C)	7943	9441	3534	55
