ORGANOMETALLICS
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Experimental section:

General. Nuclear magnetic resonance spectra were obtained on a JEOL-GX 400 instrument. Neat $HgMe_2$ was used as an external standard for the ^{199}Hg NMR spectra. The proton and carbon signals of the deuterated solvent were used as internal standard for the ^1H and ^{13}C NMR spectra, respectively. All NMR measurements were carried out at 25°C unless otherwise noted. Elemental analyses were performed by the Laboratory for Microanalysis at Technischen Universität München. When necessary, the experiments were carried out under a dry inert atmosphere of N_2 using standard Schlenk technique or a glove box (Labmaster 130, Fa. M. Braun). All melting points were measured on samples in sealed capillaries and are uncorrected. THF and THF-d_8 were dried over Na/K and distilled prior to use. Hexane was dried over CaH_2 prior distillation and use. All other sovents were used without further purification. All starting materials were purchased from Aldrich Chemicals and used without further purification.

Synthesis of 1,4-butanediylbis(mercurybromide) (1). To a suspension of magnesium (3.4 g, 0.140 mol) in THF (30 mL) was added slowly a solution of 1,4-dibromobutane (3.02 g, 0.014 mol) in THF (50 mL). After the addition was completed the mixture was stirred for 0.5 h at room temperature and then refluxed for 2 h. The resulting solution was filtered at room temperature and slowly added to a cooled (0 °C) solution of $HgBr_2$ (10.0 g, 0.028 mol) in THF (25 mL). The reaction proceeded immediately as indicated by the formation of a white precipitate. The resulting mixture was stirred for 12 h at room temperature and refluxed for 2 h. The precipitate was filtered, washed three times with water (25 mL), one time with THF (20 mL) and finally with pentane (20 mL) before being dried under vacuum to afford a 30% yield (2.63 g) of colorless powdery **1**, mp 330 - 332 °C (dec.). Anal. Calc. for $C_4H_8Br_2Hg_2$: C, 7.78; H, 1.30;. Found C, 7.49; H, 1.63. CIMS (isobutane): *m/z* 617 (M^+, 5%), 595 ($M^+ - C_2H_4$, 100%).

Synthesis of 1,5-pentandiylbis(mercurybromide) (2). Compound **2** was prepared in the same way as **1** using magnesium-turnings (3.4 g, 0.140 mol), 1,5-dibromopentane (3.22 g, 0.014 mol) and $HgBr_2$ (10 g, 0.028 mol). Yield: 2.8 g (32%) of colorless, powdery solid, mp 152 °C (lit. 150 °C see Hilpert, S.; Grüttner, G. *Chem. Ber.* **1914**, *47*, 177). Anal. Calc. for $C_5H_{10}Br_2Hg_2$: C, 9.51; H, 1.58. Found C, 9.45; H, 1.64.

^{1}H NMR (DMSO-d_6): δ 1.35 (p, ^3J 6.7 Hz, 2 H, γ-CH_2), δ 1.73 (tt, ^3J 6.7 Hz, ^3J 7.3 Hz, 4 H, β-CH_2) δ 1.82 (t, ^3J 7.3 Hz, 4 H, α-CH_2) ^{13}C{^{1}H} NMR (DMSO-d_6): δ 27.9 (γ-C) 34.3 (β-C), 39.0 (α-C). ^{199}Hg{^{1}H} NMR (DMSO-d_6): δ -1089. CIMS (isobutane): m/z 617 (M+, 5%), 595 (M^+ - C_3H_6, 100%).

Synthesis of 1,6-hexanediylbis(mercurybromide) (3). Compound **3** was prepared in the same way as **1** using magnesium-turnings (3.4 g, 0.140 mol), (3.4 g , 0.014 mol) 1,6-dibromopentane and $HgBr_2$ (10 g, 0.028 mol). Yield: 3.3 g (31%) of colorless, powdery solid, mp 285 - 286 °C (dec.). Anal. Calc. for $C_6H_{12}Br_2Hg_2$: C, 11.16; H, 1.86. Found C, 11.86; H, 2.08. CIMS (isobutane): m/z 645 (M^+, 100%).

Synthesis of 1,4-butanediylbis[bis(tetrahydrofuran)indiumdibromide] (4): InBr (0.215 g, 1.1 mmol) and **1** (0.310 g, 0.5 mmol) were stirred together at room temperature in THF (5 mL) for 3 h, after which time the reaction mixture was filtered to remove the metallic grey precipitate. Concentration of the filtrate followed by cooling to -25°C afforded a 60 % yield (0.27 g) of crystalline **4**, mp 147 °C. Anal. Calc. for $C_{20}H_{40}Br_4In_2O_4$: C, 26.87; H, 4.48. Found C, 26.80; H, 4.49. ^{1}H NMR (THF- d_8): δ 1.17 (br, 4H, α-CH_2), 1.76 (br, 4H, β-CH_2), 1.77 (m, 16H, OCH$_2$CH_2), 3.61 (m, 16H, OCH_2). ^{13}C{^{1}H} NMR (THF- d_8): δ 20.8 (br, α-C), 26.4 (OCH$_2$CH$_2$), 32.6 (β-C), 68.2 (OCH$_2$).

Synthesis of 1,5-pentanediylbis[bis(tetrahydrofuran)indiumdibromide] (5): Compound **5** was prepared in a similar fashion as **4** starting with InBr (0.215 g, 1.1 mmol) and **2** (0.315 g, 0.5 mmol). Yield: 0.11 g of colorless microcrystals (25 %), mp. 92 °C. No correct elemental analysis due to loss of part of the THF component. Anal. Calc. for $C_{21}H_{42}Br_4In_2O_4$: C, 27.78; H, 4.63. Found C, 25.24; H, 4.36. ^{1}H NMR (THF- d_8): δ 1.15 (t, ^3J 7.3 Hz, 4H, α-CH_2), 1.55 (br, ^3J 6.8 Hz, 2H, γ-CH_2), 1.76 (br, 4H, β-CH_2), 1.77 (m, 16H, OCH$_2$CH_2), 3.61 (m, 16H, OCH_2). ^{13}C{^{1}H} NMR (THF- d_8): δ 20.9 (br, α-C), 26.4 (OCH$_2$CH$_2$), 27.4 (γ-C), 39.6 (β-C), 68.2 (OCH$_2$).

Synthesis of 1,6-hexanediylbis[bis(tetrahydrofuran)indiumdibromide] (6): Compound **6** was prepared in a similar fashion as **4** starting with InBr (0.215 g, 1.1 mmol) and **3** (0.320 g, 0.5 mmol). Yield: 0.21 g of colorless crystals (46 %), mp. 94 - 96 °C. No correct elemental analysis due to loss of part of the THF component. Anal. Calc. for

$C_{22}H_{44}Br_4In_2O_4$: C, 28.66; H, 4.78. Found C, 26.42; H, 4.56. ^1H NMR (THF- d_8): δ 1.16 (t, ^3J 7.8 Hz, 4H, α-CH_2), 1.45 (br, 4H, γ-CH_2), 1.76 (br, 4H, β-CH_2), 1.77 (m, 16H, OCH_2CH_2), 3.61 (m, 16H, OCH_2). $^{13}C\{^1H\}$ NMR (THF- d_8): δ 21.0 (br, α-*C*), 26.4 (OCH_2CH_2), 27.7 (γ-*C*), 34.7 (β-*C*), 68.2 (OCH_2).

Synthesis of bis(tetraphenylphosphonium)-bis(tribromoindato)-1,4-butane (7): Compound **4** (0.05 mmol, 44.7 mg) and tetraphenylphosphonium bromide (0.1 mmol, 42 mg) were dissolved in THF (1 mL). Compound **7** precipitated immediatly as a white powder in 90% yield (65 mg), mp. 136 °C. Anal. Calc. for $C_{52}H_{48}Br_6In_2P_2$: C, 43.24; H, 3.33. Found C, 42.92; H, 3.47. ^1H NMR (MeCN-d_3): δ 1.09 (br, 4H, α-CH_2), 1.68 (br, 4H, β-CH_2), 7.66 to 7.94 (m, 40 H, P(C_6H_5)). $^{13}C\{^1H\}$ NMR (MeCN-d_3): δ 21.7 (br, α-*C*), 31.3 (β-*C*); [Ph_4P^+] δ 118.4 (*C*-ipso), 130.3 (d, $^2J_{CP}$ 13.0 Hz, C-*meta)*, 134.6 (d, $^3J_{CP}$ 10.7 Hz, C-*ortho*), 135.4 (C-*para*).

Synthesis of bis(tetraphenylphosphonium)-bis(tribromoindato)-1,6-hexane (8): Compound **6** (0.05 mmol, 46.0 mg) and tetraphenylphosphonium bromide (0.1 mmol, 42 mg) were dissolved in THF (1 mL). The resulting solution was layered with hexane (0.5 mL) and allowed to stand for several days at room temperature. Colorless crystals of **8** formed on the wall of the vessel in 85% yield (63 mg), mp. 155 °C. Anal. Calc. for $C_{54}H_{52}Br_6In_2P_2$: C, 44.05; H, 3.54. Found C, 43.87; H, 3.58. ^1H NMR (MeCN-d_3): δ 1.08 (t, ^3J 8.1 Hz, 4H, α-CH_2), 1.36 (br, 4H, γ-CH_2), 1.60 (br, 4H, β-CH_2), 7.66 to 7.94 (m, 40 H, P(C_6H_5)). $^{13}C\{^1H\}$ NMR (MeCN-d_3): δ 21.7 (br, α-*C*), 27.0 (γ-*C*), 33.3 (α-*C*); [Ph_4P^+] δ 118.4 (*C*-ipso), 130.3 (d, $^2J_{CP}$ 13.0 Hz, C-*meta)*, 134.7 (d, $^3J_{CP}$ 10.0 Hz, C-*ortho*), 135.4 (C-*para*).

Crystal Structure Determinations. Specimens of suitable quality and size of compounds **4**, **7**, and **8** were mounted in glass capillaries and used for measurement of precise cell constants and intensity data collection on an Enraf Nonius CAD4 diffractometer [Mo-K_α radiation, λ(Mo-K_α) = 0.71073 Å]. During data collection, three standard reflections were measured periodically as a general check of crystal and instrument stability. No significant changes were observed for all three compounds. Lp correction was applied and intensity data were corrected for absorption effects. The structures were solved by direct methods (SHELXS-86) and completed by full-matrix-least squares techniques against F^2 (SHELXL-93). The thermal motion of all non-hydrogen atoms was treated anisotropically. All hydrogen atoms of compounds **7** and **8** were calculated and allowed to ride on their corresponding carbon atoms with fixed isotropic contributions ($U_{iso(fix)}$ = 1.5 x U_{eq} of the attached C atom), whereas the methylene hydrogen atoms of **4** were found and refined with isotropic contributions. Further information on crystal data, data collection and structure refinement are summarized in Table 1. Important interatomic distances and angles are shown in the corresponding Figure Captions.

Table 1. Crystal data, data collection, and structure refinement for compounds **4**, **7**, and **8**.

		4	**7**	**8**
Crystal data				
Formula		$C_{20}H_{40}Br_4In_2O_4$	$C_{52}H_{48}Br_6In_2P_2$	$C_{54}H_{52}Br_6In_2P_2$
M_r		893.80	1443.94	1472.00
Crystal system		monoclinic	monoclinic	monoclinic
Space group		$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/c$
a	(Å)	9.325(1)	12.466(2)	7.689(1)
b	(Å)	13.721(1)	7.576(1)	14.585(1)
c	(Å)	12.125(1)	28.846(4)	25.014(3)
α	(°)	90	90	90
β	(°)	109.16(1)	98.89(1)	96.59(1)
γ	(°)	90	90	90
V	(Å^3)	1465.4(2)	2691.6(7)	2786.6(5)
ρ_{calc}	(gcm^{-3})	2.026	1.782	1.754
Z		2	2	2
$F(000)$		860	1396	1428
μ(Mo K_α)	(cm^{-1})	70.48	54.03	52.20
Absorption correction		psi-scans	psi-scans	psi-scans
T_{min}/T_{max}		0.749/0.999	0.436/0.999	0.668/0.999
Data collection				
T (°C)		-74	-74	-74
Scan mode		ω-θ	ω	ω
hkl range		0→12, 0→18, -15→15	0→15, 0→9, -35→35	-9→9, -18→0, 0→31
$\sin(\theta/\lambda)_{max}$	(Å^{-1})	0.66	0.62	0.64
Measured reflections		3432	5260	5400
Refls. used for refinement		3250	5205	5283
Refinement				
Refined parameters		152	280	289
H atoms (found/calcd.)		4/16	0/24	0/26
Final R values [I>2σ(I)]				
$R1$[a]		0.0351	0.0417	0.0315
$wR2$[b]		0.0885	0.0728	0.0588
$(\text{shift/error})_{max}$		<0.001	<0.001	<0.001
ρ_{fin}(max/min)	(eÅ^{-3})	1.627/-1.134	1.137/-0.790	0.494/-0.576

[a] $R = \Sigma(\int F_o \geq -\geq F_o \int)/\Sigma|F_o|$; [b] $wR2 = \{[\Sigma w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$; $w = 1/[\sigma^2(F_o^2)+(ap)^2+bp]$; $p = (F_o^2+2F_c^2)/3$; a = 0.0553 (**4**), 0.0247 (**7**), 0.0255 (**8**); b = 2.57 (**4**), 5.85 (**7**), 2.16 (**8**).

Table 1. Crystal data and structure refinement for MART6. COMPOUND 4

Identification code	MART6
Empirical formula	$C_{20}H_{40}Br_4In_2O_4$
Formula weight	893.80
Temperature	199(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 9.325(1) Å α = 90° b = 13.721(1) Å β = 109.16(1)° c = 12.125(1) Å γ = 90°
Volume	1465.4(2) $Å^3$
Z	2
Density (calculated)	2.026 Mg/m^3
Absorption coefficient	7.048 mm^{-1}
F(000)	860
θ range for data collection	3.46 to 28.02°
Index ranges	$0 \le h \le 12$, $0 \le k \le 18$, $-15 \le \ell \le 15$
Reflections collected	3432
Independent reflections	3254 (R_{int} = 0.0415)
Absorption correction	Psi-scans
Max. and min. transmission	0.999 and 0.749
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3250 / 0 / 152
Goodness-of-fit on F^2	1.047
Final R indices [$I>2\sigma(I)$]	R1 = 0.0351, wR2 = 0.0885
R indices (all data)	R1 = 0.0436, wR2 = 0.0943
Largest diff. peak and hole	1.627 and -1.134 $eÅ^{-3}$

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [$Å^2$] for MART6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In	0.80426(3)	0.90718(2)	0.15769(2)	0.02870(10)
Br(1)	0.54791(6)	0.90173(4)	0.18944(4)	0.04399(14)
Br(2)	1.00971(6)	0.86574(4)	0.34596(4)	0.0466(2)
O(1)	0.8267(4)	1.0710(2)	0.2193(3)	0.0371(7)
C(11)	0.8477(7)	1.0968(4)	0.3403(4)	0.0498(13)
C(12)	0.7939(7)	1.1997(4)	0.3364(4)	0.0514(13)
C(13)	0.6706(7)	1.2055(5)	0.2198(5)	0.060(2)
C(14)	0.7286(7)	1.1423(4)	0.1423(4)	0.0454(12)
O(2)	0.7797(4)	0.7349(2)	0.1193(3)	0.0367(7)
C(21)	0.7723(7)	0.6663(4)	0.2081(4)	0.0448(11)
C(22)	0.6746(9)	0.5834(5)	0.1431(6)	0.067(2)
C(23)	0.5943(14)	0.6197(7)	0.0304(6)	0.133(5)
C(24)	0.6803(8)	0.7024(4)	0.0075(4)	0.057(2)
C(1)	0.8127(6)	0.9294(4)	-0.0152(4)	0.0411(11)
C(2)	0.9173(5)	1.0096(4)	-0.0327(4)	0.0372(10)

Table 3. Bond lengths [Å] and angles [°] for MART6.

In-C(1)	2.145(4)	In-O(1)	2.357(3)
In-O(2)	2.406(3)	In-Br(2)	2.5167(6)
In-Br(1)	2.5440(6)	O(1)-C(14)	1.450(6)
O(1)-C(11)	1.458(5)	C(11)-C(12)	1.494(8)
C(11)-H(111)	0.97	C(11)-H(112)	0.96
C(12)-C(13)	1.503(8)	C(12)-H(121)	0.96
C(12)-H(122)	0.96	C(13)-C(14)	1.505(8)
C(13)-H(131)	0.96	C(13)-H(132)	0.97
C(14)-H(141)	0.96	C(14)-H(142)	0.96
O(2)-C(24)	1.439(5)	O(2)-C(21)	1.449(5)
C(21)-C(22)	1.507(8)	C(21)-H(211)	0.96
C(21)-H(212)	0.96	C(22)-C(23)	1.415(10)
C(22)-H(221)	0.96	C(22)-H(222)	0.96
C(23)-C(24)	1.468(9)	C(23)-H(231)	0.97
C(23)-H(232)	0.96	C(24)-H(241)	0.96
C(24)-H(242)	0.96	C(1)-C(2)	1.531(6)
C(1)-H(11)	0.86(6)	C(1)-H(12)	0.95(6)
C(2)-C(2)#1	1.509(10)	C(2)-H(21)	1.01(6)
C(2)-H(22)	1.01(5)		

C(1)-In-O(1)	98.4(2)	C(1)-In-O(2)	89.0(2)
O(1)-In-O(2)	172.61(10)	C(1)-In-Br(2)	131.1(2)
O(1)-In-Br(2)	88.05(8)	O(2)-In-Br(2)	87.10(8)
C(1)-In-Br(1)	119.3(2)	O(1)-In-Br(1)	88.29(9)
O(2)-In-Br(1)	88.06(8)	Br(2)-In-Br(1)	109.24(2)
C(14)-O(1)-C(11)	109.4(3)	C(14)-O(1)-In	117.8(3)
C(11)-O(1)-In	121.2(3)	O(1)-C(11)-C(12)	105.3(4)
O(1)-C(11)-H(111)	110.5(3)	C(12)-C(11)-H(111)	110.6(3)
O(1)-C(11)-H(112)	110.8(3)	C(12)-C(11)-H(112)	110.4(3)
H(111)-C(11)-H(112)	109.1	C(11)-C(12)-C(13)	103.0(4)
C(11)-C(12)-H(121)	110.8(4)	C(13)-C(12)-H(121)	111.2(4)
C(11)-C(12)-H(122)	111.4(3)	C(13)-C(12)-H(122)	111.0(3)
H(121)-C(12)-H(122)	109.3	C(12)-C(13)-C(14)	103.6(5)
C(12)-C(13)-H(131)	111.2(4)	C(14)-C(13)-H(131)	110.5(3)
C(12)-C(13)-H(132)	111.1(4)	C(14)-C(13)-H(132)	111.6(4)
H(131)-C(13)-H(132)	108.8	O(1)-C(14)-C(13)	105.5(4)
O(1)-C(14)-H(141)	110.5(2)	C(13)-C(14)-H(141)	110.1(3)
O(1)-C(14)-H(142)	110.5(3)	C(13)-C(14)-H(142)	111.4(4)
H(141)-C(14)-H(142)	108.8	C(24)-O(2)-C(21)	109.0(4)
C(24)-O(2)-In	118.5(3)	C(21)-O(2)-In	121.3(3)
O(2)-C(21)-C(22)	105.6(4)	O(2)-C(21)-H(211)	110.6(3)
C(22)-C(21)-H(211)	109.4(4)	O(2)-C(21)-H(212)	110.4(3)
C(22)-C(21)-H(212)	111.8(4)	H(211)-C(21)-H(212)	109.0
C(23)-C(22)-C(21)	106.1(5)	C(23)-C(22)-H(221)	112.5(6)
C(21)-C(22)-H(221)	111.5(3)	C(23)-C(22)-H(222)	108.3(7)
C(21)-C(22)-H(222)	109.2(4)	H(221)-C(22)-H(222)	109.1
C(22)-C(23)-C(24)	107.8(6)	C(22)-C(23)-H(231)	108.0(7)
C(24)-C(23)-H(231)	108.7(7)	C(22)-C(23)-H(232)	112.0(5)
C(24)-C(23)-H(232)	111.7(5)	H(231)-C(23)-H(232)	108.5
O(2)-C(24)-C(23)	106.5(4)	O(2)-C(24)-H(241)	109.7(3)
C(23)-C(24)-H(241)	109.0(6)	O(2)-C(24)-H(242)	110.9(3)
C(23)-C(24)-H(242)	111.9(6)	H(241)-C(24)-H(242)	108.8
C(2)-C(1)-In	117.9(3)	C(2)-C(1)-H(11)	116(4)
In-C(1)-H(11)	103(4)	C(2)-C(1)-H(12)	113(3)
In-C(1)-H(12)	108(3)	H(11)-C(1)-H(12)	96(5)
C(2)#1-C(2)-C(1)	112.9(5)	C(2)#1-C(2)-H(21)	109(3)
C(1)-C(2)-H(21)	110(3)	C(2)#1-C(2)-H(22)	111(3)
C(1)-C(2)-H(22)	110(3)	H(21)-C(2)-H(22)	104(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z

Table 4. Anisotropic displacement parameters [$Å^2$] for MART6.

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	0.0371(2)	0.0294(2)	0.01814(14)	0.00027(10)	0.00706(11)	-0.00309(11)
Br(1)	0.0423(3)	0.0516(3)	0.0411(3)	0.0021(2)	0.0177(2)	-0.0036(2)
Br(2)	0.0551(3)	0.0447(3)	0.0267(2)	-0.0022(2)	-0.0048(2)	0.0082(2)
O(1)	0.051(2)	0.032(2)	0.0229(14)	-0.0048(12)	0.0049(13)	-0.0003(13)
C(11)	0.072(4)	0.045(3)	0.024(2)	-0.009(2)	0.004(2)	0.005(2)
C(12)	0.068(4)	0.047(3)	0.036(2)	-0.009(2)	0.012(2)	0.005(3)
C(13)	0.067(4)	0.061(4)	0.043(3)	-0.004(3)	0.006(3)	0.021(3)
C(14)	0.061(3)	0.037(2)	0.028(2)	0.000(2)	0.001(2)	0.005(2)
O(2)	0.055(2)	0.031(2)	0.0216(13)	-0.0005(12)	0.0087(13)	-0.0072(14)
C(21)	0.062(3)	0.037(2)	0.030(2)	0.009(2)	0.007(2)	-0.006(2)
C(22)	0.097(5)	0.048(3)	0.046(3)	0.008(3)	0.013(3)	-0.025(3)
C(23)	0.215(12)	0.097(6)	0.040(3)	0.014(4)	-0.020(5)	-0.111(7)
C(24)	0.091(4)	0.046(3)	0.023(2)	-0.003(2)	0.004(2)	-0.023(3)
C(1)	0.046(3)	0.054(3)	0.023(2)	-0.001(2)	0.010(2)	-0.016(2)
C(2)	0.046(3)	0.040(2)	0.028(2)	0.008(2)	0.014(2)	-0.003(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters [$Å^2$] for MART6.

	x/a	y/b	z/c	U(eq)
H(111)	0.9534(7)	1.0918(4)	0.3873(4)	0.075
H(112)	0.7887(7)	1.0548(4)	0.3723(4)	0.075
H(121)	0.8748(7)	1.2447(4)	0.3407(4)	0.077
H(122)	0.7545(7)	1.2130(4)	0.3990(4)	0.077
H(131)	0.6566(7)	1.2711(5)	0.1913(5)	0.089
H(132)	0.5755(7)	1.1817(5)	0.2247(5)	0.089
H(141)	0.6452(7)	1.1105(4)	0.0847(4)	0.068
H(142)	0.7844(7)	1.1798(4)	0.1030(4)	0.068
H(211)	0.7254(7)	0.6959(4)	0.2597(4)	0.067
H(212)	0.8727(7)	0.6445(4)	0.2533(4)	0.067
H(221)	0.6079(9)	0.5599(5)	0.1834(6)	0.100
H(222)	0.7387(9)	0.5310(5)	0.1350(6)	0.100
H(231)	0.4969(14)	0.6429(7)	0.0311(6)	0.199
H(232)	0.5777(14)	0.5703(7)	-0.0285(6)	0.199
H(241)	0.7396(8)	0.6804(4)	-0.0396(4)	0.085
H(242)	0.6148(8)	0.7543(4)	-0.0330(4)	0.085
H(11)	0.718(7)	0.935(4)	-0.056(5)	0.04(2)
H(12)	0.829(6)	0.868(5)	-0.046(5)	0.04(2)
H(21)	0.904(6)	1.017(4)	-0.119(5)	0.043(14)
H(22)	0.885(6)	1.075(4)	-0.011(5)	0.037(14)

Table 1. Crystal data and structure refinement for MART11. COMPOUND 4

Identification code	MART11
Empirical formula	$C_{52}H_{48}Br_6In_2P_2$
Formula weight	1443.94
Temperature	199(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 12.466(2) Å α = 90° b = 7.576(1) Å β = 98.89(1)° c = 28.846(4) Å γ = 90°
Volume	2691.6(7) $Å^3$
Z	2
Density (calculated)	1.782 Mg/m^3
Absorption coefficient	5.403 mm^{-1}
F(000)	1396
Crystal size	0.45 x 0.26 x 0.10 mm
θ range for data collection	3.05 to 26.00°
Index ranges	$0 \le h \le 15$, $0 \le k \le 9$, $-35 \le \ell \le 35$
Reflections collected	5260
Independent reflections	5253 (R_{int} = 0.0100)
Absorption correction	Psi-scans
Max. and min. transmission	0.99 and 0.44
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5205 / 0 / 280
Goodness-of-fit on F^2	1.141
Final R indices [$I>2\sigma(I)$]	R1 = 0.0417, wR2 = 0.0782
R indices (all data)	R1 = 0.0750, wR2 = 0.1034
Largest diff. peak and hole	1.137 and -0.790 $eÅ^{-3}$

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [$Å^2$] for MART11. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In	0.19610(3)	0.25060(5)	0.088941(12)	0.03332(10)
Br(1)	0.15338(5)	-0.07771(7)	0.08775(2)	0.0459(2)
Br(2)	0.35005(5)	0.28491(8)	0.04089(2)	0.0510(2)
Br(3)	0.27723(6)	0.30068(11)	0.17420(2)	0.0677(2)
P	0.27898(11)	0.5169(2)	-0.14902(4)	0.0286(3)
C(1)	0.0655(4)	0.4256(6)	0.0626(2)	0.0358(12)
C(2)	0.0419(4)	0.4309(7)	0.0093(2)	0.0362(12)
C(11)	0.3290(4)	0.6539(7)	-0.1921(2)	0.0343(12)
C(12)	0.3940(5)	0.7947(7)	-0.1756(2)	0.048(2)
C(13)	0.4384(5)	0.9014(9)	-0.2066(3)	0.060(2)
C(13)	0.4168(5)	0.8681(10)	-0.2537(3)	0.063(2)
C(13)	0.3500(5)	0.7297(10)	-0.2702(2)	0.062(2)
C(16)	0.3057(4)	0.6190(8)	-0.2396(2)	0.0427(14)
C(21)	0.1704(4)	0.3772(7)	-0.1756(2)	0.0318(11)
C(22)	0.1953(4)	0.2397(8)	-0.2043(2)	0.0433(13)
C(23)	0.1150(5)	0.1267(8)	-0.2244(2)	0.054(2)
C(24)	0.0097(5)	0.1467(9)	-0.2155(2)	0.055(2)
C(25)	-0.0155(5)	0.2830(9)	-0.1866(2)	0.050(2)
C(26)	0.0644(4)	0.3989(8)	-0.1666(2)	0.0387(13)
C(31)	0.3847(4)	0.3762(6)	-0.1215(2)	0.0291(11)
C(32)	0.4923(4)	0.4058(7)	-0.1259(2)	0.0367(12)
C(33)	0.5722(5)	0.2942(8)	-0.1045(2)	0.046(2)
C(34)	0.5449(5)	0.1529(8)	-0.0787(2)	0.048(2)
C(35)	0.4389(5)	0.1232(7)	-0.0735(2)	0.047(2)
C(36)	0.3575(5)	0.2335(7)	-0.0949(2)	0.0406(13)
C(41)	0.2337(4)	0.6639(7)	-0.1072(2)	0.0307(11)
C(42)	0.1655(4)	0.8028(7)	-0.1244(2)	0.0398(13)
C(43)	0.1307(5)	0.9220(7)	-0.0930(2)	0.0451(14)
C(44)	0.1641(5)	0.9012(8)	-0.0457(2)	0.048(2)
C(45)	0.2313(5)	0.7648(8)	-0.0290(2)	0.0476(14)
C(46)	0.2675(4)	0.6439(7)	-0.0595(2)	0.0367(12)

Table 3. Bond lengths [Å] and angles [°] for MART11.

In-C(1)	2.146(5)	In-Br(3)	2.5390(8)
In-Br(1)	2.5427(7)	In-Br(2)	2.5485(7)
P-C(31)	1.783(5)	P-C(21)	1.794(5)
P-C(41)	1.795(5)	P-C(11)	1.803(5)
C(1)-C(2)	1.520(7)	C(1)-H(1)	0.96
C(1)-H(2)	0.96	C(2)-C(2)#1	1.516(10)
C(2)-H(3)	0.96	C(2)-H(4)	0.96
C(11)-C(12)	1.378(8)	C(11)-C(16)	1.382(7)
C(12)-C(13)	1.383(8)	C(12)-H(12)	0.96
C(13)-C(13)	1.368(10)	C(13)-H(13)	0.96
C(13)-C(13)	1.378(10)	C(13)-H(13)	0.96
C(13)-C(16)	1.393(8)	C(13)-H(13)	0.96
C(16)-H(16)	0.96	C(21)-C(22)	1.396(7)
C(21)-C(26)	1.395(7)	C(22)-C(23)	1.375(8)
C(22)-H(22)	0.96	C(23)-C(24)	1.384(9)
C(23)-H(23)	0.96	C(24)-C(25)	1.392(9)
C(24)-H(24)	0.96	C(25)-C(26)	1.385(8)
C(25)-H(25)	0.96	C(26)-H(26)	0.96
C(31)-C(32)	1.385(7)	C(31)-C(36)	1.397(7)
C(32)-C(33)	1.377(7)	C(32)-H(32)	0.96
C(33)-C(34)	1.377(8)	C(33)-H(33)	0.96
C(34)-C(35)	1.371(8)	C(34)-H(34)	0.96
C(35)-C(36)	1.383(8)	C(35)-H(35)	0.96
C(36)-H(36)	0.96	C(41)-C(46)	1.384(7)
C(41)-C(42)	1.394(7)	C(42)-C(43)	1.394(7)
C(42)-H(42)	0.96	C(43)-C(44)	1.373(8)
C(43)-H(43)	0.96	C(44)-C(45)	1.370(8)
C(44)-H(44)	0.96	C(45)-C(46)	1.393(7)
C(45)-H(45)	0.96	C(46)-H(46)	0.96

C(1)-In-Br(3)	114.68(14)	C(1)-In-Br(1)	117.00(14)
Br(3)-In-Br(1)	102.15(3)	C(1)-In-Br(2)	109.77(14)
Br(3)-In-Br(2)	106.91(3)	Br(1)-In-Br(2)	105.44(2)
C(31)-P-C(21)	107.1(2)	C(31)-P-C(41)	111.1(2)
C(21)-P-C(41)	111.0(2)	C(31)-P-C(11)	109.9(2)
C(21)-P-C(11)	111.4(2)	C(41)-P-C(11)	106.5(2)
C(2)-C(1)-In	113.1(3)	C(2)-C(1)-H(1)	108.4(3)
In-C(1)-H(1)	108.65(14)	C(2)-C(1)-H(2)	109.5(3)
In-C(1)-H(2)	109.23(14)	H(1)-C(1)-H(2)	107.8
C(2)#1-C(2)-C(1)	113.0(5)	C(2)#1-C(2)-H(3)	108.1(4)
C(1)-C(2)-H(3)	108.9(3)	C(2)#1-C(2)-H(4)	108.9(4)
C(1)-C(2)-H(4)	109.8(3)	H(3)-C(2)-H(4)	107.9
C(12)-C(11)-C(16)	120.9(5)	C(12)-C(11)-P	117.1(4)
C(16)-C(11)-P	122.1(4)	C(11)-C(12)-C(13)	120.1(6)
C(11)-C(12)-H(12)	119.4(3)	C(13)-C(12)-H(12)	120.5(4)
C(13)-C(13)-C(12)	119.9(7)	C(13)-C(13)-H(13)	120.0(4)
C(12)-C(13)-H(13)	120.2(4)	C(13)-C(13)-C(13)	120.0(6)
C(13)-C(13)-H(13)	120.4(4)	C(13)-C(13)-H(13)	119.6(4)
C(13)-C(13)-C(16)	121.1(6)	C(13)-C(13)-H(13)	119.7(4)
C(16)-C(13)-H(13)	119.2(4)	C(11)-C(16)-C(13)	118.1(6)
C(11)-C(16)-H(16)	120.8(3)	C(13)-C(16)-H(16)	121.1(4)
C(22)-C(21)-C(26)	120.1(5)	C(22)-C(21)-P	118.1(4)
C(26)-C(21)-P	121.7(4)	C(23)-C(22)-C(21)	120.0(5)
C(23)-C(22)-H(22)	120.2(4)	C(21)-C(22)-H(22)	119.8(3)
C(22)-C(23)-C(24)	120.2(6)	C(22)-C(23)-H(23)	119.4(4)
C(24)-C(23)-H(23)	120.3(4)	C(23)-C(24)-C(25)	120.0(6)
C(23)-C(24)-H(24)	120.2(4)	C(25)-C(24)-H(24)	119.7(4)
C(26)-C(25)-C(24)	120.3(5)	C(26)-C(25)-H(25)	120.0(3)
C(24)-C(25)-H(25)	119.7(4)	C(25)-C(26)-C(21)	119.3(5)
C(25)-C(26)-H(26)	120.1(3)	C(21)-C(26)-H(26)	120.6(3)

C(32)-C(31)-C(36)	119.7(5)	C(32)-C(31)-P	121.5(4)
C(36)-C(31)-P	118.8(4)	C(33)-C(32)-C(31)	120.2(5)
C(33)-C(32)-H(32)	120.3(3)	C(31)-C(32)-H(32)	119.4(3)
C(34)-C(33)-C(32)	119.8(5)	C(34)-C(33)-H(33)	120.2(3)
C(32)-C(33)-H(33)	119.9(3)	C(35)-C(34)-C(33)	120.6(5)
C(35)-C(34)-H(34)	120.0(3)	C(33)-C(34)-H(34)	119.4(3)
C(34)-C(35)-C(36)	120.3(5)	C(34)-C(35)-H(35)	119.3(3)
C(36)-C(35)-H(35)	120.4(3)	C(35)-C(36)-C(31)	119.3(5)
C(35)-C(36)-H(36)	120.8(3)	C(31)-C(36)-H(36)	119.9(3)
C(46)-C(41)-C(42)	120.7(5)	C(46)-C(41)-P	121.4(4)
C(42)-C(41)-P	117.9(4)	C(41)-C(42)-C(43)	119.6(5)
C(41)-C(42)-H(42)	120.0(3)	C(43)-C(42)-H(42)	120.4(4)
C(44)-C(43)-C(42)	119.5(5)	C(44)-C(43)-H(43)	120.1(3)
C(42)-C(43)-H(43)	120.3(4)	C(45)-C(44)-C(43)	120.7(5)
C(45)-C(44)-H(44)	119.8(3)	C(43)-C(44)-H(44)	119.4(3)
C(44)-C(45)-C(46)	120.9(5)	C(44)-C(45)-H(45)	119.7(3)
C(46)-C(45)-H(45)	119.4(3)	C(41)-C(46)-C(45)	118.6(5)
C(41)-C(46)-H(46)	120.5(3)	C(45)-C(46)-H(46)	121.0(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z

Table 4. Anisotropic displacement parameters [$Å^2$] for MART11.

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	0.0415(2)	0.0269(2)	0.0308(2)	0.0018(2)	0.00289(14)	0.0019(2)
Br(1)	0.0450(3)	0.0269(3)	0.0695(4)	-0.0007(3)	0.0200(3)	-0.0001(2)
Br(2)	0.0606(4)	0.0411(3)	0.0564(4)	0.0108(3)	0.0253(3)	0.0025(3)
Br(3)	0.0830(5)	0.0827(5)	0.0335(3)	-0.0028(3)	-0.0037(3)	-0.0202(4)
P	0.0301(7)	0.0281(7)	0.0282(6)	0.0021(5)	0.0058(5)	0.0009(6)
C(1)	0.044(3)	0.021(2)	0.043(3)	0.001(2)	0.008(3)	0.000(2)
C(2)	0.039(3)	0.028(3)	0.041(3)	0.001(2)	0.006(3)	0.005(2)
C(11)	0.035(3)	0.035(3)	0.037(3)	0.010(2)	0.017(2)	0.009(2)
C(12)	0.053(4)	0.039(3)	0.057(4)	0.004(3)	0.020(3)	-0.005(3)
C(13)	0.055(4)	0.049(4)	0.081(5)	0.018(4)	0.030(4)	-0.004(3)
C(13)	0.054(4)	0.069(5)	0.071(5)	0.036(4)	0.030(4)	0.012(4)
C(13)	0.056(4)	0.091(6)	0.043(3)	0.027(4)	0.023(3)	0.031(4)
C(16)	0.039(3)	0.057(4)	0.033(3)	0.011(3)	0.008(3)	0.011(3)
C(21)	0.033(3)	0.033(3)	0.029(3)	0.006(2)	0.002(2)	-0.003(2)
C(22)	0.038(3)	0.049(3)	0.042(3)	-0.008(3)	0.003(2)	-0.002(3)
C(23)	0.058(4)	0.051(4)	0.051(4)	-0.015(3)	0.000(3)	-0.010(3)
C(24)	0.055(4)	0.056(4)	0.048(4)	0.002(3)	-0.008(3)	-0.018(3)
C(25)	0.033(3)	0.070(4)	0.046(3)	0.008(3)	0.000(3)	-0.012(3)
C(26)	0.036(3)	0.046(3)	0.034(3)	0.004(3)	0.006(2)	-0.002(3)
C(31)	0.029(3)	0.027(3)	0.030(3)	-0.003(2)	0.002(2)	0.000(2)
C(32)	0.038(3)	0.035(3)	0.037(3)	0.001(2)	0.006(2)	-0.002(2)
C(33)	0.034(3)	0.048(4)	0.055(4)	-0.002(3)	0.001(3)	0.001(3)
C(34)	0.046(4)	0.037(3)	0.057(4)	-0.003(3)	-0.003(3)	0.012(3)
C(35)	0.058(4)	0.031(3)	0.050(4)	0.012(3)	0.003(3)	0.006(3)
C(36)	0.043(3)	0.031(3)	0.049(3)	0.005(3)	0.012(3)	-0.001(3)
C(41)	0.032(3)	0.031(3)	0.030(3)	0.003(2)	0.011(2)	-0.001(2)
C(42)	0.044(3)	0.035(3)	0.042(3)	0.004(2)	0.014(3)	0.001(2)
C(43)	0.044(3)	0.031(3)	0.064(4)	0.004(3)	0.018(3)	0.004(3)
C(44)	0.054(4)	0.040(3)	0.053(4)	-0.014(3)	0.022(3)	-0.008(3)
C(45)	0.052(3)	0.053(4)	0.039(3)	-0.011(3)	0.013(3)	-0.008(3)
C(46)	0.040(3)	0.038(3)	0.032(3)	-0.002(2)	0.007(2)	0.002(3)

Table 5. Hydrogen coordinates and isotropic displacement parameters [$Å^2$] for MART11.

	x/a	y/b	z/c	U(eq)
H(1)	0.0842(4)	0.5425(6)	0.0738(2)	0.054
H(2)	0.0012(4)	0.3905(6)	0.0748(2)	0.054
H(3)	0.0149(4)	0.3178(7)	-0.0020(2)	0.054
H(4)	0.1077(4)	0.4538(7)	-0.0032(2)	0.054
H(12)	0.4075(5)	0.8183(7)	-0.1425(2)	0.073
H(13)	0.4851(5)	0.9977(9)	-0.1951(3)	0.090
H(13)	0.4471(5)	0.9418(10)	-0.2755(3)	0.094
H(13)	0.3344(5)	0.7075(10)	-0.3034(2)	0.093
H(16)	0.2585(4)	0.5233(8)	-0.2511(2)	0.064
H(22)	0.2687(4)	0.2239(8)	-0.2099(2)	0.065
H(23)	0.1323(5)	0.0352(8)	-0.2450(2)	0.082
H(24)	-0.0459(5)	0.0656(9)	-0.2286(2)	0.082
H(25)	-0.0888(5)	0.2967(9)	-0.1807(2)	0.075
H(26)	0.0466(4)	0.4933(8)	-0.1469(2)	0.058
H(32)	0.5105(4)	0.5034(7)	-0.1444(2)	0.055
H(33)	0.6466(5)	0.3145(8)	-0.1079(2)	0.069
H(34)	0.6010(5)	0.0756(8)	-0.0638(2)	0.072
H(35)	0.4217(5)	0.0255(7)	-0.0548(2)	0.070
H(36)	0.2829(5)	0.2120(7)	-0.0920(2)	0.061
H(42)	0.1424(4)	0.8153(7)	-0.1576(2)	0.060
H(43)	0.0832(5)	1.0175(7)	-0.1044(2)	0.068
H(44)	0.1413(5)	0.9848(8)	-0.0242(2)	0.072
H(45)	0.2534(5)	0.7516(8)	0.0042(2)	0.071
H(46)	0.3153(4)	0.5492(7)	-0.0479(2)	0.055

Table 1. Crystal data and structure refinement for MART9. COMPOUND 8

Identification code	MART9
Empirical formula	$C_{54}H_{52}Br_6In_2P_2$
Formula weight	1472.00
Temperature	199(2) K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 7.689(1) Å α = 90° b = 14.585(1) Å β = 96.59(1)° c = 25.014(3) Å γ = 90°
Volume	2786.6(5) $Å^3$
Z	2
Density (calculated)	1.754 Mg/m^3
Absorption coefficient	5.220 mm^{-1}
F(000)	1428
Crystal size	0.55 x 0.20 x 0.15 mm
θ range for data collection	3.01 to 26.92°
Index ranges	$-9 \le h \le 9$, $-18 \le k \le 0$, $0 \le \ell \le 31$
Reflections collected	5400
Independent reflections	5289 (R_{int} = 0.0385)
Absorption correction	Psi-scans
Max. and min. transmission	0.9983 and 0.6675
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5283 / 0 / 289
Goodness-of-fit on F^2	1.054
Final R indices [I>2σ(I)]	R1 = 0.0315, wR2 = 0.0588
R indices (all data)	R1 = 0.0530, wR2 = 0.0704
Largest diff. peak and hole	0.494 and −0.576 $eÅ^{-3}$

Table 2. Atomic coordinates und equivalent isotropic displacement parameters [$Å^2$] for MART9. U(eq) is defined as one third of the trace of the orthogonalized U_{ij}-tensor.

	x/a	y/b	z/c	U(eq)
In	0.35364(3)	0.18636(2)	0.369461(10)	0.02651(7)
Br(1)	0.35969(6)	0.33601(3)	0.31662(2)	0.03712(11)
Br(2)	0.09664(5)	0.21805(3)	0.42344(2)	0.03709(11)
Br(3)	0.23371(6)	0.06969(3)	0.29936(2)	0.04417(12)
P	0.58746(13)	0.70621(7)	0.36837(4)	0.0241(2)
C(1)	0.6007(5)	0.1454(3)	0.4118(2)	0.0362(10)
C(2)	0.5972(5)	0.1089(3)	0.4685(2)	0.0370(10)
C(3)	0.4908(5)	0.0221(3)	0.4719(2)	0.0342(9)
C(11)	0.7154(5)	0.8085(3)	0.37992(14)	0.0272(8)
C(12)	0.7840(5)	0.8325(3)	0.4321(2)	0.0307(9)
C(13)	0.8969(5)	0.9063(3)	0.4397(2)	0.0388(10)
C(14)	0.9418(6)	0.9552(3)	0.3960(2)	0.0424(11)
C(15)	0.8742(6)	0.9308(3)	0.3445(2)	0.0420(11)
C(16)	0.7594(5)	0.8579(3)	0.3360(2)	0.0353(10)
C(21)	0.4280(5)	0.7224(3)	0.31095(14)	0.0248(8)
C(22)	0.3295(5)	0.8028(3)	0.3065(2)	0.0346(9)
C(23)	0.1972(6)	0.8132(3)	0.2648(2)	0.0408(10)
C(24)	0.1637(6)	0.7442(3)	0.2273(2)	0.0399(10)
C(25)	0.2629(5)	0.6655(3)	0.2307(2)	0.0348(10)
C(26)	0.3958(5)	0.6533(3)	0.2727(2)	0.0305(9)
C(31)	0.7312(5)	0.6129(3)	0.35845(14)	0.0270(8)
C(32)	0.6712(6)	0.5229(3)	0.3606(2)	0.0338(9)
C(33)	0.7824(6)	0.4508(3)	0.3536(2)	0.0365(10)
C(34)	0.9538(6)	0.4669(3)	0.3453(2)	0.0404(10)
C(35)	1.0137(6)	0.5552(3)	0.3423(2)	0.0450(11)
C(36)	0.9030(5)	0.6287(3)	0.3484(2)	0.0385(10)
C(41)	0.4774(5)	0.6799(3)	0.42621(14)	0.0273(8)
C(42)	0.3021(5)	0.7017(3)	0.4268(2)	0.0377(10)
C(43)	0.2183(6)	0.6813(4)	0.4717(2)	0.0511(12)
C(44)	0.3090(8)	0.6413(4)	0.5156(2)	0.0580(14)
C(45)	0.4842(8)	0.6199(3)	0.5159(2)	0.0539(14)
C(46)	0.5713(6)	0.6385(3)	0.4711(2)	0.0403(10)

Table 3. Bond lengths [Å] and angles [°] for MART9.

In-C(1)	2.151(4)	In-Br(3)	2.5396(5)
In-Br(1)	2.5548(5)	In-Br(2)	2.5600(6)
P-C(31)	1.788(4)	P-C(11)	1.793(4)
P-C(21)	1.794(4)	P-C(41)	1.799(4)
C(1)-C(2)	1.519(5)	C(1)-H(11)	0.96
C(1)-H(12)	0.96	C(2)-C(3)	1.515(6)
C(2)-H(21)	0.96	C(2)-H(22)	0.96
C(3)-C(3)#1	1.537(7)	C(3)-H(31)	0.96
C(3)-H(32)	0.96	C(11)-C(16)	1.388(5)
C(11)-C(12)	1.394(5)	C(12)-C(13)	1.381(5)
C(12)-H(120)	0.96	C(13)-C(14)	1.381(6)
C(13)-H(130)	0.96	C(14)-C(15)	1.379(6)
C(14)-H(140)	0.96	C(15)-C(16)	1.382(6)
C(15)-H(150)	0.96	C(16)-H(160)	0.96
C(21)-C(26)	1.393(5)	C(21)-C(22)	1.394(5)
C(22)-C(23)	1.379(5)	C(22)-H(220)	0.96
C(23)-C(24)	1.379(6)	C(23)-H(230)	0.96
C(24)-C(25)	1.376(6)	C(24)-H(240)	0.96
C(25)-C(26)	1.389(5)	C(25)-H(250)	0.96
C(26)-H(260)	0.96	C(31)-C(36)	1.393(5)
C(31)-C(32)	1.394(5)	C(32)-C(33)	1.379(5)
C(32)-H(320)	0.96	C(33)-C(34)	1.378(6)
C(33)-H(330)	0.96	C(34)-C(35)	1.371(6)
C(34)-H(340)	0.96	C(35)-C(36)	1.388(6)
C(35)-H(350)	0.96	C(36)-H(360)	0.96
C(41)-C(42)	1.387(6)	C(41)-C(46)	1.400(5)
C(42)-C(43)	1.389(6)	C(42)-H(420)	0.96
C(43)-C(44)	1.363(7)	C(43)-H(430)	0.96
C(44)-C(45)	1.381(7)	C(44)-H(440)	0.96
C(45)-C(46)	1.398(6)	C(45)-H(450)	0.96
C(46)-H(460)	0.96		

C(1)-In-Br(3)	112.59(12)	C(1)-In-Br(1)	115.11(12)
Br(3)-In-Br(1)	104.00(2)	C(1)-In-Br(2)	118.83(11)
Br(3)-In-Br(2)	104.13(2)	Br(1)-In-Br(2)	100.35(2)
C(31)-P-C(11)	108.6(2)	C(31)-P-C(21)	111.4(2)
C(11)-P-C(21)	109.4(2)	C(31)-P-C(41)	107.7(2)
C(11)-P-C(41)	110.4(2)	C(21)-P-C(41)	109.3(2)
C(2)-C(1)-In	116.6(3)	C(2)-C(1)-H(11)	108.2(2)
In-C(1)-H(11)	108.09(12)	C(2)-C(1)-H(12)	107.9(2)
In-C(1)-H(12)	108.30(12)	H(11)-C(1)-H(12)	107.4
C(3)-C(2)-C(1)	114.4(3)	C(3)-C(2)-H(21)	108.4(2)
C(1)-C(2)-H(21)	108.3(2)	C(3)-C(2)-H(22)	108.4(2)
C(1)-C(2)-H(22)	109.4(2)	H(21)-C(2)-H(22)	107.7
C(2)-C(3)-C(3)#1	114.0(4)	C(2)-C(3)-H(31)	108.6(2)
C(3)#1-C(3)-H(31)	108.8(3)	C(2)-C(3)-H(32)	108.8(2)
C(3)#1-C(3)-H(32)	108.6(3)	H(31)-C(3)-H(32)	107.8
C(16)-C(11)-C(12)	120.7(4)	C(16)-C(11)-P	118.9(3)
C(12)-C(11)-P	120.1(3)	C(13)-C(12)-C(11)	119.2(4)
C(13)-C(12)-H(120)	120.4(2)	C(11)-C(12)-H(120)	120.3(2)
C(14)-C(13)-C(12)	120.2(4)	C(14)-C(13)-H(130)	119.7(2)
C(12)-C(13)-H(130)	120.1(2)	C(15)-C(14)-C(13)	120.2(4)
C(15)-C(14)-H(140)	120.1(3)	C(13)-C(14)-H(140)	119.7(2)
C(14)-C(15)-C(16)	120.6(4)	C(14)-C(15)-H(150)	119.4(3)
C(16)-C(15)-H(150)	120.0(3)	C(15)-C(16)-C(11)	119.0(4)
C(15)-C(16)-H(160)	120.8(3)	C(11)-C(16)-H(160)	120.2(2)
C(26)-C(21)-C(22)	120.1(3)	C(26)-C(21)-P	120.4(3)
C(22)-C(21)-P	119.3(3)	C(23)-C(22)-C(21)	120.0(4)
C(23)-C(22)-H(220)	120.4(3)	C(21)-C(22)-H(220)	119.6(2)
C(24)-C(23)-C(22)	119.8(4)	C(24)-C(23)-H(230)	120.1(3)

C(22)-C(23)-H(230)	120.1(3)	C(23)-C(24)-C(25)	120.6(4)
C(25)-C(24)-H(240)	119.7(2)	C(23)-C(24)-H(240)	119.8(3)
C(24)-C(25)-C(26)	120.5(4)	C(24)-C(25)-H(250)	119.6(2)
C(26)-C(25)-H(250)	119.9(2)	C(25)-C(26)-C(21)	118.9(4)
C(25)-C(26)-H(260)	120.9(2)	C(21)-C(26)-H(260)	120.1(2)
C(36)-C(31)-C(32)	119.2(4)	C(36)-C(31)-P	120.9(3)
C(32)-C(31)-P	119.9(3)	C(33)-C(32)-C(31)	120.0(4)
C(33)-C(32)-H(320)	120.3(2)	C(31)-C(32)-H(320)	119.7(2)
C(34)-C(33)-C(32)	120.4(4)	C(34)-C(33)-H(330)	119.8(3)
C(32)-C(33)-H(330)	119.7(2)	C(35)-C(34)-C(33)	120.1(4)
C(35)-C(34)-H(340)	120.3(3)	C(33)-C(34)-H(340)	119.6(3)
C(34)-C(35)-C(36)	120.3(4)	C(34)-C(35)-H(350)	119.7(3)
C(36)-C(35)-H(350)	120.0(3)	C(35)-C(36)-C(31)	119.9(4)
C(35)-C(36)-H(360)	120.4(3)	C(31)-C(36)-H(360)	119.7(2)
C(42)-C(41)-C(46)	120.2(4)	C(42)-C(41)-P	120.5(3)
C(46)-C(41)-P	119.3(3)	C(41)-C(42)-C(43)	120.1(4)
C(41)-C(42)-H(420)	119.6(2)	C(43)-C(42)-H(420)	120.3(3)
C(44)-C(43)-C(42)	120.1(5)	C(44)-C(43)-H(430)	119.8(3)
C(42)-C(43)-H(430)	120.1(3)	C(43)-C(44)-C(45)	120.7(4)
C(43)-C(44)-H(440)	119.8(3)	C(45)-C(44)-H(440)	119.5(3)
C(44)-C(45)-C(46)	120.5(5)	C(44)-C(45)-H(450)	120.0(3)
C(46)-C(45)-H(450)	119.5(3)	C(45)-C(46)-C(41)	118.5(5)
C(45)-C(46)-H(460)	121.6(3)	C(41)-C(46)-H(460)	119.9(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters [$Å^2$] for MART9.

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	0.02208(13	0.0289(2)	0.02829(14)	0.00173(12)	0.00179(10)	-0.00020(12)
Br(1)	0.0385(2)	0.0321(2)	0.0417(2)	0.0073(2)	0.0090(2)	-0.0004(2)
Br(2)	0.0291(2)	0.0523(3)	0.0309(2)	0.0003(2)	0.0082(2)	0.0010(2)
Br(3)	0.0467(3)	0.0437(3)	0.0436(2)	-0.0131(2)	0.0120(2)	-0.0179(2)
P	0.0260(5)	0.0227(5)	0.0234(5)	-0.0010(4)	0.0027(4)	-0.0045(4)
C(1)	0.020(2)	0.046(3)	0.041(2)	0.004(2)	-0.001(2)	0.007(2)
C(2)	0.028(2)	0.040(3)	0.040(2)	0.005(2)	-0.009(2)	0.003(2)
C(3)	0.032(2)	0.034(2)	0.034(2)	0.001(2)	-0.006(2)	0.005(2)
C(11)	0.026(2)	0.024(2)	0.031(2)	-0.001(2)	0.003(2)	-0.002(2)
C(12)	0.028(2)	0.031(2)	0.033(2)	-0.001(2)	0.005(2)	-0.006(2)
C(13)	0.032(2)	0.037(2)	0.045(3)	-0.013(2)	-0.003(2)	-0.008(2)
C(14)	0.034(2)	0.030(2)	0.063(3)	-0.006(2)	0.003(2)	-0.013(2)
C(15)	0.038(2)	0.033(2)	0.056(3)	0.009(2)	0.010(2)	-0.006(2)
C(16)	0.040(2)	0.033(2)	0.032(2)	0.003(2)	0.003(2)	-0.009(2)
C(21)	0.027(2)	0.026(2)	0.022(2)	0.001(2)	0.0045(14)	-0.005(2)
C(22)	0.039(2)	0.034(2)	0.031(2)	-0.004(2)	0.002(2)	0.000(2)
C(23)	0.039(2)	0.041(3)	0.041(2)	0.005(2)	0.001(2)	0.007(2)
C(24)	0.038(2)	0.045(3)	0.035(2)	0.007(2)	-0.007(2)	-0.006(2)
C(25)	0.037(2)	0.039(3)	0.027(2)	-0.004(2)	-0.003(2)	-0.012(2)
C(26)	0.034(2)	0.029(2)	0.028(2)	-0.003(2)	0.004(2)	-0.008(2)
C(31)	0.030(2)	0.029(2)	0.022(2)	0.000(2)	0.000(2)	0.000(2)
C(32)	0.037(2)	0.029(2)	0.036(2)	-0.003(2)	0.005(2)	-0.005(2)
C(33)	0.043(3)	0.028(2)	0.039(2)	-0.003(2)	0.006(2)	0.002(2)
C(34)	0.035(2)	0.042(3)	0.043(3)	-0.007(2)	0.000(2)	0.009(2)
C(35)	0.029(2)	0.051(3)	0.056(3)	-0.013(2)	0.008(2)	0.004(2)
C(36)	0.033(2)	0.035(2)	0.047(3)	-0.005(2)	0.004(2)	-0.007(2)
C(41)	0.035(2)	0.022(2)	0.025(2)	-0.003(2)	0.006(2)	-0.008(2)
C(42)	0.034(2)	0.045(3)	0.036(2)	-0.004(2)	0.009(2)	-0.007(2)
C(43)	0.046(3)	0.063(3)	0.048(3)	-0.007(3)	0.023(2)	-0.017(3)
C(44)	0.078(4)	0.054(3)	0.048(3)	-0.001(2)	0.034(3)	-0.018(3)
C(45)	0.091(4)	0.039(3)	0.033(2)	0.008(2)	0.013(3)	-0.006(3)
C(46)	0.057(3)	0.030(2)	0.034(2)	0.005(2)	0.007(2)	-0.003(2)

Table 5. Hydrogen coordinates and isotropic displacement parameters [$Å^2$] for MART9.

	x/a	y/b	z/c	U(eq)
H(11)	0.6780(5)	0.1973(3)	0.4135(2)	0.054
H(12)	0.6504(5)	0.0988(3)	0.3911(2)	0.054
H(21)	0.5491(5)	0.1554(3)	0.4896(2)	0.055
H(22)	0.7147(5)	0.0970(3)	0.4844(2)	0.055
H(31)	0.5266(5)	-0.0216(3)	0.4466(2)	0.051
H(32)	0.3695(5)	0.0360(3)	0.4616(2)	0.051
H(120)	0.7534(5)	0.7981(3)	0.4623(2)	0.046
H(130)	0.9452(5)	0.9235(3)	0.4753(2)	0.058
H(140)	1.0196(6)	1.0066(3)	0.4016(2)	0.064
H(150)	0.9077(6)	0.9648(3)	0.3145(2)	0.063
H(160)	0.7105(5)	0.8414(3)	0.3002(2)	0.053
H(220)	0.3553(5)	0.8510(3)	0.3324(2)	0.052
H(230)	0.1276(6)	0.8681(3)	0.2621(2)	0.061
H(240)	0.0704(6)	0.7511(3)	0.1987(2)	0.060
H(250)	0.2396(5)	0.6186(3)	0.2039(2)	0.052
H(260)	0.4656(5)	0.5986(3)	0.2752(2)	0.046
H(320)	0.5528(6)	0.5115(3)	0.3674(2)	0.051
H(330)	0.7396(6)	0.3890(3)	0.3542(2)	0.055
H(340)	1.0308(6)	0.4161(3)	0.3415(2)	0.061
H(350)	1.1333(6)	0.5659(3)	0.3366(2)	0.068
H(360)	0.9440(5)	0.6905(3)	0.3454(2)	0.058
H(420)	0.2393(5)	0.7312(3)	0.3961(2)	0.056
H(430)	0.0965(6)	0.6955(4)	0.4718(2)	0.077
H(440)	0.2507(8)	0.6274(4)	0.5465(2)	0.087
H(450)	0.5471(8)	0.5923(3)	0.5472(2)	0.081
H(460)	0.6927(6)	0.6235(3)	0.4705(2)	0.060