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Xray Crystallography:

Two data sets were collected on compound **1**, and the crystals were obtained from two separate samples. The first crystallographic data set for **1** was obtained at 130 K with MoKα (λ = 0.71073 Å) radiation: a = 7.944(2) Å, b = 16.238(3) Å, c = 25.640(5) Å, Z = 4, space group $Pna2_1$, R_1 = 0.052 for 2344 (I>2σI) data. The second crystallographic data set for **1** was obtained at 170 K with MoKα (λ = 0.71073 Å) radiation: a = 7.926(3) Å, b = 16.282(7) Å, c = 25.661(8) Å, Z = 4, space group $Pna2_1$, R_1 = 0.066 for 2118 (I>2σI) data. The X-ray data for the first data set, upon refinement, indicated the presence of 1,3-$Trip_2C_6H_4$ at the same position(s). The atom bound to C(1) was refined as a mixture of In and H. The refinement converged at occupancies of 81.4(3)% for In and 18.6(3)% for H, and afforded an In-C distance of 2.256(4) Å. The presence of the contamination probably arose from the very high reactivity of **1** and its gradual decomposition during mounting of the crystal and data collection. The tendency of derivatives of the -C_6H_3-2,6-$Trip_2$ ligand to crystallize as mixtures which afford good diffraction data has been noted previously; Wehmschulte, R.J.; Grigsby, W.J.; Schiemenz, G.; Bartlett, R.A.; Power, P.P. Inorg. Chem. 1996, 35, 6694. The second data set refined at 100% occupancy for In and afforded an In-C distance of 2.260(7) Å. No decomposition was observed during data collection. The In atom was refined anisotropically, the carbon atoms were refined isotropically. The crystallographic data given in the text are from the second data set.

Crystallographic data for **2** at 130 K with MoKα (λ = 0.71073 Å) radiation: a = 9.513(2) Å, b = 9.831 Å, c = 21.083(4), α = 86.65(3)°, β = 81.40(3)°, γ = 89.32(3)° Å, Z = 4, space group P-1, R_1 = 0.047 for 7034 I>2(σ)I data. Upon refinement, the X-ray data for **2** indicated that the cyclopentadienyl ligand bound to Mn was disordered over two positions, with occupancies of 94% (set A) and 6% (set B). This disorder was modelled using two restrained ring systems with C-C distances set at 1.42 Å.

Table 1. Crystal data for InC_6H_3-2,6-$Trip_2$.

Identification code	sth14a
Empirical formula	$C_{36}H_{49}In$
Formula weight	596.57
Crystal size	0.30 x 0.20 x 0.18 mm
Crystal habit	parallelepiped
Crystal color	orange
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 7.926(3) Å α = 90° b = 16.282(7) Å β = 90° c = 25.661(8) Å γ = 90°
Volume	3312(2) $Å^3$
Z	4
Density (calculated)	1.196 $Mg \cdot m^{-3}$
Absorption coefficient	0.734 mm^{-1}
F(000)	1256
Absorption correction	Psi Scans
Max. and min. transmission	0.900 and 0.852

1) Psi Scans were used to measure absorption correction.

Table 2. Data collection for InC_6H_3-2,6-$Trip_2$.

Diffractometer	Siemens R3m/
Temperature	168(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoK\a)
Monochromator	graphite
θ range for data collection	1.48 to 27.50°
Scan type	\w
Index ranges	$0 \leq h \leq 10$, $0 \leq k \leq 21$, $0 \leq \ell \leq 33$
Reflections collected	4319
Independent reflections	3890 (R_{int} = 0.0000)
Standard reflections	2
Percent decay of standards	less than 0.01%

Table 3. Solution and refinement of InC_6H_3-2,6-$Trip_2$.

System for solution	SHELXS-86 (Sheldrick, 1990)
Structure solution	direct
System for refinement	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data ?restraints ?parameters	3888 ?7 ?166
Goodness-of-fit on F^2	1.023
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0462P)^2 + 5.5323P$, where $P = (Fo^2 + 2Fc^2)$?
R indices (all data)	R1 = 0.1388, wR2 = 0.1650
R indices calcd from obsd data	R1 = 0.0659, wR2 = 0.1223
Observed data (>2sigma(I))	2118
Absolute structure parameter	-0.14(10)
Extinction coefficient	NA
Largest diff. peak and hole	0.653 and -0.535 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||?GS|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]?GS[w(Fo^2)^2]]^{½}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]?M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for InC_6H_3-2,6-$Trip_2$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
In	2781(1)	9237(1)	3314(2)	50(1)
C(1)	633(8)	10150(4)	3313(10)	22(2)
C(2)	-3(23)	10482(12)	2853(8)	23(5)
C(3)	-1167(23)	11118(13)	2844(8)	29(5)
C(4)	-1777(9)	11413(5)	3336(9)	28(2)
C(5)	-1202(22)	11086(12)	3785(8)	25(5)
C(6)	21(22)	10477(12)	3790(8)	20(5)
C(7)	765(20)	10138(10)	2350(7)	19(4)
C(8)	2004(23)	10549(11)	2083(7)	25(4)
C(9)	2778(19)	10153(9)	1655(6)	20(3)
C(10)	2221(16)	9429(9)	1463(6)	24(3)
C(11)	869(22)	9028(12)	1714(7)	34(5)
C(12)	138(23)	9392(11)	2162(8)	33(5)
C(13)	601(22)	10091(11)	4287(7)	25(4)
C(14)	2027(23)	10462(11)	4554(7)	26(4)
C(15)	2577(23)	10084(12)	5008(7)	40(5)
C(16)	1929(19)	9333(10)	5183(7)	34(4)
C(17)	644(21)	8996(12)	4914(7)	33(5)
C(18)	-40(20)	9337(10)	4469(7)	22(4)
C(19)	2680(28)	11961(15)	1812(9)	58(7)
C(20)	2744(29)	11319(16)	2251(10)	38(6)
C(21)	4639(19)	11228(10)	2383(7)	48(4)
C(22)	1475(16)	8991(8)	519(5)	33(3)
C(23)	2692(24)	8942(13)	969(8)	58(6)
C(24)	3449(19)	8107(9)	1069(6)	33(3)
C(25)	-1248(28)	8096(13)	2592(9)	64(6)
C(26)	-1625(20)	8982(10)	2412(7)	35(4)
C(27)	-3079(26)	9107(13)	2126(7)	66(6)
C(28)	-1023(26)	8003(11)	4107(8)	53(5)
C(29)	-1339(19)	8917(10)	4205(6)	32(4)
C(30)	-2999(22)	8952(11)	4594(6)	45(4)
C(31)	2452(26)	11976(12)	4772(7)	44(5)
C(32)	2700(27)	11330(14)	4364(9)	32(6)
C(33)	4390(23)	11301(12)	4113(7)	66(6)
C(34)	3738(25)	8265(11)	5602(7)	65(6)
C(35)	2940(19)	9047(9)	5670(6)	30(4)
C(36)	1971(20)	9168(10)	6125(6)	56(4)

Table 5. Bond lengths [Å] for InC_6H_3-2,6-$Trip_2$.

In-C(1)	2.260(7)	C(1)-C(2)	1.39(2)
C(1)-C(6)	1.42(2)	C(2)-C(3)	1.39(2)
C(2)-C(7)	1.53(3)	C(3)-C(4)	1.44(2)
C(4)-C(5)	1.35(2)	C(5)-C(6)	1.39(2)
C(6)-C(13)	1.49(3)	C(7)-C(8)	1.37(2)
C(7)-C(12)	1.40(2)	C(8)-C(9)	1.41(2)
C(8)-C(20)	1.45(3)	C(9)-C(10)	1.35(2)
C(10)-C(11)	1.41(2)	C(10)-C(23)	1.54(3)
C(11)-C(12)	1.42(3)	C(12)-C(26)	1.68(2)
C(13)-C(18)	1.41(2)	C(13)-C(14)	1.45(2)
C(14)-C(15)	1.39(3)	C(14)-C(32)	1.59(3)
C(15)-C(16)	1.40(2)	C(16)-C(17)	1.35(2)
C(16)-C(35)	1.56(2)	C(17)-C(18)	1.38(3)
C(18)-C(29)	1.41(2)	C(19)-C(20)	1.54(3)
C(20)-C(21)	1.55(3)	C(22)-C(23)	1.51(2)
C(23)-C(24)	1.51(2)	C(25)-C(26)	1.54(3)
C(26)-C(27)	1.38(2)	C(28)-C(29)	1.53(2)
C(29)-C(30)	1.65(2)	C(31)-C(32)	1.49(3)
C(32)-C(33)	1.49(3)	C(34)-C(35)	1.43(2)
C(35)-C(36)	1.41(2)		

Symmetry transformations used to generate equivalent atoms:

Table 6. Bond angles [°] for InC_6H_3-2,6-$Trip_2$.

C(2)-C(1)-C(6)	117.5(6)	C(2)-C(1)-In	121.9(14)
C(6)-C(1)-In	120.2(14)	C(3)-C(2)-C(1)	123(2)
C(3)-C(2)-C(7)	122(2)	C(1)-C(2)-C(7)	115(2)
C(2)-C(3)-C(4)	117(2)	C(5)-C(4)-C(3)	120.4(7)
C(4)-C(5)-C(6)	122(2)	C(5)-C(6)-C(1)	120(2)
C(5)-C(6)-C(13)	122(2)	C(1)-C(6)-C(13)	118(2)
C(8)-C(7)-C(12)	121(2)	C(8)-C(7)-C(2)	122(2)
C(12)-C(7)-C(2)	118(2)	C(7)-C(8)-C(9)	118(2)
C(7)-C(8)-C(20)	124(2)	C(9)-C(8)-C(20)	117(2)
C(10)-C(9)-C(8)	123(2)	C(9)-C(10)-C(11)	119(2)
C(9)-C(10)-C(23)	132.0(14)	C(11)-C(10)-C(23)	108.8(14)
C(10)-C(11)-C(12)	119(2)	C(7)-C(12)-C(11)	120(2)
C(7)-C(12)-C(26)	121(2)	C(11)-C(12)-C(26)	119(2)
C(18)-C(13)-C(14)	119(2)	C(18)-C(13)-C(6)	123(2)
C(14)-C(13)-C(6)	118(2)	C(15)-C(14)-C(13)	117(2)
C(15)-C(14)-C(32)	123(2)	C(13)-C(14)-C(32)	119(2)
C(14)-C(15)-C(16)	123(2)	C(17)-C(16)-C(15)	118(2)
C(17)-C(16)-C(35)	133(2)	C(15)-C(16)-C(35)	109.3(14)
C(16)-C(17)-C(18)	124(2)	C(17)-C(18)-C(29)	119(2)
C(17)-C(18)-C(13)	119(2)	C(29)-C(18)-C(13)	122(2)
C(8)-C(20)-C(19)	111(2)	C(8)-C(20)-C(21)	112(2)
C(19)-C(20)-C(21)	105(2)	C(22)-C(23)-C(24)	116(2)
C(22)-C(23)-C(10)	117(2)	C(24)-C(23)-C(10)	115(2)
C(27)-C(26)-C(25)	117(2)	C(27)-C(26)-C(12)	116(2)
C(25)-C(26)-C(12)	109.0(14)	C(18)-C(29)-C(28)	116(2)
C(18)-C(29)-C(30)	105.9(14)	C(28)-C(29)-C(30)	105.2(14)
C(33)-C(32)-C(31)	116(2)	C(33)-C(32)-C(14)	114(2)
C(31)-C(32)-C(14)	112(2)	C(36)-C(35)-C(34)	118(2)
C(36)-C(35)-C(16)	110.0(13)	C(34)-C(35)-C(16)	113.3(14)

Symmetry transformations used to generate equivalent atoms:

Table 7. Anisotropic displacement parameters [$Å^2$ x 10^3]
for InC_6H_3-2,6-$Trip_2$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
In	49(1)	41(1)	60(1)	-3(1)	1(2)	21(1)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for InC_6H_3-2,6-$Trip_2$.

	x	y	z	U(eq)
H(3)	-1545(23)	11350(13)	2525(8)	35
H(4)	-2591(9)	11841(5)	3346(9)	34
H(5)	-1647(22)	11278(12)	4106(8)	30
H(9)	3729(19)	10405(9)	1496(6)	25
H(11)	454(22)	8521(12)	1585(7)	41
H(15)	3430(23)	10345(12)	5208(7)	49
H(17)	181(21)	8495(12)	5037(7)	39
H(19A)	3307(128)	11757(33)	1509(18)	87
H(19B)	3189(128)	12475(26)	1933(17)	87
H(19C)	1503(30)	12060(53)	1713(32)	87
H(20)	2122(29)	11530(16)	2562(10)	46
H(21A)	5115(31)	11769(12)	2462(31)	71
H(21B)	5233(26)	10989(48)	2085(14)	71
H(21C)	4768(20)	10868(40)	2687(21)	71
H(22A)	505(45)	8634(35)	587(13)	49
H(22B)	2042(30)	8813(40)	199(7)	49
H(22C)	1088(68)	9559(12)	478(17)	49
H(23)	3682(24)	9258(13)	835(8)	69
H(24A)	4025(91)	7915(24)	753(11)	50
H(24B)	2553(23)	7719(15)	1162(33)	50
H(24C)	4263(81)	8144(14)	1355(22)	50
H(25A)	-2169(88)	7901(32)	2815(43)	95
H(25B)	-189(93)	8088(19)	2789(44)	95
H(25C)	-1148(163)	7738(20)	2287(9)	95
H(26)	-1817(20)	9293(10)	2743(7)	42
H(27A)	-3388(72)	9690(16)	2139(32)	100
H(27B)	-3996(41)	8777(47)	2273(24)	100
H(27C)	-2885(46)	8944(58)	1763(11)	100
H(28A)	0(86)	7936(12)	3896(39)	79
H(28B)	-1988(70)	7767(19)	3921(41)	79
H(28C)	-877(147)	7720(17)	4441(8)	79
H(29)	-1599(19)	9201(10)	3868(6)	38
H(30A)	-2810(48)	8592(40)	4894(17)	68
H(30B)	-4002(29)	8769(47)	4404(11)	68
H(30C)	-3168(63)	9517(14)	4715(25)	68
H(31A)	1273(42)	11974(42)	4886(29)	66
H(31B)	2732(116)	12515(14)	4626(13)	66
H(31C)	3188(98)	11861(36)	5070(18)	66
H(32)	1915(27)	11491(14)	4077(9)	38
H(33A)	4449(47)	10825(34)	3880(29)	100
H(33B)	5262(24)	11253(61)	4382(7)	100
H(33C)	4571(54)	11805(27)	3912(31)	100
H(34A)	4358(125)	8121(35)	5919(18)	97

H(34B)	4523(117)	8293(24)	5307(29)	97
H(34C)	2878(29)	7847(17)	5532(48)	97
H(35)	3892(19)	9447(9)	5700(6)	36
H(36A)	847(45)	8929(51)	6076(15)	85
H(36B)	1865(97)	9757(10)	6194(21)	85
H(36C)	2529(64)	8901(48)	6421(9)	85

Table 10. Crystal data for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

Identification code	sth12
Empirical formula	$C_{43}H_{54}InMnO_2$
Formula weight	772.62
Crystal size	0.46 x 0.40 x 0.28 mm
Crystal habit	parallelepiped
Crystal color	orange
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.513(2) Å α = 86.65(3)°
	b = 9.831(2) Å β = 81.40(3)°
	c = 21.083(4) Å γ = 89.32(3)°
Volume	1946.2(7) $Å^3$
Z	2
Density (calculated)	1.318 $Mg \cdot m^{-3}$
Absorption coefficient	0.950 mm^{-1}
F(000)	804
Absorption correction[1]	XABS2
Max. and min. transmission	0.804 and 0.678

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* 1995, 28, 53-56.

Table 11. Data collection for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

Diffractometer	Siemens R3m/V
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	0.98 to 27.49°
Scan type	ω
Index ranges	$-12 \le h \le 12$, $-12 \le k \le 12$, $0 \le \ell \le 27$
Reflections collected	8937
Independent reflections	8937 (R_{int} = 0.0000)
Standard reflections	2
Percent decay of standards	less than 0.01%

Table 12. Solution and refinement of $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

System for solution	SHELXS-86 (Sheldrick, 1990)
Structure solution	direct
System for refinement	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	8936 / 0 / 435
Goodness-of-fit on F^2	1.013
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.033700P)^2 + 1.388300P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0667, wR2 = 0.1106
R indices calcd from obsd data	R1 = 0.0474, wR2 = 0.0958
Observed data (>2sigma(I))	7034
Extinction coefficient	0.0011(2)
Largest diff. peak and hole	0.562 and -0.735 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) $\text{Goodness-of-Fit} = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 13. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
In(1)	2565(1)	2386(1)	2403(1)	22(1)
Mn(1)	1518(1)	4631(1)	2433(1)	22(1)
O(1)	-560(3)	3965(3)	1598(2)	40(1)
O(2)	3618(3)	5561(3)	1321(1)	37(1)
C(1)	3651(3)	450(3)	2399(2)	18(1)
C(2)	4213(4)	-137(3)	2924(2)	20(1)
C(3)	4977(4)	-1354(4)	2851(2)	25(1)
C(4)	5130(4)	-1982(4)	2270(2)	25(1)
C(5)	4548(4)	-1400(3)	1751(2)	21(1)
C(6)	3818(4)	-164(3)	1808(2)	19(1)
C(7)	3979(4)	576(4)	3547(2)	21(1)
C(8)	2854(4)	178(4)	4032(2)	26(1)
C(9)	2578(4)	925(4)	4577(2)	33(1)
C(10)	3375(5)	2051(4)	4662(2)	33(1)
C(11)	4495(4)	2416(4)	4185(2)	33(1)
C(12)	4822(4)	1703(4)	3628(2)	26(1)
C(13)	3288(4)	614(3)	1260(2)	18(1)
C(14)	1833(4)	612(3)	1196(2)	18(1)
C(15)	1365(4)	1493(3)	723(2)	21(1)
C(16)	2285(4)	2367(3)	318(2)	21(1)
C(17)	3715(4)	2323(3)	386(2)	21(1)
C(18)	4242(4)	1458(3)	845(2)	20(1)
C(19)	1898(4)	-1016(4)	3958(2)	30(1)
C(20)	1552(5)	-1947(4)	4566(2)	43(1)
C(21)	526(5)	-491(5)	3721(2)	40(1)
C(22)	3005(5)	2858(5)	5264(2)	42(1)
C(23)	4305(6)	3120(6)	5580(2)	61(2)
C(24)	2254(6)	4177(5)	5113(2)	56(1)
C(25)	6135(4)	2103(4)	3148(2)	30(1)
C(26)	7468(5)	1580(5)	3404(2)	48(1)
C(27)	6231(5)	3642(4)	2967(2)	40(1)
C(28)	5817(4)	1518(4)	908(2)	24(1)
C(29)	6138(4)	2792(4)	1238(2)	33(1)
C(30)	6787(4)	1427(4)	262(2)	30(1)
C(31)	803(4)	-375(4)	1603(2)	25(1)
C(32)	-706(4)	180(5)	1766(2)	42(1)
C(33)	776(5)	-1711(4)	1265(2)	37(1)
C(34)	1740(4)	3356(4)	-167(2)	21(1)
C(35)	1819(4)	4820(4)	40(2)	29(1)
C(36)	2533(4)	3234(4)	-849(2)	30(1)
C(37)	2803(4)	5154(4)	1759(2)	26(1)

C(38)	288(4)	4185(4)	1925(2)	26(1)
C(39A)	45(4)	4843(5)	3288(2)	46(2)
C(40A)	143(3)	6084(4)	2904(2)	42(2)
C(41A)	1566(4)	6553(3)	2838(2)	38(1)
C(42A)	2348(3)	5603(4)	3181(2)	37(2)
C(43A)	1409(6)	4546(3)	3459(1)	42(2)
C(39B)	395(6)	4446(4)	3464(2)	13(14)
C(40B)	35(3)	5689(5)	3149(2)	7(14)
C(41B)	1292(4)	6476(2)	2985(2)	37(27)
C(42B)	2430(3)	5719(4)	3199(2)	102(60)
C(43B)	1876(6)	4464(3)	3495(2)	42(26)

Table 14. Bond lengths [Å] for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

In(1)-C(1)	2.155(3)	In(1)-Mn(1)	2.4102(9)
Mn(1)-C(38)	1.774(4)	Mn(1)-C(37)	1.785(4)
Mn(1)-C(40A)	2.115(3)	Mn(1)-C(41A)	2.123(3)
Mn(1)-C(39A)	2.130(3)	Mn(1)-C(42A)	2.143(3)
Mn(1)-C(43A)	2.148(3)	Mn(1)-C(41B)	2.203(3)
Mn(1)-C(40B)	2.206(3)	Mn(1)-C(42B)	2.269(4)
Mn(1)-C(39B)	2.273(3)	Mn(1)-C(43B)	2.311(4)
O(1)-C(38)	1.167(5)	O(2)-C(37)	1.168(5)
C(1)-C(2)	1.393(5)	C(1)-C(6)	1.403(5)
C(2)-C(3)	1.396(5)	C(2)-C(7)	1.511(5)
C(3)-C(4)	1.391(5)	C(4)-C(5)	1.389(5)
C(5)-C(6)	1.394(5)	C(6)-C(13)	1.495(5)
C(7)-C(8)	1.408(5)	C(7)-C(12)	1.408(5)
C(8)-C(9)	1.391(5)	C(8)-C(19)	1.522(5)
C(9)-C(10)	1.383(6)	C(10)-C(11)	1.387(5)
C(10)-C(22)	1.531(5)	C(11)-C(12)	1.396(5)
C(12)-C(25)	1.525(5)	C(13)-C(18)	1.406(5)
C(13)-C(14)	1.411(5)	C(14)-C(15)	1.402(5)
C(14)-C(31)	1.521(5)	C(15)-C(16)	1.394(5)
C(16)-C(17)	1.389(5)	C(16)-C(34)	1.513(5)
C(17)-C(18)	1.396(5)	C(18)-C(28)	1.526(5)
C(19)-C(20)	1.528(6)	C(19)-C(21)	1.539(6)
C(22)-C(24)	1.513(7)	C(22)-C(23)	1.522(7)
C(25)-C(26)	1.524(6)	C(25)-C(27)	1.539(6)
C(28)-C(29)	1.524(5)	C(28)-C(30)	1.533(5)
C(31)-C(32)	1.527(5)	C(31)-C(33)	1.534(5)
C(34)-C(36)	1.530(5)	C(34)-C(35)	1.534(5)
C(39A)-C(43A)	1.42	C(39A)-C(40A)	1.42
C(40A)-C(41A)	1.42	C(41A)-C(42A)	1.42
C(42A)-C(43A)	1.42	C(39B)-C(40B)	1.42
C(39B)-C(43B)	1.42	C(40B)-C(41B)	1.42
C(41B)-C(42B)	1.42	C(42B)-C(43B)	1.42

Table 15. Bond angles [°] for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

C(1)-In(1)-Mn(1)	175.39(9)	C(38)-Mn(1)-C(37)	91.7(2)
C(38)-Mn(1)-C(40A)	93.8(2)	C(37)-Mn(1)-C(40A)	120.1(2)
C(38)-Mn(1)-C(41A)	124.2(2)	C(37)-Mn(1)-C(41A)	92.2(2)
C(40A)-Mn(1)-C(41A)	39.2	C(38)-Mn(1)-C(39A)	98.0(2)
C(37)-Mn(1)-C(39A)	157.3(2)	C(40A)-Mn(1)-C(39A)	39.08(5)
C(41A)-Mn(1)-C(39A)	65.40(7)	C(38)-Mn(1)-C(42A)	159.03(14)
C(37)-Mn(1)-C(42A)	100.2(2)	C(40A)-Mn(1)-C(42A)	65.31(7)
C(41A)-Mn(1)-C(42A)	38.88(6)	C(39A)-Mn(1)-C(42A)	65.05(7)
C(38)-Mn(1)-C(43A)	132.3(2)	C(37)-Mn(1)-C(43A)	136.0(2)
C(40A)-Mn(1)-C(43A)	65.23(7)	C(41A)-Mn(1)-C(43A)	65.09(7)
C(39A)-Mn(1)-C(43A)	38.77(5)	C(42A)-Mn(1)-C(43A)	38.65(6)
C(38)-Mn(1)-C(41B)	122.91(14)	C(37)-Mn(1)-C(41B)	102.0(2)
C(38)-Mn(1)-C(40B)	98.3(2)	C(37)-Mn(1)-C(40B)	135.2(2)
C(41B)-Mn(1)-C(40B)	37.6	C(38)-Mn(1)-C(42B)	159.09(14)
C(37)-Mn(1)-C(42B)	98.4(2)	C(41B)-Mn(1)-C(42B)	37.0
C(40B)-Mn(1)-C(42B)	61.78(6)	C(38)-Mn(1)-C(39B)	107.9(2)
C(37)-Mn(1)-C(39B)	159.2(2)	C(41B)-Mn(1)-C(39B)	61.74(6)
C(40B)-Mn(1)-C(39B)	36.9	C(42B)-Mn(1)-C(39B)	60.77(7)
C(38)-Mn(1)-C(43B)	141.6(2)	C(37)-Mn(1)-C(43B)	126.1(2)
C(41B)-Mn(1)-C(43B)	61.14(7)	C(40B)-Mn(1)-C(43B)	61.10(7)
C(42B)-Mn(1)-C(43B)	36.10(5)	C(39B)-Mn(1)-C(43B)	36.1
C(2)-C(1)-C(6)	121.4(3)	C(2)-C(1)-In(1)	123.8(2)
C(6)-C(1)-In(1)	114.7(2)	C(1)-C(2)-C(3)	118.7(3)
C(1)-C(2)-C(7)	118.5(3)	C(3)-C(2)-C(7)	122.8(3)
C(4)-C(3)-C(2)	120.3(3)	C(5)-C(4)-C(3)	120.7(3)
C(4)-C(5)-C(6)	119.9(3)	C(5)-C(6)-C(1)	118.9(3)
C(5)-C(6)-C(13)	123.9(3)	C(1)-C(6)-C(13)	117.0(3)
C(8)-C(7)-C(12)	119.5(3)	C(8)-C(7)-C(2)	120.1(3)
C(12)-C(7)-C(2)	120.2(3)	C(9)-C(8)-C(7)	119.2(4)
C(9)-C(8)-C(19)	119.5(3)	C(7)-C(8)-C(19)	121.2(3)
C(10)-C(9)-C(8)	122.3(4)	C(9)-C(10)-C(11)	117.9(4)
C(9)-C(10)-C(22)	120.2(4)	C(11)-C(10)-C(22)	121.9(4)
C(10)-C(11)-C(12)	122.3(4)	C(11)-C(12)-C(7)	118.8(3)
C(11)-C(12)-C(25)	119.3(3)	C(7)-C(12)-C(25)	121.8(3)
C(18)-C(13)-C(14)	120.1(3)	C(18)-C(13)-C(6)	118.6(3)
C(14)-C(13)-C(6)	120.9(3)	C(15)-C(14)-C(13)	118.6(3)
C(15)-C(14)-C(31)	120.3(3)	C(13)-C(14)-C(31)	121.1(3)
C(16)-C(15)-C(14)	122.3(3)	C(17)-C(16)-C(15)	117.7(3)
C(17)-C(16)-C(34)	121.1(3)	C(15)-C(16)-C(34)	121.2(3)
C(16)-C(17)-C(18)	122.5(3)	C(17)-C(18)-C(13)	118.9(3)
C(17)-C(18)-C(28)	119.1(3)	C(13)-C(18)-C(28)	121.9(3)
C(8)-C(19)-C(20)	113.9(3)	C(8)-C(19)-C(21)	110.0(3)
C(20)-C(19)-C(21)	110.7(3)	C(24)-C(22)-C(23)	111.1(4)
C(24)-C(22)-C(10)	110.9(4)	C(23)-C(22)-C(10)	112.1(4)
C(26)-C(25)-C(12)	109.7(3)	C(26)-C(25)-C(27)	111.3(4)
C(12)-C(25)-C(27)	113.5(3)	C(29)-C(28)-C(18)	110.7(3)
C(29)-C(28)-C(30)	110.9(3)	C(18)-C(28)-C(30)	112.7(3)
C(14)-C(31)-C(32)	114.3(3)	C(14)-C(31)-C(33)	109.5(3)
C(32)-C(31)-C(33)	109.9(3)	C(16)-C(34)-C(36)	112.6(3)

C(16)-C(34)-C(35)	110.1(3)	C(36)-C(34)-C(35)	110.5(3)
O(2)-C(37)-Mn(1)	176.6(3)	O(1)-C(38)-Mn(1)	176.1(3)
C(43A)-C(39A)-C(40A)	108.0	C(43A)-C(39A)-Mn(1)	71.29(13)
C(40A)-C(39A)-Mn(1)	69.87(11)	C(41A)-C(40A)-C(39A)	108.0
C(41A)-C(40A)-Mn(1)	70.73(13)	C(39A)-C(40A)-Mn(1)	71.05(12)
C(42A)-C(41A)-C(40A)	108.0	C(42A)-C(41A)-Mn(1)	71.34(12)
C(40A)-C(41A)-Mn(1)	70.11(13)	C(43A)-C(42A)-C(41A)	108.0
C(43A)-C(42A)-Mn(1)	70.85(12)	C(41A)-C(42A)-Mn(1)	69.78(11)
C(42A)-C(43A)-C(39A)	108.0	C(42A)-C(43A)-Mn(1)	70.50(12)
C(39A)-C(43A)-Mn(1)	69.95(13)	C(40B)-C(39B)-C(43B)	108.0
C(40B)-C(39B)-Mn(1)	68.95(10)	C(43B)-C(39B)-Mn(1)	73.42(12)
C(41B)-C(40B)-C(39B)	108.0	C(41B)-C(40B)-Mn(1)	71.09(12)
C(39B)-C(40B)-Mn(1)	74.12(11)	C(40B)-C(41B)-C(42B)	108.0
C(40B)-C(41B)-Mn(1)	71.33(12)	C(42B)-C(41B)-Mn(1)	74.04(12)
C(43B)-C(42B)-C(41B)	108.0	C(43B)-C(42B)-Mn(1)	73.57(11)
C(41B)-C(42B)-Mn(1)	68.96(11)	C(42B)-C(43B)-C(39B)	108.0
C(42B)-C(43B)-Mn(1)	70.33(11)	C(39B)-C(43B)-Mn(1)	70.51(12)

Table 16. Anisotropic displacement parameters [$Å^2 \times 10^3$]
for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In(1)	22(1)	22(1)	23(1)	-1(1)	-4(1)	1(1)
Mn(1)	23(1)	22(1)	22(1)	-2(1)	-2(1)	0(1)
O(1)	31(2)	51(2)	43(2)	-6(2)	-14(1)	-1(1)
O(2)	36(2)	36(2)	35(2)	0(1)	5(1)	-10(1)
C(1)	10(2)	24(2)	20(2)	1(1)	1(1)	-2(1)
C(2)	15(2)	26(2)	18(2)	1(1)	-1(1)	-3(1)
C(3)	26(2)	28(2)	21(2)	6(2)	-4(2)	4(2)
C(4)	24(2)	25(2)	24(2)	-1(2)	2(2)	6(2)
C(5)	21(2)	25(2)	18(2)	-1(1)	0(1)	-1(1)
C(6)	14(2)	24(2)	16(2)	2(1)	0(1)	-2(1)
C(7)	21(2)	29(2)	14(2)	1(1)	-2(1)	1(1)
C(8)	25(2)	30(2)	21(2)	-1(2)	0(2)	0(2)
C(9)	33(2)	39(2)	23(2)	-5(2)	10(2)	-7(2)
C(10)	45(3)	38(2)	15(2)	-5(2)	0(2)	-7(2)
C(11)	34(2)	38(2)	26(2)	-8(2)	-2(2)	-14(2)
C(12)	25(2)	36(2)	18(2)	-1(2)	-4(2)	-4(2)
C(13)	17(2)	20(2)	16(2)	-2(1)	-2(1)	-3(1)
C(14)	16(2)	23(2)	16(2)	-1(1)	-2(1)	-4(1)
C(15)	14(2)	27(2)	23(2)	-1(1)	-4(1)	-6(1)
C(16)	23(2)	22(2)	17(2)	-2(1)	-1(1)	-2(1)
C(17)	22(2)	24(2)	18(2)	4(1)	-4(1)	-6(1)
C(18)	18(2)	23(2)	19(2)	-2(1)	-5(1)	-3(1)
C(19)	26(2)	34(2)	27(2)	-6(2)	8(2)	-7(2)
C(20)	42(3)	34(2)	49(3)	3(2)	6(2)	-8(2)
C(21)	34(2)	52(3)	33(2)	-8(2)	2(2)	-12(2)
C(22)	61(3)	44(2)	18(2)	-8(2)	5(2)	-15(2)
C(23)	93(5)	68(4)	28(3)	-14(2)	-22(3)	10(3)
C(24)	60(3)	74(4)	37(3)	-29(3)	-7(2)	21(3)
C(25)	24(2)	41(2)	24(2)	-5(2)	1(2)	-12(2)
C(26)	29(2)	66(3)	47(3)	1(2)	-3(2)	-5(2)
C(27)	40(3)	43(2)	34(2)	-4(2)	6(2)	-16(2)
C(28)	18(2)	31(2)	24(2)	6(2)	-8(2)	-5(2)
C(29)	23(2)	51(2)	25(2)	-4(2)	-3(2)	-13(2)
C(30)	21(2)	37(2)	32(2)	-4(2)	-5(2)	-1(2)
C(31)	17(2)	35(2)	22(2)	6(2)	-3(2)	-6(2)
C(32)	26(2)	45(3)	47(3)	9(2)	13(2)	-3(2)
C(33)	39(3)	32(2)	39(2)	3(2)	1(2)	-19(2)
C(34)	15(2)	28(2)	20(2)	4(1)	-2(1)	0(1)
C(35)	28(2)	27(2)	31(2)	4(2)	-3(2)	2(2)
C(36)	29(2)	40(2)	20(2)	4(2)	-5(2)	5(2)
C(37)	27(2)	20(2)	33(2)	-4(2)	-8(2)	0(2)
C(38)	23(2)	28(2)	25(2)	0(2)	-1(2)	2(2)

C(39A)	48(3)	48(3)	35(3)	-13(3)	17(3)	-21(3)
C(40A)	43(3)	48(3)	35(3)	-18(3)	-4(2)	19(2)
C(41A)	58(3)	27(2)	28(3)	-9(2)	-2(3)	-1(2)
C(42A)	41(4)	43(3)	29(3)	-18(2)	-8(2)	-1(2)
C(43A)	69(5)	38(3)	20(2)	-7(2)	-7(2)	4(2)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $CpMn(CO)_2(InC_6H_3\text{-}2,6\text{-}Trip_2)$.

	x	y	z	U(eq)
H(3)	5394(4)	-1755(4)	3200(2)	30
H(4)	5637(4)	-2818(4)	2228(2)	30
H(5)	4649(4)	-1842(3)	1358(2)	26
H(9)	1816(4)	654(4)	4903(2)	39
H(11)	5061(4)	3179(4)	4239(2)	39
H(15)	386(4)	1495(3)	677(2)	25
H(17)	4359(4)	2904(3)	110(2)	25
H(19)	2415(4)	-1578(4)	3617(2)	36
H(20A)	1105(30)	-2782(14)	4463(4)	65
H(20B)	899(27)	-1477(13)	4887(6)	65
H(20C)	2431(6)	-2178(26)	4739(9)	65
H(21A)	-59(15)	-1266(5)	3651(14)	60
H(21B)	769(5)	56(26)	3316(8)	60
H(21C)	-6(16)	72(26)	4044(7)	60
H(22)	2329(5)	2295(5)	5579(2)	50
H(23A)	4012(8)	3574(35)	5981(9)	92
H(23B)	4973(19)	3703(32)	5289(8)	92
H(23C)	4768(24)	2251(6)	5675(17)	92
H(24A)	2048(35)	4685(18)	5502(5)	84
H(24B)	1363(19)	3974(5)	4957(17)	84
H(24C)	2866(16)	4725(17)	4781(13)	84
H(25)	6074(4)	1630(4)	2745(2)	35
H(26A)	8308(5)	1828(30)	3092(7)	72
H(26B)	7419(17)	586(6)	3475(15)	72
H(26C)	7533(19)	1990(26)	3812(8)	72
H(27A)	7084(18)	3829(6)	2652(11)	60
H(27B)	6284(33)	4137(5)	3353(3)	60
H(27C)	5387(16)	3939(7)	2781(14)	60
H(28)	6032(4)	712(4)	1189(2)	29
H(29A)	5873(28)	3603(4)	989(7)	49
H(29B)	7155(7)	2822(15)	1267(12)	49
H(29C)	5591(23)	2772(14)	1671(5)	49
H(30A)	7783(4)	1409(28)	332(2)	45
H(30B)	6625(21)	2222(14)	-22(5)	45
H(30C)	6573(20)	594(14)	62(6)	45
H(31)	1175(4)	-586(4)	2017(2)	30
H(32A)	-1258(10)	-440(17)	2087(11)	63
H(32B)	-1157(12)	253(30)	1376(4)	63
H(32C)	-672(5)	1081(14)	1938(14)	63
H(33A)	114(24)	-2348(12)	1528(7)	56
H(33B)	1731(8)	-2112(16)	1204(13)	56
H(33C)	465(30)	-1527(6)	845(6)	56
H(34)	717(4)	3141(4)	-173(2)	25

H(35A)	1469(26)	5452(4)	-278(7)	44
H(35B)	2808(6)	5040(10)	71(12)	44
H(35C)	1232(23)	4902(8)	460(6)	44
H(36A)	2076(17)	3821(21)	-1150(2)	45
H(36B)	2508(24)	2286(7)	-967(5)	45
H(36C)	3523(8)	3516(26)	-866(4)	45
H(39A)	-786(4)	4306(5)	3408(2)	55
H(40A)	-612(5)	6523(7)	2723(3)	50
H(41A)	1930(7)	7361(3)	2605(2)	45
H(42A)	3328(3)	5663(6)	3218(2)	44
H(43A)	1650(9)	3775(4)	3715(2)	51
H(39B)	-243(8)	3728(6)	3626(3)	16
H(40B)	-886(3)	5949(7)	3062(3)	8
H(41B)	1361(6)	7354(3)	2769(3)	44
H(42B)	3393(3)	6002(6)	3152(3)	123
H(43B)	2402(9)	3761(5)	3681(2)	51

Table 1. Original crystal data for 2,6-$Trip_2C_6H_3In$.

Identification code	sth07
Empirical formula	$C_{36}H_{49.18}In_{0.82}$
Formula weight	576.08
Crystal size	0.54 x 0.30 x 0.08 mm
Crystal habit	parallelepiped
Crystal color	orange
Crystal system	Orthorhombic
Space group	$Pna2_1$
Unit cell dimensions	a = 7.944(2) Å α = 90°
	b = 16.238(3) Å β = 90°
	c = 25.640(5) Å γ = 90°
Volume	3307(3) $Å^3$
Z	4
Density (calculated)	1.198 $Mg \cdot m^{-3}$
Absorption coefficient	0.735 mm^{-1}
F(000)	1256
Absorption correction[1]	XABS2
Max. and min. transmission	0.956 and 0.830

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* 1995, 28, 53-56.

Table 2. Original data collection for 2,6-$Trip_2C_6H_3In$.

Diffractometer	Siemens R3M/V
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	1.48 to 27.49°
Scan type	ω
Index ranges	$0 \leq h \leq 10$, $0 \leq k \leq 21$, $0 \leq \ell \leq 33$
Reflections collected	4313
Independent reflections	3885 (R_{int} = 0.0000)
Standard reflections	2
Percent decay of standards	2.25

Table 3. Original solution and refinement of 2,6-$Trip_2C_6H_3In$.

System for solution	SHELXS-86 (Sheldrick, 1990)
Structure solution	direct
System for refinement	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	3880 / 39 / 341
Goodness-of-fit on F^2	1.039
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.04999P)^2 + 0.1237P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.1110, wR2 = 0.1483
R indices calcd from obsd data	R1 = 0.0520, wR2 = 0.0993
Observed data (>2sigma(I))	2344
Absolute structure parameter	0.04(9)
Largest diff. peak and hole	0.435 and -0.300 $eÅ^{-3}$

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

The atom bound to C1 was refined as a mixture of In and H. The refinement converged to cccupancies of 81.4(3)% for In and 18.6(3)% for H. The

carbon atoms in the 2,6-$Trip_2C_6H_3$ were refined using restraints of typical values for carbon-carbon bond distances.

Table 4. Original atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 2,6-$Trip_2C_6H_3In$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
In	2803(1)	9233(1)	3313(2)	48(1)
H(1)	1517	9733	3300	30
C(1)	659(6)	10144(3)	3318(5)	28(1)
C(2)	18(18)	10473(8)	2853(4)	33(4)
C(3)	-1147(18)	11110(8)	2837(5)	27(3)
C(4)	-1755(6)	11396(3)	3310(6)	37(1)
C(5)	-1198(20)	11062(9)	3774(6)	37(4)
C(6)	24(14)	10448(7)	3791(4)	20(3)
C(7)	646(16)	10114(7)	2346(4)	29(4)
C(8)	2044(16)	10479(7)	2095(4)	25(3)
C(9)	2708(18)	10143(7)	1639(5)	34(4)
C(10)	2103(17)	9405(7)	1445(4)	27(3)
C(11)	722(19)	9049(9)	1687(5)	53(5)
C(12)	50(19)	9356(8)	2155(5)	34(4)
C(13)	728(15)	10087(7)	4290(4)	29(4)
C(14)	2011(17)	10498(8)	4569(5)	38(4)
C(15)	2667(17)	10083(8)	5001(5)	41(4)
C(16)	2076(22)	9338(9)	5192(6)	54(5)
C(17)	779(16)	8973(9)	4911(4)	31(3)
C(18)	31(20)	9346(7)	4478(5)	35(4)
C(19)	2541(16)	11992(9)	1876(6)	47(4)
C(20)	2759(16)	11302(8)	2268(5)	40(4)
C(21)	4604(15)	11252(13)	2416(6)	54(4)
C(22)	1578(19)	9054(10)	493(4)	59(4)
C(23)	2638(18)	8921(8)	962(4)	61(5)
C(24)	3585(16)	8146(8)	1042(6)	55(4)
C(25)	-1251(31)	8061(10)	2551(8)	102(8)
C(26)	-1496(18)	8958(8)	2407(6)	54(5)
C(27)	-3024(23)	9024(17)	2054(8)	69(7)
C(28)	-1064(24)	8033(7)	4071(6)	49(4)
C(29)	-1451(16)	8917(8)	4217(4)	41(4)
C(30)	-3030(22)	8973(15)	4547(10)	78(7)
C(31)	2621(26)	11930(10)	4824(6)	84(6)
C(32)	2709(20)	11321(7)	4375(5)	40(4)
C(33)	4443(22)	11212(16)	4140(8)	118(9)
C(34)	3629(24)	8215(9)	5594(6)	89(7)
C(35)	2920(15)	9047(7)	5686(5)	42(3)
C(36)	1723(23)	9071(12)	6120(5)	108(8)

Table 5. Original bond lengths [Å] for 2,6-$Trip_2C_6H_3In$.

In-C(1)	2.256(4)	C(1)-C(6)	1.403(8)
C(1)-C(2)	1.404(8)	C(2)-C(3)	1.388(8)
C(2)-C(7)	1.509(8)	C(3)-C(4)	1.384(8)
C(4)-C(5)	1.379(8)	C(5)-C(6)	1.393(8)
C(6)-C(13)	1.513(8)	C(7)-C(12)	1.406(8)
C(7)-C(8)	1.414(8)	C(8)-C(9)	1.393(8)
C(8)-C(20)	1.519(9)	C(9)-C(10)	1.384(8)
C(10)-C(11)	1.387(9)	C(10)-C(23)	1.525(8)
C(11)-C(12)	1.405(8)	C(12)-C(26)	1.531(9)
C(13)-C(14)	1.413(8)	C(13)-C(18)	1.410(8)
C(14)-C(15)	1.399(8)	C(14)-C(32)	1.530(8)
C(15)-C(16)	1.387(9)	C(16)-C(17)	1.390(9)
C(16)-C(35)	1.509(9)	C(17)-C(18)	1.397(8)
C(18)-C(29)	1.523(8)	C(19)-C(20)	1.515(9)
C(20)-C(21)	1.517(8)	C(22)-C(23)	1.484(9)
C(23)-C(24)	1.481(9)	C(25)-C(26)	1.515(9)
C(26)-C(27)	1.518(9)	C(28)-C(29)	1.515(9)
C(29)-C(30)	1.515(9)	C(31)-C(32)	1.519(9)
C(32)-C(33)	1.514(9)	C(34)-C(35)	1.483(9)
C(35)-C(36)	1.465(9)		

Table 6. Original bond angles [°] for 2,6-$Trip_2C_6H_3In$.

C(6)-C(1)-C(2)	118.1(4)	C(6)-C(1)-In	120.5(7)
C(2)-C(1)-In	121.2(8)	C(3)-C(2)-C(1)	123.3(10)
C(3)-C(2)-C(7)	118.9(11)	C(1)-C(2)-C(7)	117.7(11)
C(2)-C(3)-C(4)	117.2(10)	C(5)-C(4)-C(3)	120.7(5)
C(4)-C(5)-C(6)	122.2(10)	C(1)-C(6)-C(5)	118.3(9)
C(1)-C(6)-C(13)	117.4(9)	C(5)-C(6)-C(13)	124.2(10)
C(12)-C(7)-C(8)	118.2(10)	C(12)-C(7)-C(2)	121.8(10)
C(8)-C(7)-C(2)	119.3(10)	C(9)-C(8)-C(20)	116.6(10)
C(9)-C(8)-C(7)	121.0(10)	C(20)-C(8)-C(7)	122.0(9)
C(8)-C(9)-C(10)	120.6(10)	C(11)-C(10)-C(9)	118.3(10)
C(11)-C(10)-C(23)	111.6(10)	C(9)-C(10)-C(23)	129.9(10)
C(10)-C(11)-C(12)	122.3(11)	C(7)-C(12)-C(11)	118.7(11)
C(7)-C(12)-C(26)	119.5(10)	C(11)-C(12)-C(26)	121.0(11)
C(14)-C(13)-C(18)	120.9(10)	C(14)-C(13)-C(6)	120.8(10)
C(18)-C(13)-C(6)	118.3(10)	C(13)-C(14)-C(15)	116.3(11)
C(13)-C(14)-C(32)	120.7(11)	C(15)-C(14)-C(32)	122.9(12)
C(16)-C(15)-C(14)	125.0(12)	C(15)-C(16)-C(17)	116.1(12)
C(15)-C(16)-C(35)	114.7(10)	C(17)-C(16)-C(35)	129.2(11)
C(18)-C(17)-C(16)	122.8(13)	C(17)-C(18)-C(13)	118.4(12)
C(17)-C(18)-C(29)	118.6(10)	C(13)-C(18)-C(29)	123.0(10)
C(8)-C(20)-C(21)	112.8(13)	C(8)-C(20)-C(19)	114.4(12)
C(21)-C(20)-C(19)	108.4(11)	C(24)-C(23)-C(22)	121.5(12)
C(24)-C(23)-C(10)	117.9(11)	C(22)-C(23)-C(10)	115.1(11)
C(25)-C(26)-C(27)	109(2)	C(25)-C(26)-C(12)	114.0(14)
C(27)-C(26)-C(12)	111.1(14)	C(18)-C(29)-C(30)	111.6(13)
C(18)-C(29)-C(28)	112.6(12)	C(30)-C(29)-C(28)	111.2(14)
C(31)-C(32)-C(33)	115(2)	C(31)-C(32)-C(14)	107.8(12)
C(33)-C(32)-C(14)	110.9(14)	C(36)-C(35)-C(16)	109.9(12)
C(36)-C(35)-C(34)	113.0(12)	C(16)-C(35)-C(34)	108.7(12)

Table 7. Original anisotropic displacement parameters [$Å^2$ x 10^3] for 2,6-$Trip_2C_6H_3In$.

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
In	44(1)	37(1)	63(1)	2(1)	0(1)	20(1)
C(1)	27(3)	28(3)	30(3)	7(8)	23(7)	2(2)
C(2)	49(8)	29(8)	23(7)	4(6)	-2(7)	-10(7)
C(4)	31(3)	37(3)	43(3)	-1(12)	-7(11)	7(2)
C(5)	34(5)	37(5)	39(5)	-11(4)	8(4)	9(4)
C(6)	3(5)	25(7)	33(8)	4(6)	-2(5)	4(5)
C(7)	41(8)	24(7)	21(7)	11(5)	4(6)	-4(6)
C(8)	30(8)	22(6)	22(6)	-2(5)	10(5)	4(6)
C(9)	49(9)	22(5)	30(7)	2(5)	7(6)	-13(5)
C(10)	37(5)	26(4)	17(4)	-5(3)	13(3)	11(3)
C(11)	84(12)	29(7)	45(8)	-18(6)	-22(8)	7(7)
C(12)	32(9)	39(9)	31(9)	6(8)	3(8)	4(7)
C(13)	20(7)	39(8)	28(8)	9(6)	11(5)	15(6)
C(14)	32(9)	58(9)	25(7)	-14(7)	16(6)	1(7)
C(15)	23(7)	70(10)	31(8)	-3(7)	-6(6)	26(6)
C(17)	39(7)	31(6)	22(5)	-10(4)	-7(5)	9(5)
C(18)	51(11)	23(8)	32(9)	5(7)	7(9)	-6(7)
C(19)	36(7)	44(7)	59(8)	-9(6)	-6(5)	11(5)
C(20)	22(7)	54(10)	45(10)	3(8)	10(7)	0(7)
C(21)	31(6)	65(10)	66(8)	25(7)	-16(6)	-14(6)
C(22)	83(9)	71(9)	22(7)	8(6)	0(6)	-8(7)
C(23)	97(12)	70(9)	16(5)	-2(5)	11(6)	34(9)
C(24)	39(7)	58(8)	69(11)	-16(7)	0(7)	-10(6)
C(25)	100(17)	92(14)	113(18)	57(12)	-8(13)	-27(12)
C(26)	59(12)	21(6)	82(11)	-5(7)	23(9)	-17(7)
C(27)	49(13)	83(16)	76(14)	-11(11)	12(10)	-13(11)
C(28)	49(8)	34(7)	64(11)	0(7)	-9(7)	-3(6)
C(29)	47(10)	58(10)	19(6)	13(6)	6(6)	-6(7)
C(30)	38(12)	73(12)	124(18)	-37(13)	10(12)	-14(9)
C(31)	163(17)	30(6)	60(9)	-8(6)	4(10)	-25(9)
C(32)	51(11)	36(9)	33(8)	8(7)	1(8)	-15(8)
C(33)	107(16)	69(13)	176(22)	2(15)	83(15)	-26(12)
C(34)	138(15)	95(11)	35(8)	22(8)	7(8)	95(10)
C(35)	33(5)	30(5)	64(8)	10(4)	-23(5)	-15(4)
C(36)	150(16)	127(14)	45(10)	30(9)	14(10)	122(12)

Table 8. Original hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 2,6-$Trip_2C_6H_3In$.

	x	y	z	U(eq)
H(3)	-1512(18)	11340(8)	2516(5)	32
H(4)	-2565(6)	11826(3)	3315(6)	45
H(5)	-1664(20)	11258(9)	4092(6)	44
H(9)	3585(18)	10423(7)	1460(5)	40
H(11)	213(19)	8580(9)	1531(5)	63
H(15)	3588(17)	10330(8)	5178(5)	50
H(17)	385(16)	8447(9)	5017(4)	37
H(19A)	3068(59)	11835(16)	1545(8)	70
H(19B)	3076(60)	12493(12)	2009(10)	70
H(19C)	1339(16)	12094(24)	1820(17)	70
H(20)	2130(16)	11468(8)	2589(5)	48
H(21A)	4946(24)	11766(18)	2586(21)	81
H(21B)	5283(17)	11166(39)	2102(7)	81
H(21C)	4776(20)	10790(24)	2657(19)	81
H(22A)	447(52)	8835(76)	557(20)	88
H(22B)	2082(92)	8769(69)	195(13)	88
H(22C)	1506(141)	9645(11)	419(31)	88
H(23)	3609(18)	9277(8)	857(4)	73
H(24A)	4031(139)	7954(43)	707(10)	83
H(24B)	2832(44)	7726(25)	1187(48)	83
H(24C)	4518(100)	8243(20)	1284(40)	83
H(25A)	-2214(93)	7872(25)	2758(46)	152
H(25B)	-217(101)	8001(16)	2756(47)	152
H(25C)	-1164(171)	7730(15)	2233(8)	152
H(26)	-1749(18)	9267(8)	2735(6)	65
H(27A)	-3178(60)	9599(19)	1948(25)	104
H(27B)	-4026(30)	8836(49)	2242(14)	104
H(27C)	-2854(52)	8682(43)	1744(18)	104
H(28A)	-116(75)	8020(8)	3827(27)	74
H(28B)	-2055(44)	7784(17)	3907(30)	74
H(28C)	-772(106)	7722(15)	4386(8)	74
H(29)	-1684(16)	9219(8)	3885(4)	50
H(30A)	-2792(37)	8766(50)	4898(14)	117
H(30B)	-3922(41)	8640(46)	4388(21)	117
H(30C)	-3396(63)	9548(17)	4568(28)	117
H(31A)	1542(44)	11868(35)	5005(20)	127
H(31B)	2719(109)	12492(10)	4689(7)	127
H(31C)	3544(59)	11822(33)	5068(17)	127
H(32)	1945(20)	11525(7)	4093(5)	48
H(33A)	4341(23)	10947(58)	3798(19)	176
H(33B)	5129(46)	10866(57)	4370(21)	176
H(33C)	4981(58)	11751(17)	4100(39)	176
H(34A)	4446(172)	8086(47)	5869(41)	134

H(34B)	4190(199)	8202(33)	5254(32)	134
H(34C)	2719(39)	7807(16)	5600(70)	134
H(35)	3869(15)	9431(7)	5767(5)	50
H(36A)	795(143)	8689(98)	6051(40)	161
H(36B)	1277(206)	9631(31)	6157(54)	161
H(36C)	2295(71)	8910(132)	6443(16)	161