JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1997, 119(9), 2172-2181, DOI:10.1021/ja9640859

Solution-Phase Decomposition of [*t*-$Bu_2In(\mu$-$PH_2)]_3$ (4) at Room Temperature.

Compound **4** (0.68 g, 0.87 mmol) was dissolved in hexane (20 mL) and kept at room temperature. The colorless solution slowly darkened to orange red in 10 h and then an orange-red precipitate formed during the next 10 h. The reaction mixture was stirred for a total of 48 h and then the insoluble precipitate was collected by filtration, washed with 10 mL hexane, and dried in vacuo (yield 0.38 g). Anal. Calcd for $[t\text{-}Bu_{1.3}InPH_{1.3}]_n$: C, 28.22; H, 5.92. Found: C, 28.29; H, 5.98. IR (cm^{-1}, KBr): 2940 s, 2909 s, 2829 vs, 2762 w, 2704 w, $\nu_{P\text{-}H}$ 2295 w, 1460 s, 1361 w, 1249 vw, 1150 s, 1038 w, 1010 m, 836 w, 805 w, 626 vw, 441 vw.

The orange-red powder (0.20 g) was heated in vacuo (10^{-2} Torr) at 200 ° C for 3h and then 700 ° C for 12 h to yield crystalline InP (0.11 g) along with a small quantity of In metal as determined by XRD. Anal. Found: C, 1.35; H, 0.05.

Solution-Phase Decomposition of [*t*-$Bu_2In(\mu$-$PH_2)]_3$ (4) at 203 °C. Compound **4** was generated *in situ* from *t*-Bu_3In (0.368 g, 1.29 mmol) and PH_3 as described in the preceding experimental description, but in 1,3-diisopropylbenzene (15 mL) as the solvent. The solution was refluxed for 21 h to yield a black insoluble precipitate, which was collected by filtration, washed with hexane, and dried in vacuo (yield 0.165 g, theoretical weight yield for InP 0.188 g). Anal. Found: C, 1.24; H, 0.14.

The XRD pattern of the black solid exhibited considerably broadened reflections indicating an average InP crystallite coherence length of 9 nm. A small amount of In metal was also detected.

Methanolysis of $\{Me_2In[\mu\text{-}P(SiMe_3)_2]\}_2$. MeOH (226 μL, 0.18 g, 5.6 mmol) was added to a toluene (30 mL) suspension of $\{Me_2In[\mu\text{-}P(SiMe_3)_2]\}_2$ (0.90 g, 1.40 mmol) and the mixture was stirred at room temperature for 12 h to give a pale yellow solution. The reaction mixture was then refluxed for 24 h in a heating mantle. A yellow-orange solid precipitated in the first 30 min of heating, which ultimately became dark brown. The solid product was collected by filtration, washed with hexane (2 × 5 mL), and dried in vacuo (yield 0.32 g). Anal. Found: C, 10.18; H, 1.92.

The brown powder exhibited a very broad XRD pattern. Further heating of the brown solid in refluxing mesitylene did not improve its crystallinity as determined by XRD.

Reaction of $(2,4,6\text{-}Me_3C_6H_2)_3In$ and PH_3 in the Presence of MeOH. The general procedure for the catalyzed reactions of *t*-Bu_3In and PH_3 was followed using compound $(2,4,6\text{-}Me_3C_6H_2)_3In$ (0.567 g, 1.22 mmol), toluene (10 mL), and MeOH (10 μL, 0.25 mmol). The reaction mixture was refluxed with a heating mantle for 48 h. The XRD pattern of the resulting brown precipitate was very broad, indicating an amorphous product.

Reaction of Et_3In and PH_3. A faint yellow soln. of Et_3In (0.363 g, 1.80 mmol) in 1,3-diisopropylbenzene (15.0 mL) was prepared at room temperature. Excess PH_3 was bubbled through the solution, and a white suspension formed. Then, the solution was sparged with N_2 and stirred for 15 h. The suspension became a faint yellow. The solution was refluxed for 24 h in an oil bath and produced a dark brown precipitate, which was subsequently collected by filtration, washed with hexane, and dried in vacuo (yield 0.299 g).

The XRD pattern for the solid indicated essentially amorphous InP (less than 2 nm coherence length). No In metal was detected.

Reaction of $[EtMe_2C]_3In$ and PH_3. A faint yellow soln. of $[EtMe_2C]_3In$ (0.406 g, mmol) in 1,3-diisopropylbenzene (25 mL) was prepared at room temperature. Excess PH_3 was bubbled through the solution, and it became darker yellow. The solution was sparged with N_2 with no further change in appearance, and then it was heated to reflux in an oil bath for 15 min. a dark-grey precipitate was obtained, which was collected by filtration, washed with hexane, and dried in vacuo (yield 0.092 g).

The XRD pattern for the solid contained InP (average coherence length 8 nm) and In reflections.

Reaction of Et_3In and PH_3 in the Presence of PhSH and *t*-Bu_3In. A pale yellow solution of Et_3In (0.350 g, 1.73 mmol) in 1,3-diisopropylbenzene (15 mL) was prepared at room temperature. PH_3 was bubbled through the solution until it became cloudy and white. Excess PH_3 was then removed by sparging the solution with N_2, and the solution became an opaque, yellow suspension. *t*-Bu_3In (0.10 g, 0.35 mmol) and PhSH (20 μL, 0.20 mmol) were added to the suspension, which was then stirred for 14 h and subsequently refluxed for 26 h. A brown precipitate was obtained, which was collected by filtration, washed with hexane, and dried in vacuo (yield 0.273 g).

The XRD pattern for the solid contained reflections for In and InP; the data indicated an average coherence length of 9 nm for InP.

STRUCTURE DETERMINATION SUMMARY FOR 2

Crystal Data

Empirical Formula	$C_{18}H_{42}In_2O_2$
Color; Habit	Colorless; irregular
Crystal size (mm)	0.2 x 0.3 x 0.4
Crystal System	Monoclinic
Space Group	C2/m
Unit Cell Dimensions	$\underline{a}$ = 14.598(6) Å
	$\underline{b}$ = 10.814(5) Å
	$\underline{c}$ = 9.748(3) Å
	β = 129.11(2)°
Volume	1194.0(8) Å^3
Z	2
Formula weight	520.2
Density(calc.)	1.447 g/cm^3
Absorption Coefficient	19.36 cm^{-1}
F(000)	528

Data Collection for 2

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	295
Monochromator	Highly oriented graphite crystal
2θ Range	3.5 to 50.0°
Scan Type	2θ–θ
Scan Speed	Variable; 3.97 to 14.65°/min. in ω
Scan Range (ω)	1.40° plus Kα-separation
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$-17 \le h \le 13$, $-12 \le k \le 12$ $0 \le l \le 7$
Reflections Collected	1735
Independent Reflections	846 (R_{int} = 1.23%)
Observed Reflections	812 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

Solution and Refinement for 2

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, refined isotropic U for hydrogen atoms bonded to c7, otherwise hydrogen atoms were located and refined isotropically.
Weighting Scheme	N/A
Number of Parameters Refined	100
Final R Indices (obs. data)	R = 1.32 %, wR = 1.48 %
R Indices (all data)	R = 1.43 %, wR = 1.57 %
Goodness-of-Fit	1.01
Largest and Mean Δ/σ	0.002, 0.000
Data-to-Parameter Ratio	8.1:1
Largest Difference Peak	0.43 $e\text{Å}^{-3}$
Largest Difference Hole	-0.33 $e\text{Å}^{-3}$

Table 3. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
In(1)	3576(1)	0	8088(1)	27(1)
O(1)	5000	1215(2)	10000	31(1)
C(1)	2255(3)	0	8478(5)	33(2)
C(2)	2819(5)	0	10394(7)	63(4)
C(3)	1490(3)	1147(4)	7596(7)	67(3)
C(4)	3286(3)	0	5591(5)	31(2)
C(5)	3823(3)	-1149(3)	5448(5)	45(2)
C(6)	1958(3)	0	4057(6)	41(3)
C(7)	5000	2508(3)	10000	51(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 4. Bond lengths (Å)

In(1)-O(1)	2.153 (2)	In(1)-C(1)	2.188 (6)
In(1)-C(4)	2.191 (5)	In(1)-O(1A)	2.153 (2)
O(1)-C(7)	1.398 (4)	O(1)-In(1A)	2.153 (2)
C(1)-C(2)	1.492 (8)	C(1)-C(3)	1.522 (4)
C(1)-C(3A)	1.522 (4)	C(4)-C(5)	1.522 (5)
C(4)-C(6)	1.528 (4)	C(4)-C(5A)	1.522 (5)

Table 5. Bond angles (°)

O(1)-In(1)-C(1)	109.0(1)	O(1)-In(1)-C(4)	111.5(1)
C(1)-In(1)-C(4)	128.2(1)	O(1)-In(1)-O(1A)	75.2(1)
C(1)-In(1)-O(1A)	109.0(1)	C(4)-In(1)-O(1A)	111.5(1)
In(1)-O(1)-C(7)	127.6(1)	In(1)-O(1)-In(1A)	104.8(1)
C(7)-O(1)-In(1A)	127.6(1)	In(1)-C(1)-C(2)	111.5(3)
In(1)-C(1)-C(3)	108.4(4)	C(2)-C(1)-C(3)	109.6(4)
In(1)-C(1)-C(3A)	108.4(4)	C(2)-C(1)-C(3A)	109.6(4)
C(3)-C(1)-C(3A)	109.2(3)	In(1)-C(4)-C(5)	110.6(2)
In(1)-C(4)-C(6)	108.9(4)	C(5)-C(4)-C(6)	108.6(2)
In(1)-C(4)-C(5A)	110.6(2)	C(5)-C(4)-C(5A)	109.4(5)
C(6)-C(4)-C(5A)	108.6(2)		

Table 6. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	24(1)	32(1)	24(1)	0	15(1)	0
O(1)	30(1)	25(1)	28(1)	0	14(1)	0
C(1)	28(2)	50(2)	25(3)	0	19(2)	0
C(2)	52(3)	110(5)	42(4)	0	37(3)	0
C(3)	61(2)	80(3)	81(4)	28(2)	54(2)	20(2)
C(4)	30(2)	37(2)	27(2)	0	18(2)	0
C(5)	51(2)	46(2)	44(2)	6(1)	33(2)	-2(1)
C(6)	38(2)	53(3)	23(3)	0	14(2)	0
C(7)	56(3)	31(2)	48(3)	0	24(2)	0

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 7. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(2A)	3243(27)	760(28)	10939(42)	66(10)
H(2B)	2272(42)	0	10649(65)	71(15)
H(3A)	908(29)	1164(30)	7787(42)	73(10)
H(3B)	1960(32)	1927(37)	8243(50)	102(15)
H(3C)	1100(32)	1159(37)	6357(51)	99(16)
H(5A)	3474(23)	-1892(27)	5468(37)	50(8)
H(5B)	4631(26)	-1181(27)	6335(39)	56(9)
H(5C)	3704(24)	-1149(27)	4349(42)	55(11)
H(6A)	1575(24)	731(26)	4037(37)	59(9)
H(6B)	1808(34)	0	2898(63)	52(15)
H(7A)	5756	2804	11015	44(15)
H(7B)	4846	2804	8944	36(15)
H(7C)	4398	2804	10041	59(19)

STRUCTURE DETERMINATION SUMMARY FOR 3

Crystal Data

Chemical Formula	$C_{22} H_{56} P_2 Si_2 In_2$
Color; Habit	Colorless prism
Crystal Size (mm)	0.40 x 0.46 x 0.50
Crystal System	Monoclinic
Space Group	$P2_1/n$
Unit Cell Dimensions	$\underline{a}$ = 8.643(1) Å
	$\underline{b}$ = 11.181(2) Å
	$\underline{c}$ = 18.237(2) Å
	β = 94.19(1)°
Volume	1757.7(4) $Å^3$
Z	2
Formula weight	668.4
Density(calc.)	1.263 g/cm^3
Absorption Coefficient	14.56 cm^{-1}
F(000)	688

Data Collection for 3

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	295
Monochromator	Highly oriented graphite crystal
2θ Range	3.5 to 55.0°
Scan Type	ω
Scan Speed	Variable; 4.88 to 14.65°/min. in ω
Scan Range (ω)	1.20°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$0 \leq h \leq 11$, $0 \leq k \leq 14$ $-23 \leq \ell \leq 23$
Reflections Collected	4816
Independent Reflections	4062 (R_{int} = 1.17%)
Observed Reflections	2630 ($F > 6.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.7072 / 0.7746

Solution and Refinement for 3

System Used	Siemens SHELXTL PLUS (VMS)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Poistions and U of H1 was refined; all other H atoms assume riding model with a common isotropic U refined
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0020F^2$
Number of Parameters refined	132
Final R indices (obs. data)	R = 2.93 %, wR = 4.52 %
R Indices (all data)	R = 5.49 %, wR = 6.00 %
Goodness-of-Fit	0.80
Largest and Mean Δ/σ	0.022, 0.001
Data-to-Parameter Ratio	19.9:1
Largest Difference Peak	0.31 $e\text{Å}^{-3}$
Largest Difference Hole	-0.35 $e\text{Å}^{-3}$

Table 8. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
In(1)	214(1)	4456(1)	8990(1)	55(1)
P(1)	-1366(1)	3858(1)	10118(1)	54(1)
Si(1)	-2098(2)	2024(1)	10444(1)	67(1)
C(1)	-1426(6)	5126(5)	8113(2)	68(2)
C(2)	-535(10)	5819(7)	7563(3)	120(3)
C(3)	-2257(10)	4084(7)	7746(4)	131(3)
C(4)	-2630(7)	5965(6)	8415(3)	95(2)
C(5)	2095(6)	3194(5)	8802(3)	84(2)
C(6)	2838(13)	2783(13)	9480(5)	296(9)
C(7)	1421(10)	2141(7)	8362(6)	152(4)
C(8)	3210(11)	3757(9)	8353(8)	204(7)
C(9)	-443(8)	1262(6)	10931(4)	119(3)
C(10)	-3727(8)	2175(7)	11054(3)	120(3)
C(11)	-2759(8)	1165(6)	9605(4)	104(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 9. Bond lengths (Å)

In(1)-P(1)	2.638 (1)	In(1)-C(1)	2.190 (5)
In(1)-C(5)	2.198 (6)	In(1)-P(1A)	2.637 (1)
P(1)-Si(1)	2.239 (2)	P(1)-In(1A)	2.637 (1)
Si(1)-C(9)	1.837 (6)	Si(1)-C(10)	1.866 (7)
Si(1)-C(11)	1.860 (7)	C(1)-C(2)	1.520 (9)
C(1)-C(3)	1.500 (9)	C(1)-C(4)	1.533 (8)
C(5)-C(6)	1.427 (11)	C(5)-C(7)	1.516 (10)
C(5)-C(8)	1.453 (13)		

Table 10. Bond angles (°)

P(1)-In(1)-C(1)	108.2(1)	P(1)-In(1)-C(5)	112.9(1)
C(1)-In(1)-C(5)	123.5(2)	P(1)-In(1)-P(1A)	83.9(1)
C(1)-In(1)-P(1A)	113.7(1)	C(5)-In(1)-P(1A)	107.8(1)
In(1)-P(1)-Si(1)	127.7(1)	In(1)-P(1)-In(1A)	96.1(1)
Si(1)-P(1)-In(1A)	126.3(1)	P(1)-Si(1)-C(9)	109.1(2)
P(1)-Si(1)-C(10)	108.4(3)	C(9)-Si(1)-C(10)	110.4(3)
P(1)-Si(1)-C(11)	109.3(2)	C(9)-Si(1)-C(11)	109.9(3)
C(10)-Si(1)-C(11)	109.7(3)	In(1)-C(1)-C(2)	108.9(4)
In(1)-C(1)-C(3)	108.9(4)	C(2)-C(1)-C(3)	110.6(5)
In(1)-C(1)-C(4)	111.5(3)	C(2)-C(1)-C(4)	108.3(5)
C(3)-C(1)-C(4)	108.6(5)	In(1)-C(5)-C(6)	111.3(6)
In(1)-C(5)-C(7)	108.7(4)	C(6)-C(5)-C(7)	109.9(7)
In(1)-C(5)-C(8)	109.7(5)	C(6)-C(5)-C(8)	110.7(7)
C(7)-C(5)-C(8)	106.4(7)		

Table 11. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	60(1)	60(1)	44(1)	11(1)	5(1)	-2(1)
P(1)	59(1)	54(1)	49(1)	3(1)	4(1)	5(1)
Si(1)	80(1)	57(1)	62(1)	-7(1)	-3(1)	7(1)
C(1)	81(3)	71(3)	49(2)	-5(2)	-10(2)	6(2)
C(2)	147(6)	148(6)	65(3)	6(5)	18(4)	42(4)
C(3)	161(7)	110(5)	113(5)	-17(5)	-57(5)	-18(4)
C(4)	86(4)	107(4)	91(4)	24(3)	-7(3)	20(3)
C(5)	79(3)	94(4)	79(3)	28(3)	15(3)	-12(3)
C(6)	313(15)	451(22)	120(7)	334(17)	-17(8)	-29(10)
C(7)	155(7)	101(5)	207(9)	30(5)	54(6)	-56(6)
C(8)	135(7)	126(7)	370(18)	9(6)	146(10)	-28(10)
C(9)	131(6)	65(3)	152(7)	-1(3)	-54(5)	24(4)
C(10)	133(5)	142(6)	89(4)	-26(5)	35(4)	24(4)
C(11)	111(5)	89(4)	108(5)	-6(4)	-10(4)	-25(4)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 12. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1)	-2962(68)	4238(48)	9820(34)	105(19)
H(2A)	-1244	6120	7176	173(7)
H(2B)	0	6475	7808	173(7)
H(2C)	203	5299	7358	173(7)
H(3A)	-2991	4353	7361	173(7)
H(3B)	-1504	3574	7542	173(7)
H(3C)	-2790	3646	8104	173(7)
H(4A)	-3335	6243	8020	173(7)
H(4B)	-3197	5544	8768	173(7)
H(4C)	-2104	6635	8648	173(7)
H(6A)	3648	2238	9371	173(7)
H(6B)	3260	3401	9802	173(7)
H(6C)	2047	2359	9717	173(7)
H(7A)	2225	1578	8273	173(7)
H(7B)	650	1759	8634	173(7)
H(7C)	951	2424	7901	173(7)
H(8A)	4027	3203	8268	173(7)
H(8B)	2706	3999	7890	173(7)
H(8C)	3637	4446	8608	173(7)
H(9A)	-750	475	11071	173(7)
H(9B)	395	1204	10615	173(7)
H(9C)	-109	1711	11363	173(7)
H(10A)	-4059	1397	11200	173(7)
H(10B)	-3391	2630	11483	173(7)
H(10C)	-4575	2579	10790	173(7)
H(11A)	-3074	376	9740	173(7)
H(11B)	-3621	1572	9355	173(7)
H(11C)	-1926	1108	9287	173(7)

STRUCTURE DETERMINATION SUMMARY FOR 4

Crystal Data

Empirical Formula	$C_{24}\ H_{54}\ In_3\ P_3$
Color; Habit	Pale yellow prism
Crystal Size (mm)	0.05 x 0.25 x 0.38
Crystal System	Hexagonal
Space Group	$P\bar{6}2m$ (No.189)
Unit Cell Dimensions	a = 11.327(3) Å
	c = 16.962(7) Å
Volume	1884.6(15) $Å^3$
Z	2
Formula weight	780.0
Density(calc.)	1.375 g/cm^3
Absorption Coefficient	19.28 cm^{-1}
F(000)	780

Data Collection for 4

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	-100
Monochromator	Highly oriented graphite crystal
2θ Range	3.50 to 55.0°
Scan Type	2θ-θ
Scan Speed	Variable; 4.19 to 9.77°/min. in ω
Scan Range (ω)	1.20° plus Kα-separation
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$-5\leq h\leq 0$, $-3\leq k\leq 0$, $-10\leq \ell\leq 0$ and $0\leq h\leq 12$, $0\leq k\leq 12$, $0\leq \ell\leq 22$
Reflections Collected	1844
Independent Reflections	1003 (R_{int} = 3.15%)
Observed Reflections	721 ($F > 6.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.8044 / 0.9606

Solution and Refinement for 4

System Used	Siemens SHELXTL PLUS (VMS)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0050F^2$
Number of Parameters refined	44
Final R indices (obs. data)	R = 5.82 %, wR = 7.92 %
R Indices (all data)	R = 7.84 %, wR = 11.12 %
Goodness-of-Fit	0.98
Largest and Mean Δ/σ	0.090, 0.015
Data-to-Parameter Ratio	16.4:1
Largest Difference Peak	1.96 $eÅ^{-3}$
Largest Difference Hole	-1.17 $eÅ^{-3}$

Table 13. Atomic coordinates ($x10^5$) and equivalent isotropic displacement coefficients ($Å^2 x10^4$)

	x	y	z	U(eq)
In(1)	25070(12)	0	0	352(6)
P(1)	0	-20693(76)	0	650(34)
C(1)	33787(135)	0	11591(90)	392(52)
C(2)	47484(189)	12194(174)	12418(131)	1257(111)
C(3)	24342(242)	0	17710(161)	1321(168)
In(2)	66240(27)	8174(28)	50000	492(12)
P(2)	46428(139)	13227(124)	50000	1075(90)
C(4)	69460	0	39570	1926(222)
C(5)	82370	0	39540	1210(119)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table 14. Bond lengths (Å)

In(1)-P(1)	2.627 (3)	In(1)-C(1)	2.200 (15)
In(1)-P(1A)	2.627 (6)	In(1)-C(1A)	2.200 (15)
P(1)-In(1A)	2.627 (3)	C(1)-C(2)	1.480 (17)
C(1)-C(3)	1.491 (31)	C(1)-C(2A)	1.480 (25)
In(2)-P(2)	2.578 (18)	In(2)-C(4)	2.111 (2)
In(2)-In(2B)	1.604 (5)	In(2)-P(2A)	2.618 (11)
In(2)-C(4A)	2.111 (2)	P(2)-In(2A)	2.618 (17)
P(2)-P(2B)	2.595 (24)	C(4)-C(5)	1.462 (1)
C(4)-In(2B)	2.111 (2)		

Table15. Bond angles (°)

P(1)-In(1)-C(1)	106.6(2)	P(1)-In(1)-P(1A)	101.2(3)
C(1)-In(1)-P(1A)	106.6(2)	P(1)-In(1)-C(1A)	106.6(2)
C(1)-In(1)-C(1A)	126.7(8)	P(1A)-In(1)-C(1A)	106.6(2)
In(1)-P(1)-In(1A)	138.8(4)	In(1)-C(1)-C(2)	110.2(11)
In(1)-C(1)-C(3)	107.5(13)	C(2)-C(1)-C(3)	110.6(13)
In(1)-C(1)-C(2A)	110.2(10)	C(2)-C(1)-C(2A)	107.8(18)
C(3)-C(1)-C(2A)	110.6(12)	P(2)-In(2)-C(4)	117.2(1)
P(2)-In(2)-In(2B)	101.1(3)	C(4)-In(2)-In(2B)	67.7(1)
P(2)-In(2)-P(2A)	99.2(6)	C(4)-In(2)-P(2A)	102.7(2)
In(2B)-In(2)-P(2A)	159.7(4)	P(2)-In(2)-C(4A)	117.2(1)
C(4)-In(2)-C(4A)	113.8(2)	In(2B)-In(2)-C(4A)	67.7(1)
P(2A)-In(2)-C(4A)	102.7(2)	In(2)-P(2)-In(2A)	140.8(4)
In(2)-P(2)-P(2B)	78.9(6)	In(2A)-P(2)-P(2B)	140.3(4)
In(2)-C(4)-C(5)	113.3(1)	In(2)-C(4)-In(2B)	44.6(1)
C(5)-C(4)-In(2B)	113.3(1)		

Table 16. Anisotropic displacement coefficients ($Å^2 x 10^4$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
In(1)	191(5)	282(9)	614(10)	141(5)	0	0
P(1)	150(28)	294(27)	1459(87)	75(14)	0	0
C(1)	437(63)	377(72)	342(78)	189(36)	-89(54)	0
C(2)	864(110	924(134	1375(178	-10(119	-688(123	-54(127)
C(3)	1468(227	891(205	1412(264	446(103	529(187	0
In(2)	389(13)	336(14)	773(20)	198(11)	0	0
P(2)	464(65)	338(54)	2431(233	206(54)	0	0

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table 17. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(2A)	5070	1199	1762	60
H(2B)	5357	1189	859	60
H(2C)	4714	2043	1174	60
H(3A)	2778	0	2288	60
H(3B)	2354	799	1707	60
H(3C)	1555	-799	1707	60