Electronic Supplementary Information (ESI)

Paddlewheel 1,2,4-Diazaphospholide Dibismuthanes with Very Short Bismuth–Bismuth Single Bonds

Minggang Zhao,[a] Lixia Wang,[a] Pangpang Li,[a] Xiang Zhang,[a] Ying Yang,[b] and Wenjun Zheng[a,c,*]

[a]*Institute of Organic Chemistry & College of Chemical and Materials Science, Shanxi Normal Univeristy, Gongyuan Street 1, Linfen, Shanxi Province 041004, China*

[b]*School of Chemistry and Chemical Engineering, Central South University, Lushannan Road 932, Changsha, Hunan Province 410083, China*

[c]*Key Laboratory of Magnetic Molecules and Magnetic Information Material, Ministry of Education, Gongyuan Street 1, Linfen, Shanxi Province 041004, China*

Email: wjzheng@sxnu.edu.cn, wjzheng_sxnu@qq.com

Table of the Content

General Information

All manipulations were carried out in a nitrogen atmosphere under anaerobic conditions using standard Schlenk, vacuum line and glove box techniques. The solvents were thoroughly dried, deoxygenated and distilled in a nitrogen atmosphere prior to use. THF-d_8 and C_6D_6 were dried with metallic potassium before use. The ^{1}H NMR, ^{13}C{^{1}H} NMR and ^{31}P{^{1}H} NMR spectra were recorded with a Bruker DRX-600 spectrometer. IR measurements were carried out on a NICOLET 360 FT-IR spectrometer from Nujol mulls prepared in a dry box. Elemental analysis was performed on an Elementar vario MACRO cube (Germany). Melting points were measured in sealed argon-filled capillaries without temperature correction with an apparatus XT4-100A (Electronic and Optical Instruments, Beijing). $BiCl_3$ were purchased from Aldrich and used as received. K[3,5-*t*Bu$_2$dp], K[3,5-*i*Pr$_2$dp], and K[3,5-Ph$_2$dp] were prepared according to the literature.[1,2]

1. Synthetic Procedures, Spectral Data, and Analytical Data for **2**, **4**, **5**, and **6**

Preparation of K[3,5-*i*Pr$_2$dp] (2): To a mixture of 1*H*-3,5-di-isopropyl-1,2,4-diazaphosphole (H[3,5-*i*Pr$_2$dp]) (0.655 g, 3.84 mmol)[1] and KH (0.201 g, 5.0 mmol) was added THF (20 mL) via syringe at room temperature. After the evolution of gas ceased the solution was filtered through Celite and the volatile components were removed in high vacuum (0.01 mmHg) to yield **2** as off-white pure solids (0.59 g, 73.7%). M.p. > 250°C, decomp.. ^{1}H NMR (600 MHz, DMSO-d_6, 23°C): δ = 3.04–2.99 (m, 2 H, C*H* for *i*Pr), 1.20–1.19 (d, $^1J_{H–H}$ = 7.2 Hz, 12 H, CH_3 for *i*Pr) ppm; ^{13}C{^{1}H} NMR (150 MHz, DMSO-d_6, 23°C): δ = 185.55, 185.23 (d, $^1J_{C–P}$ = 48.0 Hz, P*C*N), 32.20, 32.05 (d, $^2J_{C–P}$ = 22.5 Hz, *C*H), 26.55, 26.41 (d, $^3J_{C–P}$ = 21.0 Hz, *C*H$_3$) ppm; ^{31}P{^{1}H} NMR (243 MHz, DMSO-d_6, 23°C): δ = 46.27 (s) ppm. IR (KBr, Nujol mull, cm^{-1}): 2960(s), 2923(s), 2854(m), 1459(w), 1413(w), 1376(w), 1261(s), 1093(s), 1020(s), 863(w), 800(s), 665(w); Anal. calcd for $C_8H_{14}KN_2P$: C 46.13, H 6.78, N 13.45; Found: C 45.98, H 6.49, N 13.17.

Preparation of {η^1,η^1-3,5-*t*Bu$_2$dp}$_2$(Bi-Bi){η^1,η^1-3,5-*t*Bu$_2$dp}$_2$ (4): To a mixture of $BiCl_3$ (0.315 g, 1.0 mmol) and K[3,5-*t*Bu$_2$dp][1] (**1**, 0.709 g, 3.0 mmol) was added 30 mL tetrahydrofuran (THF) via syringe. After the mixture was stirred for 48 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (4 × 10 mL) and the orange-red solution was filtered through Celite. The filtrate was concentrated under the reduced pressure to about 25 mL to give **4** as orange-red crystals at room temperature. The mother liquid was further concentrated to afford another portion of **4** and a group of colorless free ligand H[3,5-*t*Bu$_2$dp] (0.095 g, 15.9%) at –20°C. The total yield of **4** is 0.307 g (50.8%). Mp: > 210°C, turn red, decomp.. ^{1}H NMR (600 MHz, THF-d_8, 23°C): δ = 1.38, 1.25 (2s, 72 H, –CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz, THF-d_8, 23°C): δ = 199.34 (d, $^1J_{C–P}$ = 60.0 Hz, P*C*N), 186.54 (d, $^1J_{C–P}$ = 55.5 Hz, P*C*N), 32.88, 32.77 (2s, *C*CH$_3$), 30.94–30.06 (2s, overlapped, *C*H$_3$); ^{31}P{^{1}H} NMR (243 MHz,THF-d_8, 23°C): 79.11(s); ^{1}H NMR (600 MHz, C_6D_6, 23°C): δ = 1.28 (s, 72 H, –CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 23°C): δ = 201.40 (d, $^1J_{C–P}$ = 58.5 Hz, P*C*N), 34.84 (d, $^2J_{C–P}$ = 72.0 Hz, *C*CH$_3$), 33.22 (d, $^3J_{C–P}$ = 36.0 Hz, *C*H$_3$); ^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 23°C): 80.20(s); IR (KBr, Nujol mull, cm^{-1}): 2923(s), 2854(s), 1619(w), 1461(m), 1376(w), 1261(s), 1093(s), 1020(s), 800(s), 680(w); Anal. calcd for $C_{40}H_{72}Bi_2P_4N_8$: C 39.81, H 6.01, N 9.28; Found: C 38.99, H 5.81, N 8.97.

Preparation of {η¹,η¹-3,5-*i*Pr₂dp}₂(Bi-Bi){η¹,η¹-3,5-*i*Pr₂dp}₂ (5α, 5β): To a mixture of $BiCl_3$ (0.297 g, 0.942 mmol) and **2** (0.59 g, 2.83 mmol) was added THF (20 mL) via syringe. After the mixture was stirred for 48 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (3 × 10 mL). The orange-red solution was filtered through Celite and the filtrate was concentrated to about 15 mL to give **5** as orange-red crystals at –15°C. The mother liquor was further concentrated to afford another portion of **5** and small amount of colorless crystals H[3,5-*i*Pr₂dp] at –30°C. The total yield of **5** was 0.238 g (46.1%). Mp: 218–220°C. ^{1}H NMR (600 MHz, C_6D_6, 23°C): δ = 2.98–2.95 (m, slightly overlapped, $^2J_{P-H}$ = 6.6 Hz, 8 H, C*H*), 1.311 (d, $^3J_{P-H}$ = 7.2 Hz, 48 H, CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 23°C): δ = 200.97 (br., overlapped, N*C*P), 34.63 (s, *C*H), 25.60 (d, $^3J_{P-C}$ = 6.0 Hz, *C*H$_3$) ppm; ^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 23°C): δ = 61.44(s) ppm; IR (KBr, Nujol mull, cm^{-1}): 2960(s), 2923(s), 2854(m), 1461(m), 1411(w), 1376(w), 1261(m), 1093(s), 1020(s), 863(w), 798(s), 686(w); Anal. calcd for $C_{32}H_{56}Bi_2P_4N_8$: C 35.11, H 5.16, N 10.24; Found: C 34.97, H 5.05, N 10.18.

Preparation of {η¹,η¹-3,5-Ph₂dp}₂(Bi-Bi){η¹,η¹-3,5-Ph₂dp}₂ (6): To a mixture of $BiCl_3$(0.315 g, 1.0 mmol) and K[3,5-Ph$_2$dp]·0.67THF[2] (**3**, 0.973 g, 3.0 mmol) was added THF (50 mL) via syringe. After the mixture was stirred for 48 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (5 × 10 mL) and the orange-red solution was filtered through Celite. The filtrate was concentrated to about 40 mL to give free ligand 1*H*-3,5-di-phenyl-1,2,4-diazaphosphole (H[3,5-Ph$_2$dp]) as white solid at room temperature. The mother liquor was further concentrated to afford **6** as orange-red crystals at room temperature (0.274 g, 40.2%). M.p. > 215°C, turn dark, decomp.. ^{1}H NMR (600 MHz,THF-d_8, 23°C): δ = 8.04 (d, 16 H, C*H*), 7.74–7.22 (t, 16 H, C*H*), 7.09–7.07 (t, 8 H, C*H*) ppm; ^{13}C{^{1}H} NMR (150 MHz, THF-d_8, 23°C): δ = 178.12 (d, $^1J_{C-P}$ = 43.5 Hz, P*C*N), 144.29 (d, $^1J_{C-C}$ = 22.5 Hz, *C*H for Ph ring), 127.39–124.72 (m, *C*H for Ph ring) ppm; ^{31}P{^{1}H} NMR (243 MHz, THF-d_8, 23°C): 67.24(s) ppm; IR (KBr, Nujol mull, cm^{-1}): 2960(s), 2923(vs), 2854(s), 1461(m), 1376(w) 1261(m), 1091(m), 1020(m), 865(vw), 798(m), 694(vw); Anal. calcd for $C_{56}H_{40}Bi_2P_4N_8$: C 49.21, H 2.95, N 8.20; Found: C 48.97, H 2.77, N 7.95.

2. ^{1}H, $^{31}P\{^{1}H\}$, $^{13}C\{^{1}H\}$ NMR data for **4**, **5**, and **6**

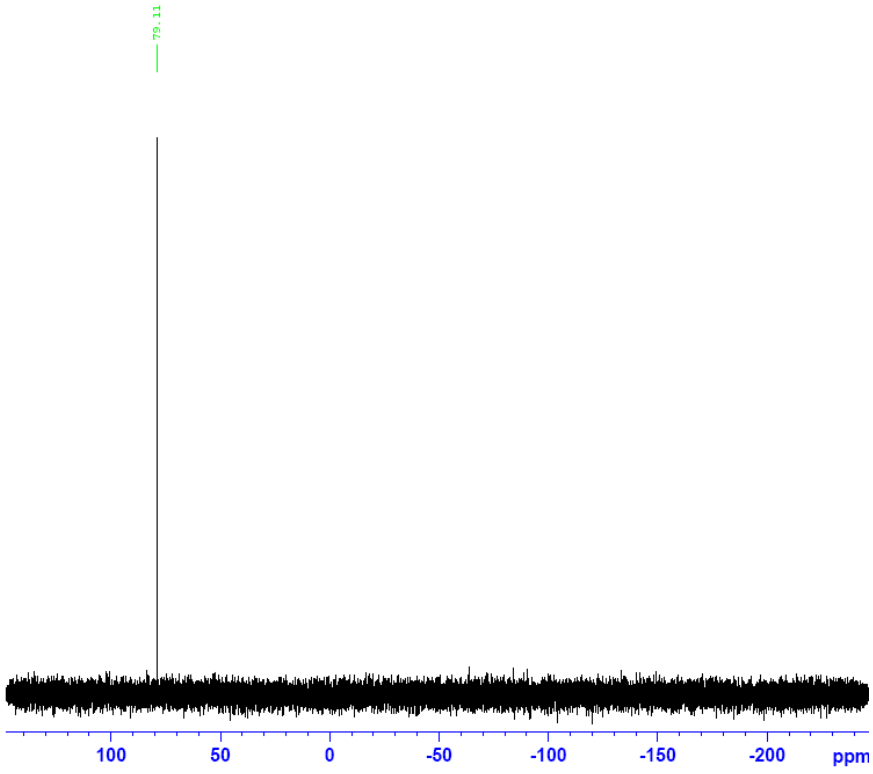

Figure 1. The ^{31}P NMR spectrum of compound **4** in THF-d_8

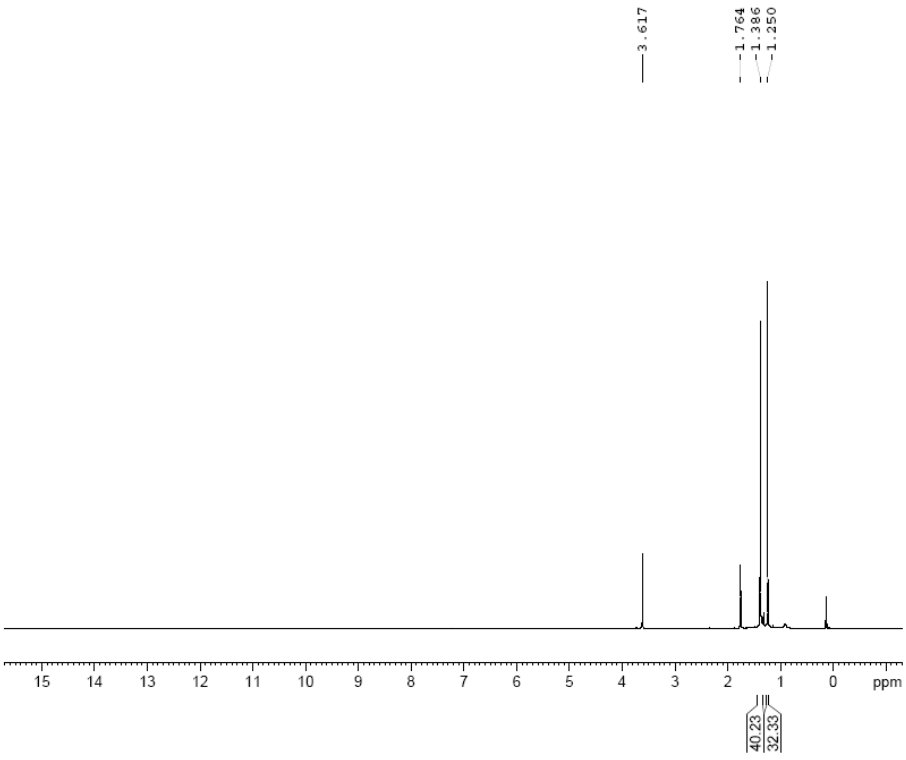

Figure 2. The ^{1}H NMR spectrum of compound **4** in THF-d_8

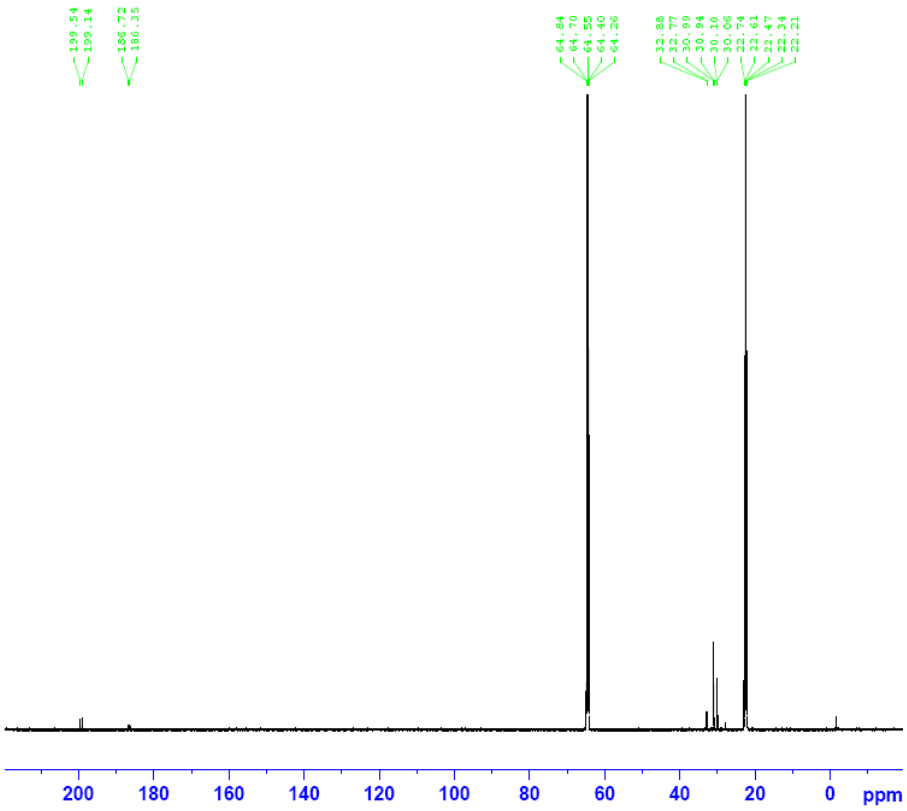

Figure 3. The ^{13}C NMR spectrum of compound **4** in THF-d_8

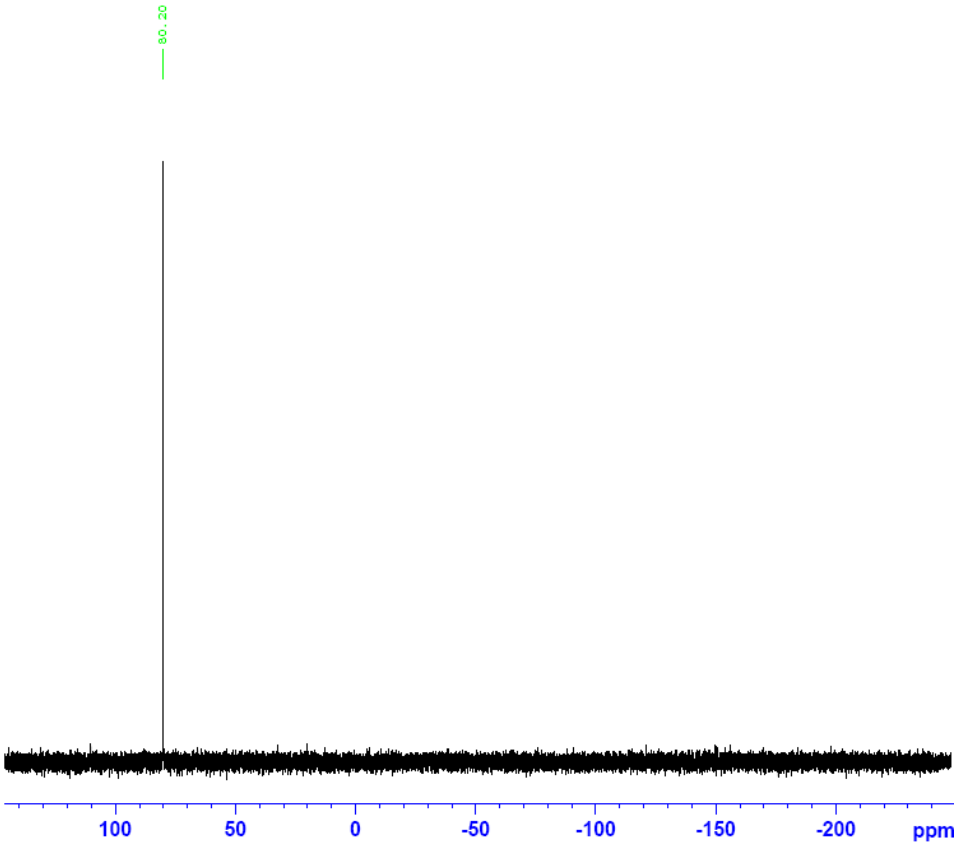

Figure 4. The ^{31}P NMR spectrum of compound **4** in C_6D_6

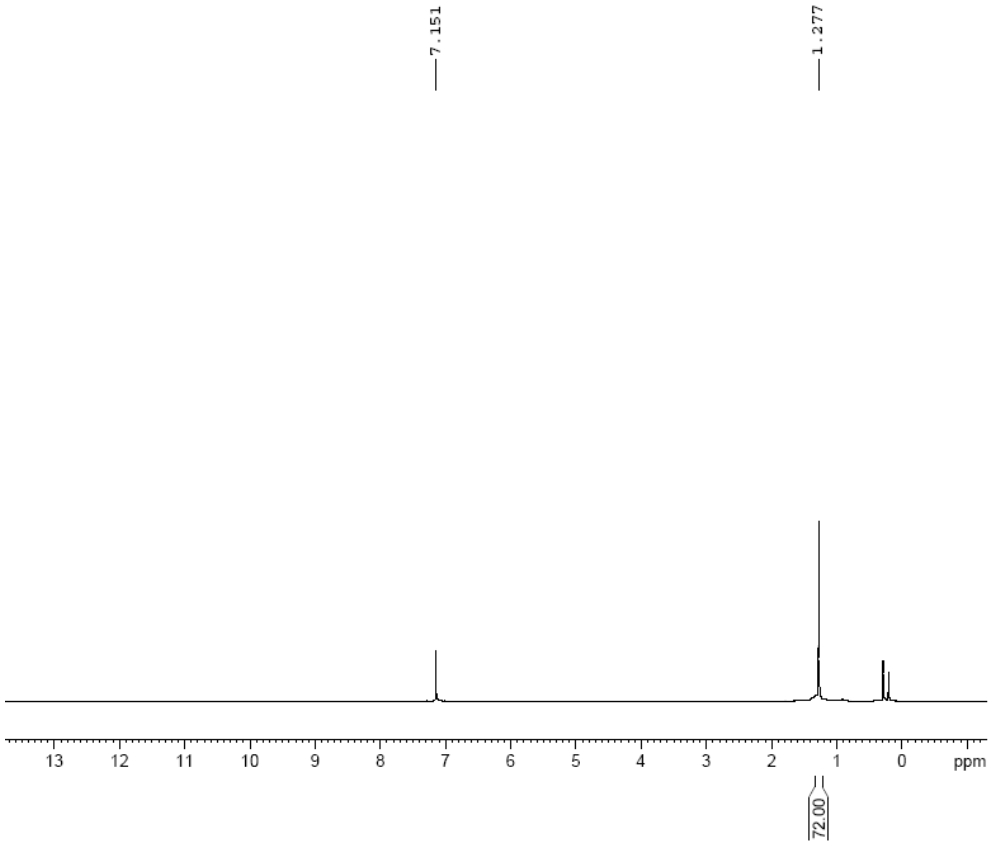

Figure 5. The ^{1}H NMR spectrum of compound **4** in C_6D_6

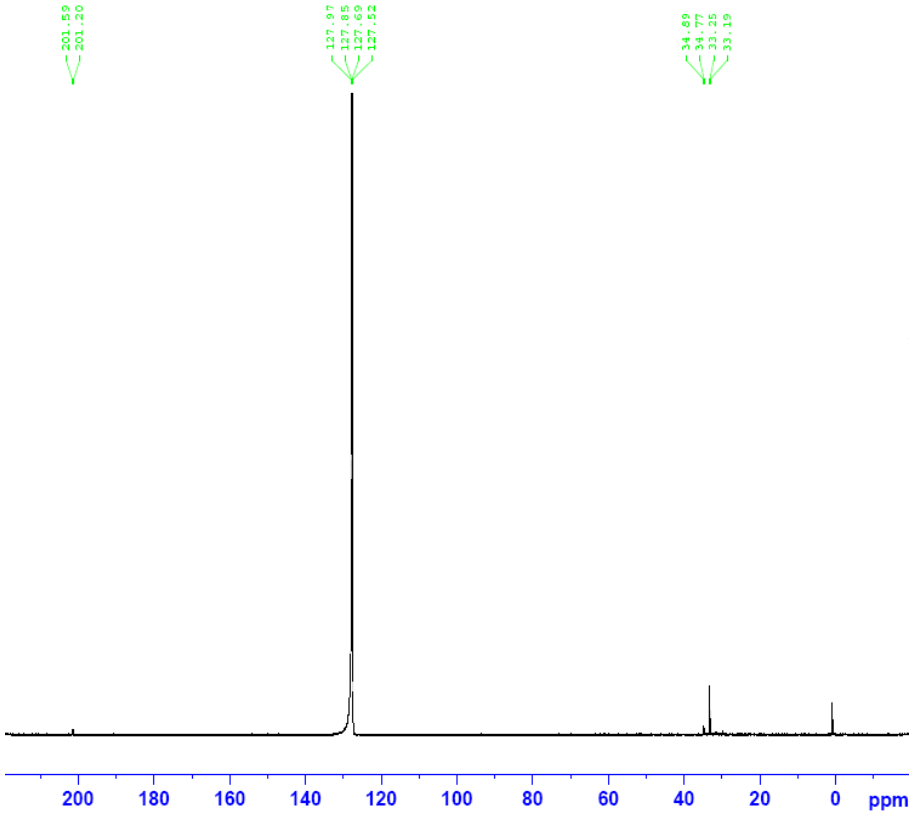

Figure 6. The ^{13}C NMR spectrum of compound **4** in C_6D_6

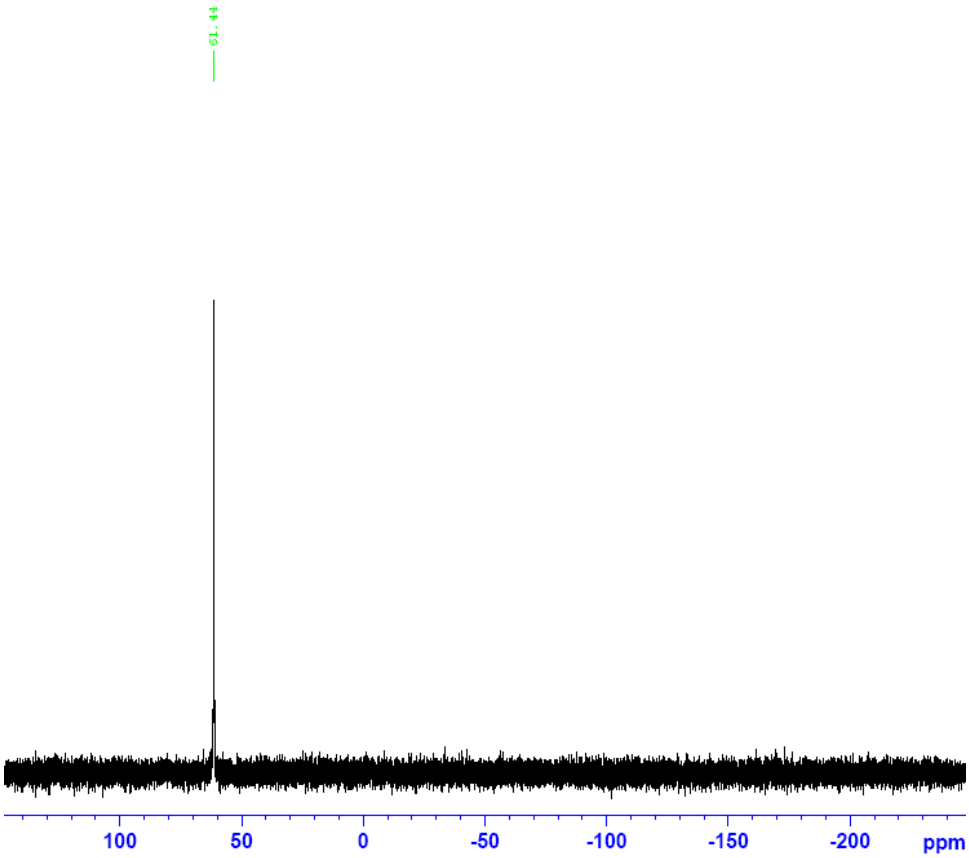

Figure 7. The ^{31}P NMR spectrum of compound **5** in C_6D_6

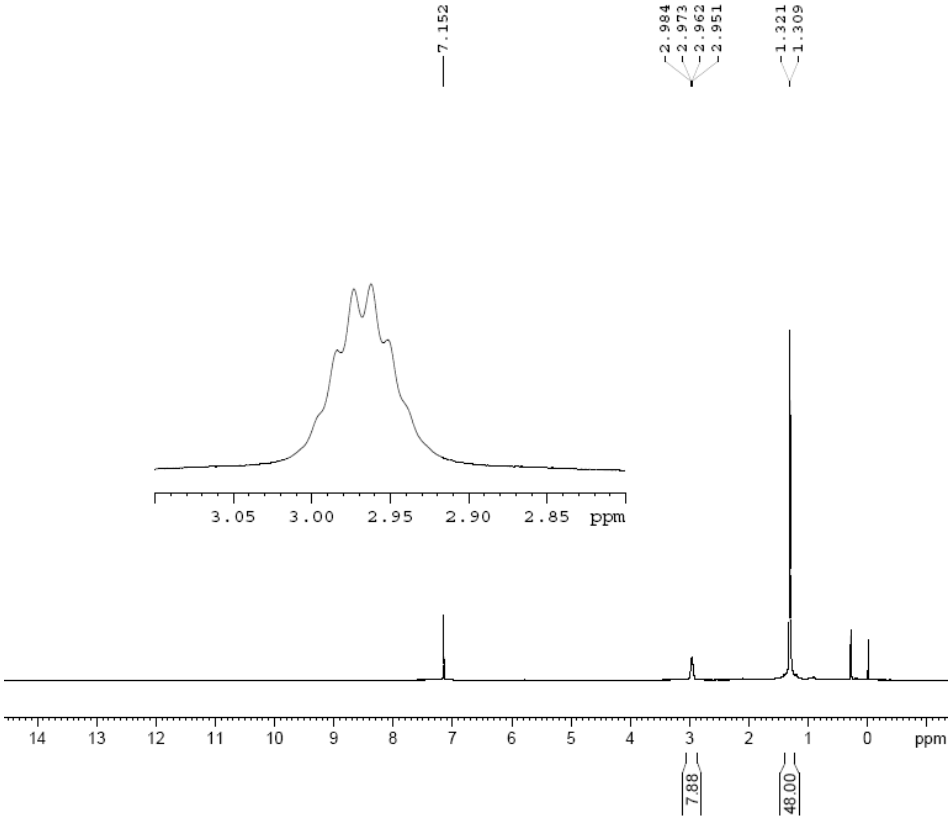

Figure 8. The ^{1}H NMR spectrum of compound **5** in C_6D_6

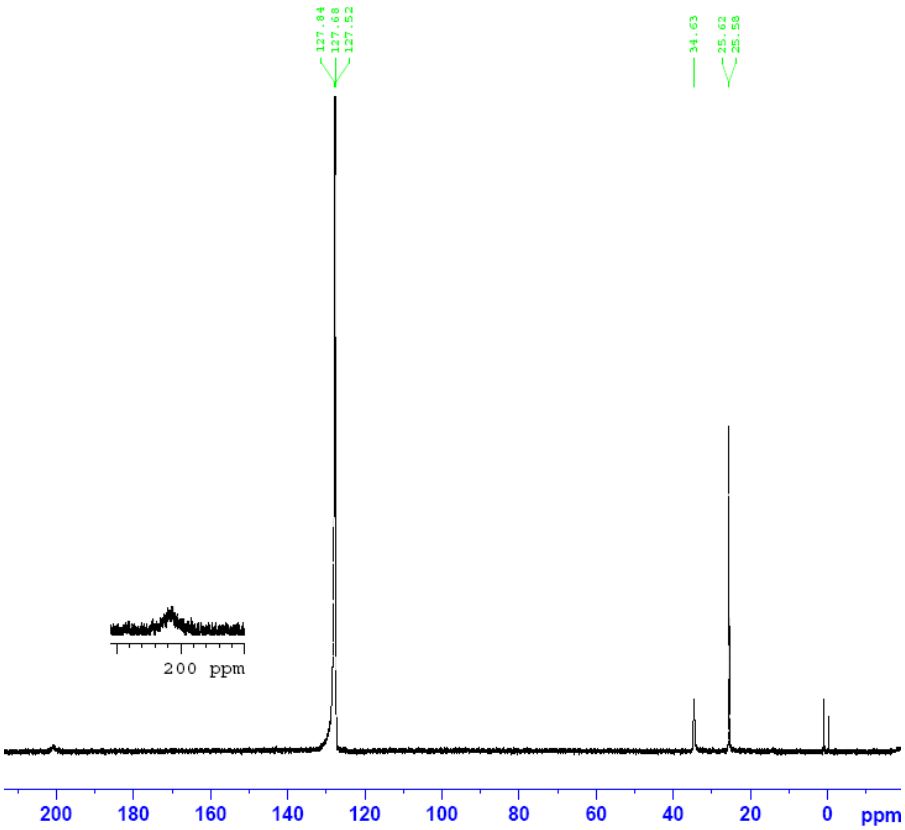

Figure 9. The ^{13}C NMR spectrum of compound **5** in C_6D_6

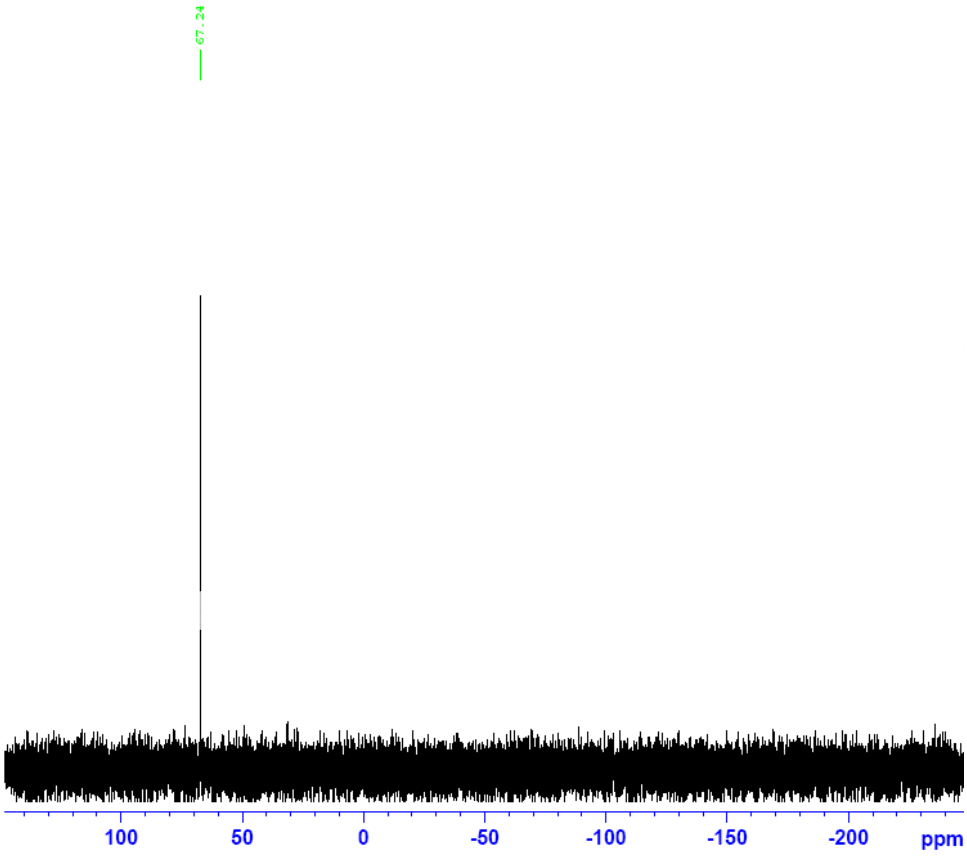

Figure 10. The ^{31}P NMR spectrum of compound **6** in THF-d_8

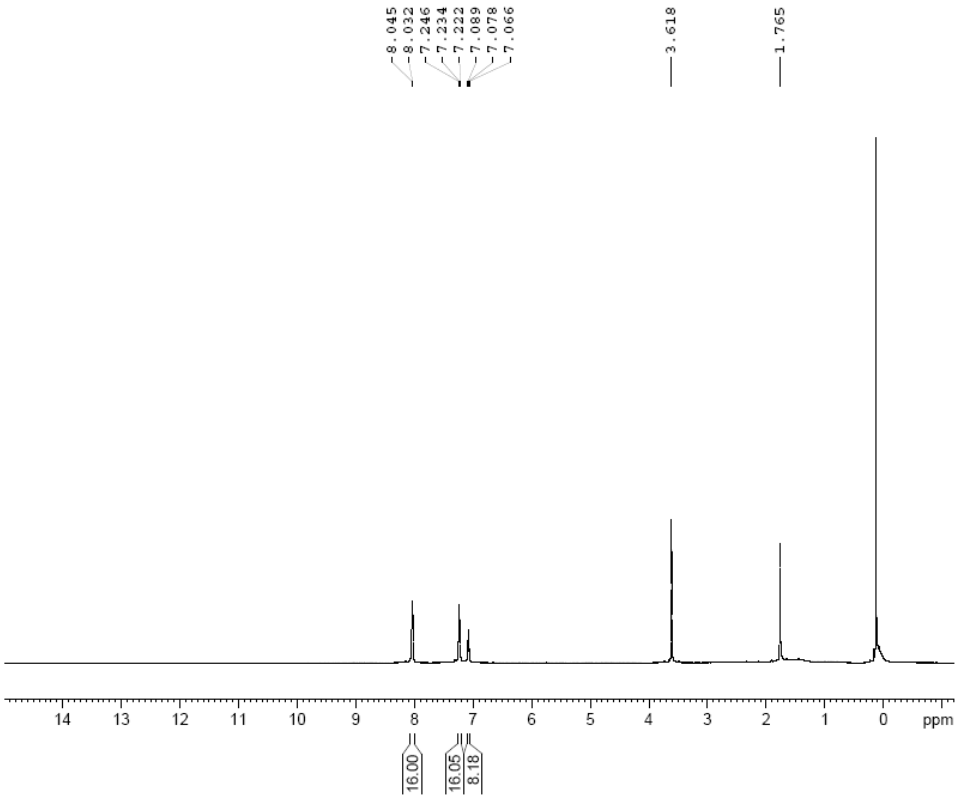

Figure 11. The ^{1}H NMR spectrum of compound **6** in THF-d_8

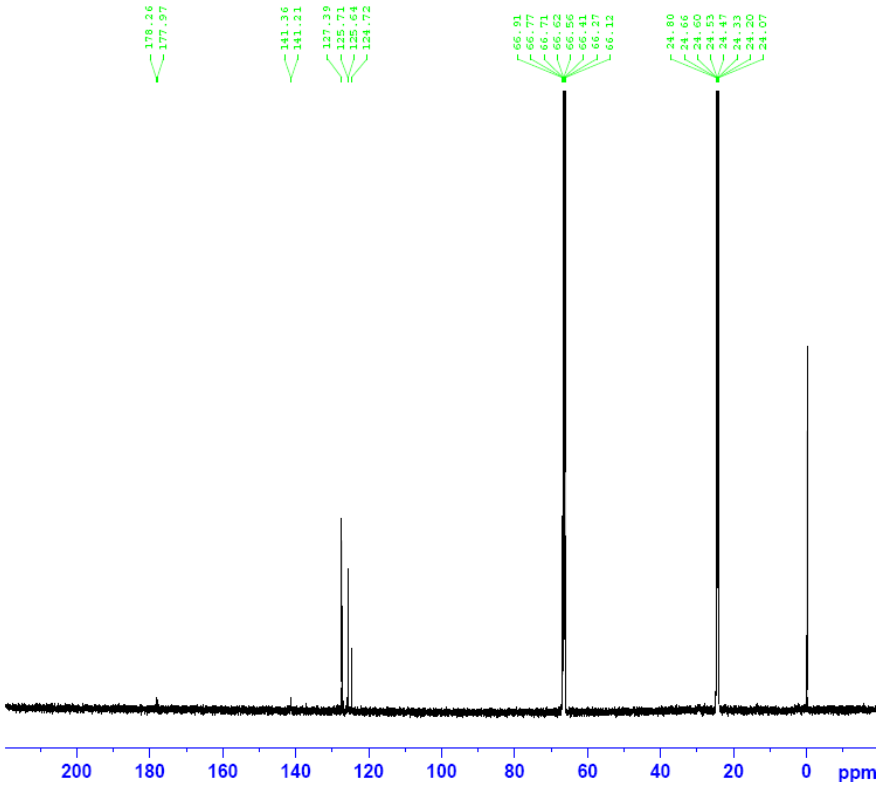

Figure 12. The ^{13}C NMR spectrum of compound **6** in THF-d_8

3. Crystal structural analysis data for **4**, **5**, and **6**

3.1 Crystal structural analysis data for **4**

Table 1. Crystal data and structure refinement for **4**.

Identification code	140731-1a
Empirical formula	$C_{40}H_{72}Bi_2N_8P_4$
Formula weight	1206.90
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, *P*21/*c*
Unit cell dimensions	*a* = 23.3993(14) Å α = 90 deg. *b* = 10.7452(5) Å β = 114.212(8) deg. *c* = 21.7187(17) Å γ = 90 deg.
Volume	4980.4(5) Å^3
Z, Calculated density	4, 1.610 Mg/m^3
Absorption coefficient	7.220 mm^{-1}
F(000)	2376
Crystal size	0.20 × 0.15 × 0.10 mm
Theta range for data collection	2.86 to 26.50 deg.
Limiting indices	$-29 \le h \le 26$, $-12 \le k \le 13$, $-26 \le l \le 27$
Reflections collected / unique	23479 / 10295 [*R*(int) = 0.0671]
Completeness to theta = 26.50	99.6 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	0.5321 and 0.3261
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10295 / 0 / 505
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R_1 = 0.0561, wR_2 = 0.0898
R indices (all data)	R_1 = 0.0956, wR_2 = 0.1042
Largest diff. peak and hole	1.585 and -2.066 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Bi(1)	2703(1)	1993(1)	2396(1)	30(1)
Bi(2)	2302(1)	-387(1)	2560(1)	30(1)
P(1)	4039(1)	749(2)	4792(1)	39(1)
P(2)	1005(1)	2516(2)	3249(1)	41(1)
P(3)	4017(1)	-1003(2)	1756(1)	47(1)
P(4)	936(1)	903(2)	177(1)	42(1)
N(1)	3425(3)	1193(6)	3512(3)	30(2)
N(2)	3067(3)	367(6)	3685(3)	32(2)
N(3)	1595(3)	1117(5)	2738(3)	26(2)
N(4)	1937(3)	2194(6)	2913(4)	36(2)
N(5)	3246(3)	458(5)	1971(3)	28(2)
N(6)	3236(3)	-599(6)	2304(4)	33(2)
N(7)	1751(3)	213(6)	1349(4)	30(2)
N(8)	1736(3)	1493(5)	1368(3)	25(2)
C(1)	3957(3)	1480(7)	4039(4)	27(2)
C(2)	3313(4)	54(7)	4334(4)	28(2)
C(3)	2958(4)	-810(8)	4598(5)	42(2)
C(4)	2883(6)	-2074(9)	4304(6)	101(5)
C(5)	3308(5)	-934(10)	5360(5)	70(3)

C(6)	2328(5)	-241(10)	4465(6)	93(5)
C(7)	4458(4)	2269(7)	3955(5)	35(2)
C(8)	4980(4)	2596(9)	4649(5)	65(2)
C(9)	4196(4)	3461(9)	3574(5)	65(2)
C(10)	4741(4)	1493(9)	3558(5)	60(3)
C(11)	1074(4)	1138(7)	2852(4)	31(2)
C(12)	1689(3)	3023(7)	3185(4)	26(2)
C(13)	2007(4)	4269(7)	3446(5)	37(2)
C(14)	1766(5)	4844(9)	3930(6)	76(4)
C(15)	1852(5)	5155(8)	2848(6)	69(4)
C(16)	2721(4)	4135(9)	3809(5)	66(3)
C(17)	596(4)	110(8)	2622(5)	35(2)
C(18)	135(5)	239(10)	2940(6)	83(4)
C(19)	245(5)	235(11)	1861(6)	93(4)
C(20)	878(5)	-1183(9)	2767(7)	98(5)
C(21)	3614(4)	403(7)	1638(4)	34(2)
C(22)	3620(3)	-1470(7)	2251(4)	28(2)
C(23)	3744(4)	-2683(8)	2639(5)	39(2)
C(24)	4083(6)	-2430(10)	3377(5)	92(4)
C(25)	3138(5)	-3360(10)	2508(7)	113(6)
C(26)	4144(5)	-3546(9)	2431(6)	69(3)
C(27)	3637(4)	1457(9)	1194(5)	46(3)
C(28)	4054(5)	1112(9)	839(5)	77(4)
C(29)	3914(5)	2633(10)	1620(5)	75(4)
C(30)	2983(5)	1727(10)	689(6)	77(4)
C(31)	1366(4)	-239(7)	769(5)	34(2)
C(32)	1331(4)	1998(7)	798(4)	28(2)
C(33)	1218(4)	3383(8)	750(5)	39(2)
C(34)	832(5)	3754(9)	26(5)	77(4)
C(35)	844(4)	3686(9)	1161(5)	61(3)
C(36)	1829(4)	4136(8)	1009(6)	67(3)
C(37)	1337(4)	-1634(7)	621(4)	32(2)
C(38)	888(5)	-1882(8)	-103(5)	67(3)
C(39)	1110(5)	-2313(8)	1090(5)	68(3)
C(40)	1989(4)	-2031(7)	714(5)	54(3)

Table 3. Bond lengths [A] and angles [deg] for **4**.

Bi(1)-N(1)	2.472(7)
Bi(1)-N(5)	2.480(6)
Bi(1)-N(4)	2.483(6)

Bi(1)-N(8)	2.500(6)
Bi(1)-Bi(2)	2.7964(4)
Bi(2)-N(3)	2.454(6)
Bi(2)-N(6)	2.475(5)
Bi(2)-N(7)	2.492(7)
Bi(2)-N(2)	2.499(7)
P(1)-C(2)	1.746(8)
P(1)-C(1)	1.753(8)
P(2)-C(12)	1.748(7)
P(2)-C(11)	1.753(8)
P(3)-C(21)	1.743(8)
P(3)-C(22)	1.756(7)
P(4)-C(32)	1.743(8)
P(4)-C(31)	1.765(8)
N(1)-C(1)	1.336(9)
N(1)-N(2)	1.374(8)
N(2)-C(2)	1.329(9)
N(3)-C(11)	1.341(8)
N(3)-N(4)	1.368(8)
N(4)-C(12)	1.328(9)
N(5)-C(21)	1.334(9)
N(5)-N(6)	1.352(8)
N(6)-C(22)	1.336(9)
N(7)-C(31)	1.305(10)
N(7)-N(8)	1.377(8)
N(8)-C(32)	1.328(9)
C(1)-C(7)	1.517(10)
C(2)-C(3)	1.507(10)
C(3)-C(4)	1.481(12)
C(3)-C(6)	1.509(11)
C(3)-C(5)	1.521(12)
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-C(9)	1.511(11)
C(7)-C(10)	1.530(11)
C(7)-C(8)	1.543(12)
C(8)-H(8A)	0.9600

C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(17)	1.504(10)
C(12)-C(13)	1.524(10)
C(13)-C(14)	1.513(11)
C(13)-C(15)	1.529(12)
C(13)-C(16)	1.534(11)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(18)	1.508(10)
C(17)-C(20)	1.515(12)
C(17)-C(19)	1.521(13)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-C(27)	1.503(11)
C(22)-C(23)	1.514(11)
C(23)-C(24)	1.494(13)
C(23)-C(25)	1.513(12)
C(23)-C(26)	1.513(11)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600

C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-C(30)	1.502(13)
C(27)-C(28)	1.514(11)
C(27)-C(29)	1.543(13)
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(37)	1.529(10)
C(32)-C(33)	1.507(10)
C(33)-C(34)	1.509(12)
C(33)-C(35)	1.519(11)
C(33)-C(36)	1.535(11)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-C(38)	1.514(12)
C(37)-C(40)	1.515(10)
C(37)-C(39)	1.515(11)
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600

N(1)-Bi(1)-N(5)	83.4(2)

N(1)-Bi(1)-N(4)	85.2(2)
N(5)-Bi(1)-N(4)	143.23(19)
N(1)-Bi(1)-N(8)	143.7(2)
N(5)-Bi(1)-N(8)	86.5(2)
N(4)-Bi(1)-N(8)	82.3(2)
N(1)-Bi(1)-Bi(2)	71.80(14)
N(5)-Bi(1)-Bi(2)	71.87(13)
N(4)-Bi(1)-Bi(2)	71.35(14)
N(8)-Bi(1)-Bi(2)	71.90(14)
N(3)-Bi(2)-N(6)	144.1(2)
N(3)-Bi(2)-N(7)	84.6(2)
N(6)-Bi(2)-N(7)	84.8(2)
N(3)-Bi(2)-N(2)	83.8(2)
N(6)-Bi(2)-N(2)	84.5(2)
N(7)-Bi(2)-N(2)	143.2(2)
N(3)-Bi(2)-Bi(1)	72.57(13)
N(6)-Bi(2)-Bi(1)	71.50(14)
N(7)-Bi(2)-Bi(1)	71.61(14)
N(2)-Bi(2)-Bi(1)	71.61(15)
C(2)-P(1)-C(1)	87.2(4)
C(12)-P(2)-C(11)	87.3(4)
C(21)-P(3)-C(22)	87.0(4)
C(32)-P(4)-C(31)	86.7(4)
C(1)-N(1)-N(2)	111.9(7)
C(1)-N(1)-Bi(1)	141.4(5)
N(2)-N(1)-Bi(1)	104.1(4)
C(2)-N(2)-N(1)	114.0(6)
C(2)-N(2)-Bi(2)	141.2(5)
N(1)-N(2)-Bi(2)	102.5(5)
C(11)-N(3)-N(4)	114.0(6)
C(11)-N(3)-Bi(2)	139.7(5)
N(4)-N(3)-Bi(2)	104.2(4)
C(12)-N(4)-N(3)	112.2(6)
C(12)-N(4)-Bi(1)	142.0(5)
N(3)-N(4)-Bi(1)	104.4(4)
C(21)-N(5)-N(6)	114.3(6)
C(21)-N(5)-Bi(1)	140.7(5)
N(6)-N(5)-Bi(1)	103.6(4)
C(22)-N(6)-N(5)	112.4(6)
C(22)-N(6)-Bi(2)	140.5(5)
N(5)-N(6)-Bi(2)	104.7(4)
C(31)-N(7)-N(8)	112.6(7)
C(31)-N(7)-Bi(2)	140.9(5)
N(8)-N(7)-Bi(2)	103.6(5)

C(32)-N(8)-N(7)	113.4(7)
C(32)-N(8)-Bi(1)	141.6(5)
N(7)-N(8)-Bi(1)	102.5(5)
N(1)-C(1)-C(7)	121.3(7)
N(1)-C(1)-P(1)	113.7(6)
C(7)-C(1)-P(1)	124.7(6)
N(2)-C(2)-C(3)	119.6(7)
N(2)-C(2)-P(1)	113.1(5)
C(3)-C(2)-P(1)	127.3(7)
C(4)-C(3)-C(2)	112.7(7)
C(4)-C(3)-C(6)	110.9(9)
C(2)-C(3)-C(6)	108.9(8)
C(4)-C(3)-C(5)	107.7(9)
C(2)-C(3)-C(5)	109.5(7)
C(6)-C(3)-C(5)	107.0(8)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(9)-C(7)-C(1)	112.4(6)
C(9)-C(7)-C(10)	109.0(8)
C(1)-C(7)-C(10)	107.3(7)
C(9)-C(7)-C(8)	108.8(7)
C(1)-C(7)-C(8)	110.5(7)
C(10)-C(7)-C(8)	108.8(7)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(3)-C(11)-C(17)	122.4(7)
N(3)-C(11)-P(2)	112.2(6)
C(17)-C(11)-P(2)	125.3(6)
N(4)-C(12)-C(13)	121.2(6)
N(4)-C(12)-P(2)	114.1(6)
C(13)-C(12)-P(2)	124.6(6)
C(14)-C(13)-C(12)	110.6(7)
C(14)-C(13)-C(15)	108.0(8)
C(12)-C(13)-C(15)	108.8(7)
C(14)-C(13)-C(16)	108.6(8)
C(12)-C(13)-C(16)	111.9(7)
C(15)-C(13)-C(16)	108.9(8)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(13)-C(16)-H(16A)	109.5
C(13)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(13)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(11)-C(17)-C(18)	110.7(7)

C(11)-C(17)-C(20)	113.8(7)
C(18)-C(17)-C(20)	108.8(8)
C(11)-C(17)-C(19)	107.0(7)
C(18)-C(17)-C(19)	108.7(8)
C(20)-C(17)-C(19)	107.6(9)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(5)-C(21)-C(27)	121.1(7)
N(5)-C(21)-P(3)	112.9(6)
C(27)-C(21)-P(3)	126.0(6)
N(6)-C(22)-C(23)	122.4(7)
N(6)-C(22)-P(3)	113.4(6)
C(23)-C(22)-P(3)	123.9(6)
C(24)-C(23)-C(25)	109.4(9)
C(24)-C(23)-C(26)	108.1(8)
C(25)-C(23)-C(26)	107.2(9)
C(24)-C(23)-C(22)	109.7(8)
C(25)-C(23)-C(22)	111.0(7)
C(26)-C(23)-C(22)	111.2(7)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5

C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(30)-C(27)-C(21)	108.7(8)
C(30)-C(27)-C(28)	110.6(9)
C(21)-C(27)-C(28)	110.0(7)
C(30)-C(27)-C(29)	109.4(8)
C(21)-C(27)-C(29)	110.4(8)
C(28)-C(27)-C(29)	107.8(8)
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(27)-C(29)-H(29A)	109.5
C(27)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
N(7)-C(31)-C(37)	121.4(8)
N(7)-C(31)-P(4)	114.0(6)
C(37)-C(31)-P(4)	124.4(7)
N(8)-C(32)-C(33)	120.4(8)
N(8)-C(32)-P(4)	113.3(5)
C(33)-C(32)-P(4)	126.2(6)
C(32)-C(33)-C(34)	110.3(8)
C(32)-C(33)-C(35)	107.3(7)
C(34)-C(33)-C(35)	108.2(8)
C(32)-C(33)-C(36)	112.6(7)
C(34)-C(33)-C(36)	108.2(8)

C(35)-C(33)-C(36)	110.2(8)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(38)-C(37)-C(40)	108.8(7)
C(38)-C(37)-C(39)	109.1(8)
C(40)-C(37)-C(39)	112.7(8)
C(38)-C(37)-C(31)	110.0(7)
C(40)-C(37)-C(31)	107.0(6)
C(39)-C(37)-C(31)	109.2(7)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(37)-C(40)-H(40A)	109.5
C(37)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(37)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Aˆ2 x 10ˆ3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 piˆ2 [hˆ2 a*ˆ2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Bi(1)	28(1)	23(1)	39(1)	2(1)	16(1)	-3(1)
Bi(2)	28(1)	22(1)	42(1)	2(1)	17(1)	-2(1)
P(1)	34(1)	44(1)	33(2)	7(1)	8(1)	-9(1)
P(2)	32(1)	38(1)	63(2)	-10(1)	28(1)	-2(1)
P(3)	50(2)	46(2)	62(2)	18(1)	39(2)	21(1)
P(4)	41(1)	36(1)	35(2)	-5(1)	2(1)	4(1)
N(1)	22(4)	40(4)	27(4)	10(3)	9(3)	-15(3)
N(2)	24(4)	46(4)	28(5)	-6(4)	12(3)	-11(3)
N(3)	23(4)	20(3)	38(5)	0(3)	15(3)	-2(3)
N(4)	25(4)	20(4)	70(6)	14(4)	28(4)	8(3)
N(5)	29(4)	21(3)	33(5)	12(3)	12(3)	3(3)
N(6)	31(4)	25(4)	59(6)	-1(3)	34(4)	-3(3)
N(7)	36(4)	18(3)	33(5)	-4(3)	12(4)	-4(3)
N(8)	22(3)	18(3)	38(5)	-2(3)	14(3)	-1(3)
C(1)	19(4)	22(4)	38(6)	1(4)	9(4)	0(3)
C(2)	27(4)	25(4)	31(6)	-3(4)	11(4)	-7(4)
C(3)	36(5)	45(6)	51(7)	-5(5)	23(5)	-13(5)
C(4)	192(15)	57(7)	104(12)	-22(7)	112(11)	-59(9)
C(5)	86(8)	79(8)	47(8)	4(6)	28(7)	-41(7)
C(6)	58(7)	114(10)	131(13)	63(9)	65(8)	10(7)
C(7)	22(4)	32(5)	51(7)	-2(4)	14(4)	-8(4)
C(8)	33(4)	57(5)	93(7)	27(5)	12(4)	-19(4)
C(9)	33(4)	57(5)	93(7)	27(5)	12(4)	-19(4)
C(10)	44(6)	82(8)	63(8)	-5(6)	33(6)	-15(6)
C(11)	22(4)	33(5)	35(6)	-3(4)	9(4)	-6(4)
C(12)	21(4)	23(4)	33(5)	7(4)	9(4)	9(4)
C(13)	43(5)	27(5)	49(7)	-11(4)	27(5)	-5(4)
C(14)	73(8)	50(7)	126(12)	-49(7)	63(8)	-34(6)
C(15)	78(8)	29(5)	99(11)	-12(6)	34(8)	-28(6)
C(16)	34(6)	62(7)	86(10)	-39(7)	9(6)	-16(5)
C(17)	20(4)	33(5)	56(7)	-7(5)	19(5)	-14(4)

C(18)	68(8)	75(8)	141(13)	-37(8)	79(9)	-41(7)
C(19)	71(8)	101(10)	73(10)	-4(8)	-6(7)	-62(7)
C(20)	41(7)	53(7)	178(15)	-18(8)	21(8)	-22(6)
C(21)	25(4)	38(5)	44(6)	8(4)	19(4)	4(4)
C(22)	23(4)	29(4)	35(5)	-10(4)	14(4)	-13(4)
C(23)	32(5)	40(5)	49(7)	21(5)	20(5)	19(4)
C(24)	152(13)	71(8)	44(9)	37(7)	32(8)	53(9)
C(25)	78(9)	63(8)	219(19)	54(10)	82(11)	15(7)
C(26)	89(9)	51(6)	84(10)	21(6)	53(8)	31(6)
C(27)	37(5)	46(6)	59(8)	23(5)	25(5)	7(5)
C(28)	99(9)	77(8)	94(10)	46(7)	77(9)	33(7)
C(29)	97(9)	72(8)	74(10)	23(7)	52(8)	-7(7)
C(30)	78(9)	80(8)	87(11)	31(7)	48(8)	11(7)
C(31)	36(5)	28(5)	46(6)	9(4)	26(5)	6(4)
C(32)	30(5)	17(4)	35(6)	12(4)	12(4)	12(4)
C(33)	39(5)	35(5)	39(6)	-2(5)	11(5)	4(4)
C(34)	93(9)	43(6)	65(9)	16(6)	2(7)	28(6)
C(35)	67(7)	44(6)	87(10)	-2(6)	46(7)	11(6)
C(36)	60(7)	29(5)	118(11)	18(6)	42(7)	11(5)
C(37)	38(5)	21(4)	31(6)	-11(4)	7(4)	-1(4)
C(38)	86(8)	35(6)	69(9)	-8(6)	22(7)	0(6)
C(39)	118(10)	28(5)	82(10)	1(6)	67(8)	-8(6)
C(40)	63(7)	34(5)	67(8)	-21(5)	29(6)	14(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(4A)	2687	-2018	3820	151
H(4B)	2627	-2567	4460	151
H(4C)	3287	-2457	4440	151
H(5A)	3062	-1416	5534	106
H(5B)	3382	-122	5562	106
H(5C)	3702	-1343	5464	106
H(6A)	2129	16	4001	139
H(6B)	2385	469	4753	139
H(6C)	2070	-844	4555	139
H(8A)	4806	3073	4905	98

H(8B)	5298	3076	4587	98
H(8C)	5161	1844	4888	98
H(9A)	3846	3272	3158	98
H(9B)	4515	3874	3479	98
H(9C)	4062	3995	3844	98
H(10A)	4884	710	3782	89
H(10B)	5087	1933	3533	89
H(10C)	4428	1347	3111	89
H(14A)	1322	4968	3702	114
H(14B)	1969	5630	4085	114
H(14C)	1855	4299	4308	114
H(15A)	2039	4852	2558	104
H(15B)	2014	5968	3011	104
H(15C)	1406	5202	2601	104
H(16A)	2823	3610	4198	99
H(16B)	2906	4941	3950	99
H(16C)	2880	3771	3508	99
H(18A)	358	298	3422	124
H(18B)	-136	-475	2830	124
H(18C)	-112	977	2772	124
H(19A)	55	1044	1754	140
H(19B)	-74	-392	1696	140
H(19C)	532	134	1651	140
H(20A)	1086	-1354	2476	147
H(20B)	552	-1785	2688	147
H(20C)	1176	-1231	3229	147
H(24A)	4487	-2080	3467	138
H(24B)	4135	-3194	3624	138
H(24C)	3845	-1855	3516	138
H(25A)	3228	-4121	2762	169
H(25B)	2926	-3545	2036	169
H(25C)	2875	-2843	2644	169
H(26A)	4526	-3131	2488	104
H(26B)	3920	-3775	1966	104
H(26C)	4240	-4281	2707	104
H(28A)	4476	1006	1168	116
H(28B)	4040	1762	530	116
H(28C)	3908	348	596	116
H(29A)	3643	2905	1826	113
H(29B)	3952	3280	1335	113
H(29C)	4321	2444	1965	113
H(30A)	2806	991	431	115
H(30B)	2993	2380	391	115
H(30C)	2731	1984	921	115

H(34A)	1054	3543	-245	116
H(34B)	757	4634	3	116
H(34C)	439	3319	-139	116
H(35A)	785	4570	1163	92
H(35B)	1068	3398	1616	92
H(35C)	444	3281	964	92
H(36A)	2077	3886	772	101
H(36B)	2059	3986	1483	101
H(36C)	1733	5006	935	101
H(38A)	474	-1623	-169	100
H(38B)	885	-2755	-197	100
H(38C)	1019	-1423	-402	100
H(39A)	725	-1947	1059	102
H(39B)	1420	-2249	1546	102
H(39C)	1041	-3174	962	102
H(40A)	1992	-2910	636	81
H(40B)	2281	-1843	1166	81
H(40C)	2106	-1591	399	81

Table 6. Torsion angles [deg] for **4**.

N(1)-Bi(1)-Bi(2)-N(3)	103.7(2)
N(5)-Bi(1)-Bi(2)-N(3)	-167.4(2)
N(4)-Bi(1)-Bi(2)-N(3)	12.6(2)
N(8)-Bi(1)-Bi(2)-N(3)	-75.2(2)
N(1)-Bi(1)-Bi(2)-N(6)	-75.7(2)
N(5)-Bi(1)-Bi(2)-N(6)	13.2(2)
N(4)-Bi(1)-Bi(2)-N(6)	-166.8(2)
N(8)-Bi(1)-Bi(2)-N(6)	105.5(2)
N(1)-Bi(1)-Bi(2)-N(7)	-166.3(2)
N(5)-Bi(1)-Bi(2)-N(7)	-77.4(2)
N(4)-Bi(1)-Bi(2)-N(7)	102.6(2)
N(8)-Bi(1)-Bi(2)-N(7)	14.9(2)
N(1)-Bi(1)-Bi(2)-N(2)	14.6(2)
N(5)-Bi(1)-Bi(2)-N(2)	103.5(2)
N(4)-Bi(1)-Bi(2)-N(2)	-76.5(2)
N(8)-Bi(1)-Bi(2)-N(2)	-164.3(2)
N(5)-Bi(1)-N(1)-C(1)	101.4(9)
N(4)-Bi(1)-N(1)-C(1)	-113.6(9)
N(8)-Bi(1)-N(1)-C(1)	176.3(7)
Bi(2)-Bi(1)-N(1)-C(1)	174.4(9)

N(5)-Bi(1)-N(1)-N(2)	-99.7(5)
N(4)-Bi(1)-N(1)-N(2)	45.3(4)
N(8)-Bi(1)-N(1)-N(2)	-24.8(6)
Bi(2)-Bi(1)-N(1)-N(2)	-26.7(4)
C(1)-N(1)-N(2)-C(2)	1.7(9)
Bi(1)-N(1)-N(2)-C(2)	-164.3(5)
C(1)-N(1)-N(2)-Bi(2)	-164.8(5)
Bi(1)-N(1)-N(2)-Bi(2)	29.2(4)
N(3)-Bi(2)-N(2)-C(2)	100.2(8)
N(6)-Bi(2)-N(2)-C(2)	-113.9(8)
N(7)-Bi(2)-N(2)-C(2)	172.4(7)
Bi(1)-Bi(2)-N(2)-C(2)	173.8(8)
N(3)-Bi(2)-N(2)-N(1)	-99.9(4)
N(6)-Bi(2)-N(2)-N(1)	46.1(4)
N(7)-Bi(2)-N(2)-N(1)	-27.6(6)
Bi(1)-Bi(2)-N(2)-N(1)	-26.2(4)
N(6)-Bi(2)-N(3)-C(11)	176.6(7)
N(7)-Bi(2)-N(3)-C(11)	103.2(8)
N(2)-Bi(2)-N(3)-C(11)	-111.8(9)
Bi(1)-Bi(2)-N(3)-C(11)	175.6(9)
N(6)-Bi(2)-N(3)-N(4)	-21.8(7)
N(7)-Bi(2)-N(3)-N(4)	-95.2(5)
N(2)-Bi(2)-N(3)-N(4)	49.8(5)
Bi(1)-Bi(2)-N(3)-N(4)	-22.8(4)
C(11)-N(3)-N(4)-C(12)	2.4(10)
Bi(2)-N(3)-N(4)-C(12)	-164.7(5)
C(11)-N(3)-N(4)-Bi(1)	-167.4(5)
Bi(2)-N(3)-N(4)-Bi(1)	25.5(4)
N(1)-Bi(1)-N(4)-C(12)	100.3(9)
N(5)-Bi(1)-N(4)-C(12)	172.6(8)
N(8)-Bi(1)-N(4)-C(12)	-113.9(9)
Bi(2)-Bi(1)-N(4)-C(12)	172.7(10)
N(1)-Bi(1)-N(4)-N(3)	-95.1(5)
N(5)-Bi(1)-N(4)-N(3)	-22.8(7)
N(8)-Bi(1)-N(4)-N(3)	50.7(5)
Bi(2)-Bi(1)-N(4)-N(3)	-22.7(4)
N(1)-Bi(1)-N(5)-C(21)	-115.6(9)
N(4)-Bi(1)-N(5)-C(21)	171.5(8)
N(8)-Bi(1)-N(5)-C(21)	99.3(9)
Bi(2)-Bi(1)-N(5)-C(21)	171.4(9)
N(1)-Bi(1)-N(5)-N(6)	48.9(5)
N(4)-Bi(1)-N(5)-N(6)	-23.9(7)
N(8)-Bi(1)-N(5)-N(6)	-96.1(5)
Bi(2)-Bi(1)-N(5)-N(6)	-24.0(4)

C(21)-N(5)-N(6)-C(22)	2.5(10)
Bi(1)-N(5)-N(6)-C(22)	-166.8(5)
C(21)-N(5)-N(6)-Bi(2)	-163.8(6)
Bi(1)-N(5)-N(6)-Bi(2)	26.9(4)
N(3)-Bi(2)-N(6)-C(22)	174.9(8)
N(7)-Bi(2)-N(6)-C(22)	-111.8(9)
N(2)-Bi(2)-N(6)-C(22)	103.5(9)
Bi(1)-Bi(2)-N(6)-C(22)	175.9(9)
N(3)-Bi(2)-N(6)-N(5)	-25.3(7)
N(7)-Bi(2)-N(6)-N(5)	48.1(5)
N(2)-Bi(2)-N(6)-N(5)	-96.7(5)
Bi(1)-Bi(2)-N(6)-N(5)	-24.3(4)
N(3)-Bi(2)-N(7)-C(31)	-111.3(8)
N(6)-Bi(2)-N(7)-C(31)	103.1(8)
N(2)-Bi(2)-N(7)-C(31)	176.7(7)
Bi(1)-Bi(2)-N(7)-C(31)	175.3(9)
N(3)-Bi(2)-N(7)-N(8)	46.3(4)
N(6)-Bi(2)-N(7)-N(8)	-99.3(4)
N(2)-Bi(2)-N(7)-N(8)	-25.6(6)
Bi(1)-Bi(2)-N(7)-N(8)	-27.1(4)
C(31)-N(7)-N(8)-C(32)	0.6(9)
Bi(2)-N(7)-N(8)-C(32)	-164.3(5)
C(31)-N(7)-N(8)-Bi(1)	-165.4(5)
Bi(2)-N(7)-N(8)-Bi(1)	29.6(4)
N(1)-Bi(1)-N(8)-C(32)	172.2(7)
N(5)-Bi(1)-N(8)-C(32)	-113.9(8)
N(4)-Bi(1)-N(8)-C(32)	101.2(8)
Bi(2)-Bi(1)-N(8)-C(32)	174.1(8)
N(1)-Bi(1)-N(8)-N(7)	-28.6(6)
N(5)-Bi(1)-N(8)-N(7)	45.3(4)
N(4)-Bi(1)-N(8)-N(7)	-99.6(4)
Bi(2)-Bi(1)-N(8)-N(7)	-26.8(4)
N(2)-N(1)-C(1)-C(7)	173.5(6)
Bi(1)-N(1)-C(1)-C(7)	-28.6(13)
N(2)-N(1)-C(1)-P(1)	-1.0(8)
Bi(1)-N(1)-C(1)-P(1)	156.9(5)
C(2)-P(1)-C(1)-N(1)	0.1(6)
C(2)-P(1)-C(1)-C(7)	-174.2(7)
N(1)-N(2)-C(2)-C(3)	177.7(7)
Bi(2)-N(2)-C(2)-C(3)	-23.7(12)
N(1)-N(2)-C(2)-P(1)	-1.6(9)
Bi(2)-N(2)-C(2)-P(1)	156.9(5)
C(1)-P(1)-C(2)-N(2)	0.9(6)
C(1)-P(1)-C(2)-C(3)	-178.4(7)

N(2)-C(2)-C(3)-C(4)	64.9(12)
P(1)-C(2)-C(3)-C(4)	-115.8(10)
N(2)-C(2)-C(3)-C(6)	-58.5(11)
P(1)-C(2)-C(3)-C(6)	120.7(9)
N(2)-C(2)-C(3)-C(5)	-175.2(8)
P(1)-C(2)-C(3)-C(5)	4.0(11)
N(1)-C(1)-C(7)-C(9)	51.0(11)
P(1)-C(1)-C(7)-C(9)	-135.1(8)
N(1)-C(1)-C(7)-C(10)	-68.7(10)
P(1)-C(1)-C(7)-C(10)	105.2(8)
N(1)-C(1)-C(7)-C(8)	172.8(7)
P(1)-C(1)-C(7)-C(8)	-13.3(10)
N(4)-N(3)-C(11)-C(17)	172.7(7)
Bi(2)-N(3)-C(11)-C(17)	-26.9(13)
N(4)-N(3)-C(11)-P(2)	-3.9(9)
Bi(2)-N(3)-C(11)-P(2)	156.5(5)
C(12)-P(2)-C(11)-N(3)	3.3(6)
C(12)-P(2)-C(11)-C(17)	-173.2(8)
N(3)-N(4)-C(12)-C(13)	177.3(7)
Bi(1)-N(4)-C(12)-C(13)	-18.9(14)
N(3)-N(4)-C(12)-P(2)	0.3(9)
Bi(1)-N(4)-C(12)-P(2)	164.1(6)
C(11)-P(2)-C(12)-N(4)	-2.0(7)
C(11)-P(2)-C(12)-C(13)	-178.9(8)
N(4)-C(12)-C(13)-C(14)	-161.0(9)
P(2)-C(12)-C(13)-C(14)	15.7(11)
N(4)-C(12)-C(13)-C(15)	80.6(10)
P(2)-C(12)-C(13)-C(15)	-102.8(8)
N(4)-C(12)-C(13)-C(16)	-39.7(11)
P(2)-C(12)-C(13)-C(16)	136.9(7)
N(3)-C(11)-C(17)-C(18)	168.2(8)
P(2)-C(11)-C(17)-C(18)	-15.6(12)
N(3)-C(11)-C(17)-C(20)	45.2(13)
P(2)-C(11)-C(17)-C(20)	-138.6(8)
N(3)-C(11)-C(17)-C(19)	-73.5(10)
P(2)-C(11)-C(17)-C(19)	102.7(9)
N(6)-N(5)-C(21)-C(27)	174.7(8)
Bi(1)-N(5)-C(21)-C(27)	-21.7(14)
N(6)-N(5)-C(21)-P(3)	-3.0(9)
Bi(1)-N(5)-C(21)-P(3)	160.5(5)
C(22)-P(3)-C(21)-N(5)	2.0(7)
C(22)-P(3)-C(21)-C(27)	-175.6(9)
N(5)-N(6)-C(22)-C(23)	173.4(7)
Bi(2)-N(6)-C(22)-C(23)	-27.8(14)

N(5)-N(6)-C(22)-P(3)	-0.9(9)
Bi(2)-N(6)-C(22)-P(3)	157.9(6)
C(21)-P(3)-C(22)-N(6)	-0.6(7)
C(21)-P(3)-C(22)-C(23)	-174.8(8)
N(6)-C(22)-C(23)-C(24)	-66.1(11)
P(3)-C(22)-C(23)-C(24)	107.5(8)
N(6)-C(22)-C(23)-C(25)	55.0(12)
P(3)-C(22)-C(23)-C(25)	-131.4(8)
N(6)-C(22)-C(23)-C(26)	174.3(8)
P(3)-C(22)-C(23)-C(26)	-12.0(12)
N(5)-C(21)-C(27)-C(30)	-54.7(12)
P(3)-C(21)-C(27)-C(30)	122.8(8)
N(5)-C(21)-C(27)-C(28)	-175.9(9)
P(3)-C(21)-C(27)-C(28)	1.6(13)
N(5)-C(21)-C(27)-C(29)	65.3(11)
P(3)-C(21)-C(27)-C(29)	-117.3(8)
N(8)-N(7)-C(31)-C(37)	176.0(6)
Bi(2)-N(7)-C(31)-C(37)	-27.6(12)
N(8)-N(7)-C(31)-P(4)	-0.2(8)
Bi(2)-N(7)-C(31)-P(4)	156.2(5)
C(32)-P(4)-C(31)-N(7)	-0.2(6)
C(32)-P(4)-C(31)-C(37)	-176.3(7)
N(7)-N(8)-C(32)-C(33)	175.2(6)
Bi(1)-N(8)-C(32)-C(33)	-27.0(12)
N(7)-N(8)-C(32)-P(4)	-0.8(8)
Bi(1)-N(8)-C(32)-P(4)	157.0(5)
C(31)-P(4)-C(32)-N(8)	0.5(6)
C(31)-P(4)-C(32)-C(33)	-175.2(7)
N(8)-C(32)-C(33)-C(34)	170.0(7)
P(4)-C(32)-C(33)-C(34)	-14.6(11)
N(8)-C(32)-C(33)-C(35)	-72.4(10)
P(4)-C(32)-C(33)-C(35)	103.0(8)
N(8)-C(32)-C(33)-C(36)	49.0(11)
P(4)-C(32)-C(33)-C(36)	-135.6(7)
N(7)-C(31)-C(37)-C(38)	-175.8(7)
P(4)-C(31)-C(37)-C(38)	0.0(10)
N(7)-C(31)-C(37)-C(40)	-57.8(10)
P(4)-C(31)-C(37)-C(40)	118.0(7)
N(7)-C(31)-C(37)-C(39)	64.5(10)
P(4)-C(31)-C(37)-C(39)	-119.8(8)

Symmetry transformations used to generate equivalent atoms:

a) Crystal structural analysis data for **5**

Table 1. Crystal data and structure refinement for **5**.

Identification code	150209-1
Empirical formula	$C_{32}H_{56}Bi_2N_8P_4$
Formula weight	1094.69
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, $P\,\bar{1}$
Unit cell dimensions	a = 10.5121(2) Å α = 90.269(2) deg. b = 13.7719(3) Å β = 101.428(2) deg. c = 15.2443(3) Å γ = 93.926(2) deg.
Volume	2157.73(8) Å^3
Z, Calculated density	2, 1.685 Mg/m^3
Absorption coefficient	8.324 mm^{-1}
F(000)	1060
Crystal size	0.26 × 0.15 × 0.10 mm
Theta range for data collection	2.93 to 26.37 deg.
Limiting indices	-13<=h<=13, -17<=k<=17, -17<=l<=19
Reflections collected / unique	26642 / 8798 [R(int) = 0.0404]
Completeness to theta = 26.37	99.8 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	1.00000 and 0.24037
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8798 / 6 / 425
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R_1 = 0.0345, wR_2 = 0.0671
R indices (all data)	R_1 = 0.0603, wR_2 = 0.0765
Largest diff. peak and hole	1.457 and -0.798 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Bi(1)	4473(1)	9392(1)	4232(1)	36(1)
Bi(2)	5327(1)	4149(1)	506(1)	39(1)
C(1)	3425(10)	8974(7)	8470(5)	110(3)
C(2)	4249(8)	9298(5)	7810(4)	59(2)
C(3)	5668(9)	9184(7)	8175(5)	110(3)
C(4)	3803(7)	8772(4)	6915(4)	45(2)
C(5)	3040(6)	7795(4)	5576(4)	43(2)
C(6)	2502(7)	7130(4)	4793(4)	47(2)
C(7)	1980(10)	6158(5)	5067(5)	99(3)
C(8)	1456(7)	7583(5)	4140(4)	63(2)
C(9)	7266(9)	6380(5)	4069(5)	82(3)
C(10)	6630(7)	7322(4)	3991(4)	50(2)
C(11)	6812(9)	7795(5)	3104(4)	86(3)
C(12)	7160(6)	8010(4)	4763(4)	39(1)
C(13)	8235(6)	9049(4)	6003(4)	42(1)
C(14)	9054(7)	9631(5)	6770(4)	59(2)
C(15)	10304(8)	10056(6)	6516(5)	81(2)
C(16)	9369(9)	9022(6)	7600(5)	98(3)
C(17)	2424(12)	8139(6)	1706(7)	136(3)
C(18)	2961(9)	7533(5)	1042(5)	77(2)
C(19)	4063(12)	8132(6)	810(7)	136(3)
C(20)	3415(7)	6580(4)	1456(4)	49(2)
C(21)	3999(6)	5122(4)	2226(4)	45(2)
C(22)	4278(7)	4218(5)	2775(4)	60(2)
C(23)	3341(9)	3377(5)	2425(5)	92(3)
C(24)	4262(10)	4406(6)	3748(5)	99(3)
C(25)	2274(11)	1395(5)	-918(6)	113(3)
C(26)	2294(10)	2178(5)	-244(5)	87(3)
C(27)	1215(10)	1944(7)	255(6)	126(4)
C(28)	2148(7)	3152(4)	-692(4)	49(2)
C(29)	1717(7)	4637(4)	-1466(4)	50(2)
C(30)	1275(8)	5544(5)	-1963(5)	68(2)
C(31)	412(9)	5316(6)	-2856(5)	84(3)

C(32)	590(14)	6160(8)	-1407(7)	170(6)
N(1)	4173(5)	9178(3)	6209(3)	43(1)
N(2)	6496(5)	8767(3)	4876(3)	38(1)
N(3)	3730(5)	8610(3)	5444(3)	39(1)
N(4)	7115(5)	9364(3)	5591(3)	42(1)
N(5)	2845(5)	4684(3)	-906(3)	45(1)
N(6)	4296(5)	5145(3)	1420(3)	40(1)
N(7)	3103(5)	3836(3)	-467(3)	43(1)
N(8)	3955(5)	5986(3)	967(3)	45(1)
P(1)	3263(2)	6139(1)	2497(1)	62(1)
P(2)	855(2)	3512(2)	-1490(2)	76(1)
P(3)	2869(2)	7671(1)	6686(1)	57(1)
P(4)	8617(2)	7963(1)	5537(1)	58(1)

Table 3. Bond lengths [A] and angles [deg] for **5**.

Bi(1)-N(2)	2.378(5)
Bi(1)-N(3)	2.379(4)
Bi(1)-N(4)#1	2.522(5)
Bi(1)-N(1)#1	2.523(5)
Bi(1)-Bi(1)#1	2.8630(4)
Bi(2)-N(5)#2	2.398(5)
Bi(2)-N(6)	2.405(4)
Bi(2)-N(8)#2	2.516(5)
Bi(2)-N(7)	2.517(5)
Bi(2)-Bi(2)#2	2.8611(4)
C(1)-C(2)	1.503(10)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(3)	1.504(10)
C(2)-C(4)	1.517(8)
C(2)-H(2)	0.9800
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-N(1)	1.329(7)
C(4)-P(3)	1.743(6)
C(5)-N(3)	1.332(7)
C(5)-C(6)	1.495(8)
C(5)-P(3)	1.744(6)

C(6)-C(8)	1.502(8)
C(6)-C(7)	1.504(9)
C(6)-H(6)	0.9800
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(10)	1.494(8)
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-C(12)	1.501(8)
C(10)-C(11)	1.543(8)
C(10)-H(10)	0.9800
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-N(2)	1.323(7)
C(12)-P(4)	1.744(6)
C(13)-N(4)	1.322(7)
C(13)-C(14)	1.500(9)
C(13)-P(4)	1.758(6)
C(14)-C(16)	1.515(9)
C(14)-C(15)	1.523(9)
C(14)-H(14)	0.9800
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-C(18)	1.524(10)
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(19)	1.476(12)
C(18)-C(20)	1.524(9)
C(18)-H(18)	0.9800
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(20)-N(8)	1.331(7)

C(20)-P(1)	1.735(6)
C(21)-N(6)	1.328(7)
C(21)-C(22)	1.515(8)
C(21)-P(1)	1.732(6)
C(22)-C(23)	1.492(10)
C(22)-C(24)	1.509(9)
C(22)-H(22)	0.9800
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.481(10)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-C(27)	1.504(11)
C(26)-C(28)	1.511(8)
C(26)-H(26)	0.9800
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-N(7)	1.320(7)
C(28)-P(2)	1.737(7)
C(29)-N(5)	1.314(7)
C(29)-C(30)	1.516(8)
C(29)-P(2)	1.737(6)
C(30)-C(31)	1.498(9)
C(30)-C(32)	1.508(12)
C(30)-H(30)	0.9800
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
N(1)-N(3)	1.383(6)
N(1)-Bi(1)#1	2.523(5)
N(2)-N(4)	1.388(6)
N(4)-Bi(1)#1	2.522(5)
N(5)-N(7)	1.365(6)
N(5)-Bi(2)#2	2.398(5)
N(6)-N(8)	1.383(6)

N(8)-Bi(2)#2	2.516(5)
N(2)-Bi(1)-N(3)	84.17(16)
N(2)-Bi(1)-N(4)#1	144.82(14)
N(3)-Bi(1)-N(4)#1	84.59(15)
N(2)-Bi(1)-N(1)#1	85.56(16)
N(3)-Bi(1)-N(1)#1	144.88(14)
N(4)#1-Bi(1)-N(1)#1	84.76(16)
N(2)-Bi(1)-Bi(1)#1	74.37(11)
N(3)-Bi(1)-Bi(1)#1	74.82(11)
N(4)#1-Bi(1)-Bi(1)#1	70.52(11)
N(1)#1-Bi(1)-Bi(1)#1	70.07(10)
N(5)#2-Bi(2)-N(6)	85.01(17)
N(5)#2-Bi(2)-N(8)#2	85.22(17)
N(6)-Bi(2)-N(8)#2	145.04(14)
N(5)#2-Bi(2)-N(7)	144.52(14)
N(6)-Bi(2)-N(7)	86.16(16)
N(8)#2-Bi(2)-N(7)	82.63(16)
N(5)#2-Bi(2)-Bi(2)#2	73.47(11)
N(6)-Bi(2)-Bi(2)#2	73.89(10)
N(8)#2-Bi(2)-Bi(2)#2	71.15(11)
N(7)-Bi(2)-Bi(2)#2	71.06(10)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(1)-C(2)-C(3)	111.5(7)
C(1)-C(2)-C(4)	111.6(7)
C(3)-C(2)-C(4)	111.0(6)
C(1)-C(2)-H(2)	107.5
C(3)-C(2)-H(2)	107.5
C(4)-C(2)-H(2)	107.5
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(1)-C(4)-C(2)	117.3(5)
N(1)-C(4)-P(3)	114.6(4)
C(2)-C(4)-P(3)	128.1(5)
N(3)-C(5)-C(6)	118.7(5)

N(3)-C(5)-P(3)	112.7(4)
C(6)-C(5)-P(3)	128.5(5)
C(5)-C(6)-C(8)	111.4(5)
C(5)-C(6)-C(7)	112.6(5)
C(8)-C(6)-C(7)	109.4(6)
C(5)-C(6)-H(6)	107.8
C(8)-C(6)-H(6)	107.8
C(7)-C(6)-H(6)	107.8
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(10)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(9)-C(10)-C(12)	112.9(6)
C(9)-C(10)-C(11)	108.3(6)
C(12)-C(10)-C(11)	110.2(5)
C(9)-C(10)-H(10)	108.5
C(12)-C(10)-H(10)	108.5
C(11)-C(10)-H(10)	108.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(10)	118.4(6)
N(2)-C(12)-P(4)	114.1(4)
C(10)-C(12)-P(4)	127.5(4)
N(4)-C(13)-C(14)	119.6(5)
N(4)-C(13)-P(4)	113.5(4)
C(14)-C(13)-P(4)	126.8(5)

C(13)-C(14)-C(16)	111.5(6)
C(13)-C(14)-C(15)	110.5(6)
C(16)-C(14)-C(15)	110.1(6)
C(13)-C(14)-H(14)	108.2
C(16)-C(14)-H(14)	108.2
C(15)-C(14)-H(14)	108.2
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-H(17A)	109.5
C(18)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(18)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(17)	106.3(7)
C(19)-C(18)-C(20)	110.6(7)
C(17)-C(18)-C(20)	110.8(7)
C(19)-C(18)-H(18)	109.7
C(17)-C(18)-H(18)	109.7
C(20)-C(18)-H(18)	109.7
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(8)-C(20)-C(18)	117.9(6)
N(8)-C(20)-P(1)	114.6(4)
C(18)-C(20)-P(1)	127.5(5)
N(6)-C(21)-C(22)	117.8(5)
N(6)-C(21)-P(1)	114.1(4)
C(22)-C(21)-P(1)	128.1(4)
C(23)-C(22)-C(24)	109.8(6)
C(23)-C(22)-C(21)	111.8(6)

C(24)-C(22)-C(21)	111.3(6)
C(23)-C(22)-H(22)	107.9
C(24)-C(22)-H(22)	107.9
C(21)-C(22)-H(22)	107.9
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(26)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(25)-C(26)-C(27)	108.9(8)
C(25)-C(26)-C(28)	110.5(6)
C(27)-C(26)-C(28)	110.9(7)
C(25)-C(26)-H(26)	108.8
C(27)-C(26)-H(26)	108.8
C(28)-C(26)-H(26)	108.8
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(7)-C(28)-C(26)	118.2(7)
N(7)-C(28)-P(2)	113.7(4)
C(26)-C(28)-P(2)	128.2(6)
N(5)-C(29)-C(30)	119.0(6)
N(5)-C(29)-P(2)	113.4(4)
C(30)-C(29)-P(2)	127.5(5)
C(31)-C(30)-C(32)	109.8(8)
C(31)-C(30)-C(29)	112.6(6)
C(32)-C(30)-C(29)	110.7(7)
C(31)-C(30)-H(30)	107.9

C(32)-C(30)-H(30)	107.9
C(29)-C(30)-H(30)	107.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(4)-N(1)-N(3)	111.2(5)
C(4)-N(1)-Bi(1)#1	142.0(4)
N(3)-N(1)-Bi(1)#1	106.8(3)
C(12)-N(2)-N(4)	112.6(5)
C(12)-N(2)-Bi(1)	138.2(4)
N(4)-N(2)-Bi(1)	109.1(3)
C(5)-N(3)-N(1)	114.1(4)
C(5)-N(3)-Bi(1)	137.6(4)
N(1)-N(3)-Bi(1)	108.3(3)
C(13)-N(4)-N(2)	112.8(5)
C(13)-N(4)-Bi(1)#1	140.9(4)
N(2)-N(4)-Bi(1)#1	105.8(3)
C(29)-N(5)-N(7)	113.4(5)
C(29)-N(5)-Bi(2)#2	136.5(4)
N(7)-N(5)-Bi(2)#2	109.9(4)
C(21)-N(6)-N(8)	112.8(5)
C(21)-N(6)-Bi(2)	138.1(4)
N(8)-N(6)-Bi(2)	109.1(3)
C(28)-N(7)-N(5)	112.5(5)
C(28)-N(7)-Bi(2)	142.0(4)
N(5)-N(7)-Bi(2)	105.5(3)
C(20)-N(8)-N(6)	111.5(5)
C(20)-N(8)-Bi(2)#2	142.5(4)
N(6)-N(8)-Bi(2)#2	105.9(3)
C(21)-P(1)-C(20)	87.0(3)
C(28)-P(2)-C(29)	87.0(3)
C(4)-P(3)-C(5)	87.3(3)
C(12)-P(4)-C(13)	87.0(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1 #2 -x+1,-y+1,-z

Table 4. Anisotropic displacement parameters (Aˆ2 x 10ˆ3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 piˆ2 [hˆ2 a*ˆ2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Bi(1)	39(1)	38(1)	31(1)	-6(1)	3(1)	1(1)
Bi(2)	44(1)	35(1)	38(1)	5(1)	7(1)	6(1)
C(1)	146(10)	141(8)	49(5)	-14(5)	39(6)	4(7)
C(2)	97(7)	43(4)	35(4)	-1(3)	7(4)	11(4)
C(3)	93(8)	156(9)	64(6)	-35(5)	-27(5)	18(7)
C(4)	60(5)	34(3)	42(4)	2(3)	10(3)	13(3)
C(5)	43(4)	38(3)	50(4)	2(3)	12(3)	6(3)
C(6)	46(4)	41(4)	54(4)	-12(3)	8(3)	-1(3)
C(7)	163(10)	41(4)	80(6)	-10(4)	0(6)	-19(5)
C(8)	63(6)	66(5)	56(4)	-16(3)	4(4)	0(4)
C(9)	114(8)	46(4)	86(6)	-4(4)	19(5)	19(4)
C(10)	52(5)	45(4)	57(4)	-4(3)	21(3)	4(3)
C(11)	136(9)	73(5)	50(5)	0(4)	23(5)	6(5)
C(12)	46(4)	33(3)	43(3)	3(3)	18(3)	1(3)
C(13)	34(4)	44(3)	45(4)	3(3)	3(3)	2(3)
C(14)	45(5)	73(5)	52(4)	-8(3)	-5(3)	7(4)
C(15)	62(6)	87(6)	86(6)	4(4)	-3(5)	-13(5)
C(16)	100(8)	118(7)	61(5)	18(5)	-11(5)	-25(6)
C(17)	206(10)	69(4)	162(7)	12(4)	91(7)	50(5)
C(18)	93(7)	47(4)	87(6)	-13(4)	8(5)	14(4)
C(19)	206(10)	69(4)	162(7)	12(4)	91(7)	50(5)
C(20)	55(5)	42(4)	47(4)	-13(3)	1(3)	10(3)
C(21)	41(4)	59(4)	33(3)	0(3)	9(3)	0(3)
C(22)	54(5)	82(5)	49(4)	17(4)	20(4)	18(4)
C(23)	126(9)	62(5)	83(6)	9(4)	14(6)	-17(5)
C(24)	140(10)	110(7)	52(5)	20(5)	28(5)	12(6)
C(25)	193(8)	61(4)	90(5)	13(4)	36(5)	16(5)
C(26)	162(8)	40(4)	65(5)	12(3)	35(5)	7(4)
C(27)	142(11)	116(8)	122(8)	68(7)	35(8)	-8(7)
C(28)	54(5)	38(3)	52(4)	2(3)	7(3)	-5(3)
C(29)	46(5)	49(4)	49(4)	4(3)	-1(3)	4(3)

C(30)	55(5)	59(4)	80(5)	19(4)	-13(4)	5(4)
C(31)	90(7)	93(6)	63(5)	18(4)	-6(5)	14(5)
C(32)	259(17)	132(9)	114(9)	-3(7)	-13(10)	124(11)
N(1)	50(4)	39(3)	36(3)	-7(2)	3(2)	-2(2)
N(2)	34(3)	37(3)	42(3)	-7(2)	3(2)	4(2)
N(3)	47(3)	36(3)	35(3)	-1(2)	8(2)	2(2)
N(4)	43(3)	42(3)	38(3)	-6(2)	1(2)	9(2)
N(5)	45(4)	37(3)	49(3)	7(2)	2(3)	6(2)
N(6)	44(3)	44(3)	36(3)	2(2)	13(2)	10(2)
N(7)	47(4)	45(3)	37(3)	2(2)	6(2)	2(3)
N(8)	52(4)	41(3)	42(3)	-3(2)	6(3)	9(3)
P(1)	72(2)	71(1)	49(1)	-8(1)	21(1)	20(1)
P(2)	57(2)	63(1)	90(2)	16(1)	-19(1)	-13(1)
P(3)	79(2)	45(1)	49(1)	6(1)	21(1)	-3(1)
P(4)	49(1)	56(1)	67(1)	-3(1)	4(1)	20(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(1A)	3393	8278	8509	165
H(1B)	2560	9177	8275	165
H(1C)	3795	9261	9047	165
H(2)	4146	9993	7710	71
H(3A)	5783	8527	8366	165
H(3B)	5970	9623	8675	165
H(3C)	6157	9328	7717	165
H(6)	3213	7015	4483	57
H(7A)	2664	5847	5451	149
H(7B)	1653	5756	4543	149
H(7C)	1289	6250	5380	149
H(8A)	729	7676	4419	95
H(8B)	1180	7163	3624	95
H(8C)	1790	8201	3961	95
H(9A)	8150	6491	3995	122
H(9B)	6803	5931	3614	122
H(9C)	7255	6113	4648	122
H(10)	5696	7183	3967	60

H(11A)	6520	8441	3082	129
H(11B)	6315	7412	2610	129
H(11C)	7716	7825	3070	129
H(14)	8561	10171	6908	70
H(15A)	10823	9538	6409	122
H(15B)	10783	10469	6996	122
H(15C)	10094	10431	5984	122
H(16A)	8578	8802	7784	148
H(16B)	9914	9409	8073	148
H(16C)	9817	8471	7470	148
H(17A)	3080	8263	2237	204
H(17B)	1678	7790	1858	204
H(17C)	2175	8746	1441	204
H(18)	2289	7396	503	92
H(19A)	4636	8373	1349	204
H(19B)	3740	8670	456	204
H(19C)	4529	7742	475	204
H(22)	5152	4041	2734	72
H(23A)	2484	3516	2496	138
H(23B)	3596	2805	2752	138
H(23C)	3340	3270	1802	138
H(24A)	4887	4934	3975	149
H(24B)	4479	3832	4083	149
H(24C)	3410	4573	3806	149
H(25A)	1479	1389	-1356	170
H(25B)	2329	778	-627	170
H(25C)	3001	1511	-1207	170
H(26)	3128	2201	180	105
H(27A)	439	1721	-161	189
H(27B)	1056	2518	565	189
H(27C)	1462	1445	679	189
H(30)	2052	5928	-2064	81
H(31A)	852	4924	-3207	127
H(31B)	208	5911	-3161	127
H(31C)	-377	4968	-2773	127
H(32A)	376	6753	-1712	255
H(32B)	1150	6310	-838	255
H(32C)	-193	5808	-1317	255

Table 6. Torsion angles [deg] for **5**.

C(1)-C(2)-C(4)-N(1)	160.4(6)
C(3)-C(2)-C(4)-N(1)	-74.5(8)
C(1)-C(2)-C(4)-P(3)	-20.6(9)
C(3)-C(2)-C(4)-P(3)	104.4(7)
N(3)-C(5)-C(6)-C(8)	-68.0(8)
P(3)-C(5)-C(6)-C(8)	110.7(6)
N(3)-C(5)-C(6)-C(7)	168.7(6)
P(3)-C(5)-C(6)-C(7)	-12.6(9)
C(9)-C(10)-C(12)-N(2)	-165.3(6)
C(11)-C(10)-C(12)-N(2)	73.5(7)
C(9)-C(10)-C(12)-P(4)	17.2(8)
C(11)-C(10)-C(12)-P(4)	-104.0(6)
N(4)-C(13)-C(14)-C(16)	125.0(7)
P(4)-C(13)-C(14)-C(16)	-56.9(8)
N(4)-C(13)-C(14)-C(15)	-112.2(7)
P(4)-C(13)-C(14)-C(15)	65.9(8)
C(19)-C(18)-C(20)-N(8)	-60.0(9)
C(17)-C(18)-C(20)-N(8)	-177.6(8)
C(19)-C(18)-C(20)-P(1)	122.5(7)
C(17)-C(18)-C(20)-P(1)	4.9(11)
N(6)-C(21)-C(22)-C(23)	-73.3(8)
P(1)-C(21)-C(22)-C(23)	103.8(7)
N(6)-C(21)-C(22)-C(24)	163.5(6)
P(1)-C(21)-C(22)-C(24)	-19.4(9)
C(25)-C(26)-C(28)-N(7)	-118.8(8)
C(27)-C(26)-C(28)-N(7)	120.4(8)
C(25)-C(26)-C(28)-P(2)	61.2(10)
C(27)-C(26)-C(28)-P(2)	-59.7(9)
N(5)-C(29)-C(30)-C(31)	150.8(7)
P(2)-C(29)-C(30)-C(31)	-33.4(10)
N(5)-C(29)-C(30)-C(32)	-85.9(10)
P(2)-C(29)-C(30)-C(32)	89.9(9)
C(2)-C(4)-N(1)-N(3)	178.4(5)
P(3)-C(4)-N(1)-N(3)	-0.7(6)
C(2)-C(4)-N(1)-Bi(1)#1	2.9(10)
P(3)-C(4)-N(1)-Bi(1)#1	-176.2(4)
C(10)-C(12)-N(2)-N(4)	-177.7(5)
P(4)-C(12)-N(2)-N(4)	0.2(6)
C(10)-C(12)-N(2)-Bi(1)	5.2(8)
P(4)-C(12)-N(2)-Bi(1)	-176.9(3)

N(3)-Bi(1)-N(2)-C(12)	97.1(5)
N(4)#1-Bi(1)-N(2)-C(12)	169.1(5)
N(1)#1-Bi(1)-N(2)-C(12)	-116.6(5)
Bi(1)#1-Bi(1)-N(2)-C(12)	172.9(6)
N(3)-Bi(1)-N(2)-N(4)	-80.1(3)
N(4)#1-Bi(1)-N(2)-N(4)	-8.1(6)
N(1)#1-Bi(1)-N(2)-N(4)	66.3(3)
Bi(1)#1-Bi(1)-N(2)-N(4)	-4.3(3)
C(6)-C(5)-N(3)-N(1)	179.5(5)
P(3)-C(5)-N(3)-N(1)	0.6(6)
C(6)-C(5)-N(3)-Bi(1)	-1.6(9)
P(3)-C(5)-N(3)-Bi(1)	179.5(3)
C(4)-N(1)-N(3)-C(5)	0.1(7)
Bi(1)#1-N(1)-N(3)-C(5)	177.2(4)
C(4)-N(1)-N(3)-Bi(1)	-179.1(4)
Bi(1)#1-N(1)-N(3)-Bi(1)	-2.1(4)
N(2)-Bi(1)-N(3)-C(5)	-101.8(6)
N(4)#1-Bi(1)-N(3)-C(5)	111.6(6)
N(1)#1-Bi(1)-N(3)-C(5)	-175.5(5)
Bi(1)#1-Bi(1)-N(3)-C(5)	-177.1(6)
N(2)-Bi(1)-N(3)-N(1)	77.2(4)
N(4)#1-Bi(1)-N(3)-N(1)	-69.4(4)
N(1)#1-Bi(1)-N(3)-N(1)	3.4(6)
Bi(1)#1-Bi(1)-N(3)-N(1)	1.8(3)
C(14)-C(13)-N(4)-N(2)	177.7(5)
P(4)-C(13)-N(4)-N(2)	-0.6(6)
C(14)-C(13)-N(4)-Bi(1)#1	-12.4(10)
P(4)-C(13)-N(4)-Bi(1)#1	169.3(4)
C(12)-N(2)-N(4)-C(13)	0.3(7)
Bi(1)-N(2)-N(4)-C(13)	178.2(4)
C(12)-N(2)-N(4)-Bi(1)#1	-173.1(3)
Bi(1)-N(2)-N(4)-Bi(1)#1	4.8(3)
C(30)-C(29)-N(5)-N(7)	176.8(6)
P(2)-C(29)-N(5)-N(7)	0.4(7)
C(30)-C(29)-N(5)-Bi(2)#2	-8.0(10)
P(2)-C(29)-N(5)-Bi(2)#2	175.5(3)
C(22)-C(21)-N(6)-N(8)	177.7(5)
P(1)-C(21)-N(6)-N(8)	0.2(7)
C(22)-C(21)-N(6)-Bi(2)	-4.3(10)
P(1)-C(21)-N(6)-Bi(2)	178.2(3)
N(5)#2-Bi(2)-N(6)-C(21)	-103.9(6)
N(8)#2-Bi(2)-N(6)-C(21)	-178.2(5)
N(7)-Bi(2)-N(6)-C(21)	110.5(6)
Bi(2)#2-Bi(2)-N(6)-C(21)	-178.2(6)

N(5)#2-Bi(2)-N(6)-N(8)	74.2(4)
N(8)#2-Bi(2)-N(6)-N(8)	-0.1(6)
N(7)-Bi(2)-N(6)-N(8)	-71.4(4)
Bi(2)#2-Bi(2)-N(6)-N(8)	-0.1(3)
C(26)-C(28)-N(7)-N(5)	-179.0(5)
P(2)-C(28)-N(7)-N(5)	1.0(7)
C(26)-C(28)-N(7)-Bi(2)	2.0(10)
P(2)-C(28)-N(7)-Bi(2)	-178.0(4)
C(29)-N(5)-N(7)-C(28)	-0.9(7)
Bi(2)#2-N(5)-N(7)-C(28)	-177.3(4)
C(29)-N(5)-N(7)-Bi(2)	178.5(4)
Bi(2)#2-N(5)-N(7)-Bi(2)	2.0(4)
N(5)#2-Bi(2)-N(7)-C(28)	175.8(6)
N(6)-Bi(2)-N(7)-C(28)	-108.4(7)
N(8)#2-Bi(2)-N(7)-C(28)	104.8(7)
Bi(2)#2-Bi(2)-N(7)-C(28)	177.4(7)
N(5)#2-Bi(2)-N(7)-N(5)	-3.3(6)
N(6)-Bi(2)-N(7)-N(5)	72.6(3)
N(8)#2-Bi(2)-N(7)-N(5)	-74.2(3)
Bi(2)#2-Bi(2)-N(7)-N(5)	-1.7(3)
C(18)-C(20)-N(8)-N(6)	-178.9(6)
P(1)-C(20)-N(8)-N(6)	-1.1(7)
C(18)-C(20)-N(8)-Bi(2)#2	4.1(11)
P(1)-C(20)-N(8)-Bi(2)#2	-178.1(4)
C(21)-N(6)-N(8)-C(20)	0.6(7)
Bi(2)-N(6)-N(8)-C(20)	-178.0(4)
C(21)-N(6)-N(8)-Bi(2)#2	178.7(4)
Bi(2)-N(6)-N(8)-Bi(2)#2	0.1(4)
N(6)-C(21)-P(1)-C(20)	-0.6(5)
C(22)-C(21)-P(1)-C(20)	-177.8(6)
N(8)-C(20)-P(1)-C(21)	1.0(5)
C(18)-C(20)-P(1)-C(21)	178.6(7)
N(7)-C(28)-P(2)-C(29)	-0.7(5)
C(26)-C(28)-P(2)-C(29)	179.4(6)
N(5)-C(29)-P(2)-C(28)	0.1(5)
C(30)-C(29)-P(2)-C(28)	-175.9(6)
N(1)-C(4)-P(3)-C(5)	0.9(5)
C(2)-C(4)-P(3)-C(5)	-178.1(6)
N(3)-C(5)-P(3)-C(4)	-0.8(5)
C(6)-C(5)-P(3)-C(4)	-179.6(6)
N(2)-C(12)-P(4)-C(13)	-0.4(4)
C(10)-C(12)-P(4)-C(13)	177.2(5)
N(4)-C(13)-P(4)-C(12)	0.5(5)
C(14)-C(13)-P(4)-C(12)	-177.6(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z+1 #2 -x+1,-y+1,-z

3.3 Crystal structural analysis data for 6

Table 1. Crystal data and structure refinement for 6.

Identification code	141015-3a
Empirical formula	$C_{56}H_{40}Bi_2N_8P_4$
Formula weight	1366.80
Temperature	289.70(10) K
Wavelength	0.7107 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.4968(2) Å α = 90 deg.
	b = 20.3504(4) Å β = 97.027(2) deg.
	c = 13.5884(2) Å γ = 90 deg.
Volume	2606.42(8) Å^3
Z, Calculated density	2, 1.742 Mg/m^3
Absorption coefficient	6.911 mm^{-1}
F(000)	1316
Crystal size	0.4300 × 0.2300 × 0.2100 mm
Theta range for data collection	2.78 to 26.37 deg.
Limiting indices	-11<=h<=11, -25<=k<=25, -16<=l<=16

Reflections collected / unique	26600 / 5319 [R(int) = 0.0445]
Completeness to theta = 26.37	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.81939
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5319 / 0 / 316
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R_1 = 0.0296, wR_2 = 0.0415
R indices (all data)	R_1 = 0.0574, wR_2 = 0.0462
Largest diff. peak and hole	0.948 and -0.683 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **6**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Bi(1)	-357(1)	4947(1)	8939(1)	30(1)
C(1)	-796(5)	6362(2)	7328(3)	50(1)
C(2)	-1137(5)	6329(3)	6314(3)	65(2)
C(3)	-2447(5)	6536(3)	5878(3)	62(2)
C(4)	-3411(5)	6766(3)	6463(3)	58(1)
C(5)	-3096(5)	6796(2)	7477(3)	47(1)
C(6)	-1781(5)	6591(2)	7927(3)	35(1)
C(7)	-1453(4)	6598(2)	9022(3)	34(1)
C(8)	-983(4)	6684(2)	10793(3)	34(1)
C(9)	-770(5)	6811(2)	11863(3)	38(1)
C(10)	435(5)	6586(2)	12459(3)	44(1)
C(11)	621(6)	6703(2)	13468(3)	54(1)
C(12)	-367(6)	7050(3)	13901(4)	63(2)

C(13)	-1563(6)	7281(3)	13329(4)	62(2)
C(14)	-1753(5)	7158(2)	12313(3)	50(1)
C(15)	4428(5)	6462(3)	11878(4)	71(2)
C(16)	4724(6)	6598(4)	12880(5)	94(2)
C(17)	4614(6)	6113(5)	13557(5)	96(3)
C(18)	4211(5)	5488(4)	13265(4)	79(2)
C(19)	3926(4)	5350(3)	12259(3)	56(1)
C(20)	4020(4)	5839(3)	11554(3)	47(1)
C(21)	3619(4)	5700(2)	10489(3)	40(1)
C(22)	3070(4)	5530(2)	8735(3)	36(1)
C(23)	2827(4)	5452(2)	7653(3)	37(1)
C(24)	3126(5)	5955(2)	7022(3)	51(1)
C(25)	2827(5)	5894(3)	6005(4)	63(2)
C(26)	2205(5)	5332(3)	5591(4)	63(2)
C(27)	1915(5)	4823(3)	6205(3)	58(1)
C(28)	2230(5)	4880(2)	7215(3)	48(1)
N(1)	2142(3)	5238(2)	9263(2)	36(1)
N(2)	2450(3)	5338(2)	10248(2)	39(1)
N(3)	-740(3)	6082(2)	9435(2)	34(1)
N(4)	-474(3)	6131(2)	10440(2)	35(1)
P(1)	-1833(1)	7197(1)	9869(1)	47(1)
P(2)	4433(1)	5948(1)	9463(1)	51(1)

Table 3. Bond lengths [A] and angles [deg] for **6**.

Bi(1)-N(1)	2.433(3)
Bi(1)-N(3)	2.444(3)
Bi(1)-N(4)#1	2.447(3)
Bi(1)-N(2)#1	2.458(3)
Bi(1)-Bi(1)#1	2.8873(3)
C(1)-C(2)	1.379(6)
C(1)-C(6)	1.392(6)
C(1)-H(1)	0.9300
C(2)-C(3)	1.376(6)
C(2)-H(2)	0.9300
C(3)-C(4)	1.366(6)
C(3)-H(3)	0.9300
C(4)-C(5)	1.376(6)
C(4)-H(4)	0.9300
C(5)-C(6)	1.386(5)
C(5)-H(5)	0.9300

C(6)-C(7)	1.483(5)
C(7)-N(3)	1.336(5)
C(7)-P(1)	1.743(4)
C(8)-N(4)	1.336(5)
C(8)-C(9)	1.467(5)
C(8)-P(1)	1.751(4)
C(9)-C(14)	1.373(6)
C(9)-C(10)	1.396(5)
C(10)-C(11)	1.381(6)
C(10)-H(10)	0.9300
C(11)-C(12)	1.364(6)
C(11)-H(11)	0.9300
C(12)-C(13)	1.379(6)
C(12)-H(12)	0.9300
C(13)-C(14)	1.392(6)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-C(20)	1.383(7)
C(15)-C(16)	1.384(7)
C(15)-H(15)	0.9300
C(16)-C(17)	1.362(9)
C(16)-H(16)	0.9300
C(17)-C(18)	1.372(9)
C(17)-H(17)	0.9300
C(18)-C(19)	1.390(6)
C(18)-H(18)	0.9300
C(19)-C(20)	1.392(6)
C(19)-H(19)	0.9300
C(20)-C(21)	1.477(5)
C(21)-N(2)	1.339(5)
C(21)-P(2)	1.749(4)
C(22)-N(1)	1.341(5)
C(22)-C(23)	1.468(5)
C(22)-P(2)	1.751(4)
C(23)-C(24)	1.386(6)
C(23)-C(28)	1.396(6)
C(24)-C(25)	1.382(6)
C(24)-H(24)	0.9300
C(25)-C(26)	1.375(7)
C(25)-H(25)	0.9300
C(26)-C(27)	1.377(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.374(6)
C(27)-H(27)	0.9300

C(28)-H(28)	0.9300
N(1)-N(2)	1.351(4)
N(2)-Bi(1)#1	2.458(3)
N(3)-N(4)	1.362(4)
N(4)-Bi(1)#1	2.447(3)

N(1)-Bi(1)-N(3)	83.99(11)
N(1)-Bi(1)-N(4)#1	83.64(11)
N(3)-Bi(1)-N(4)#1	143.58(10)
N(1)-Bi(1)-N(2)#1	143.20(10)
N(3)-Bi(1)-N(2)#1	86.79(11)
N(4)#1-Bi(1)-N(2)#1	82.98(12)
N(1)-Bi(1)-Bi(1)#1	72.35(8)
N(3)-Bi(1)-Bi(1)#1	71.32(7)
N(4)#1-Bi(1)-Bi(1)#1	72.30(7)
N(2)#1-Bi(1)-Bi(1)#1	70.94(7)
C(2)-C(1)-C(6)	120.5(4)
C(2)-C(1)-H(1)	119.7
C(6)-C(1)-H(1)	119.7
C(3)-C(2)-C(1)	120.3(5)
C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	119.3(4)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	121.2(4)
C(3)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(4)-C(5)-C(6)	120.1(4)
C(4)-C(5)-H(5)	119.9
C(6)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	118.5(4)
C(5)-C(6)-C(7)	120.4(4)
C(1)-C(6)-C(7)	121.1(4)
N(3)-C(7)-C(6)	116.5(4)
N(3)-C(7)-P(1)	114.1(3)
C(6)-C(7)-P(1)	129.4(3)
N(4)-C(8)-C(9)	119.4(4)
N(4)-C(8)-P(1)	113.6(3)
C(9)-C(8)-P(1)	127.0(3)
C(14)-C(9)-C(10)	117.7(4)
C(14)-C(9)-C(8)	120.9(4)
C(10)-C(9)-C(8)	121.4(4)
C(11)-C(10)-C(9)	121.1(5)

C(11)-C(10)-H(10)	119.5
C(9)-C(10)-H(10)	119.5
C(12)-C(11)-C(10)	120.4(5)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.8(5)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
C(12)-C(13)-C(14)	119.7(5)
C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1
C(9)-C(14)-C(13)	121.4(5)
C(9)-C(14)-H(14)	119.3
C(13)-C(14)-H(14)	119.3
C(20)-C(15)-C(16)	120.8(6)
C(20)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(17)-C(16)-C(15)	119.8(7)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	121.2(6)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(17)-C(18)-C(19)	119.1(6)
C(17)-C(18)-H(18)	120.5
C(19)-C(18)-H(18)	120.5
C(18)-C(19)-C(20)	120.7(6)
C(18)-C(19)-H(19)	119.6
C(20)-C(19)-H(19)	119.6
C(15)-C(20)-C(19)	118.4(5)
C(15)-C(20)-C(21)	121.0(5)
C(19)-C(20)-C(21)	120.5(4)
N(2)-C(21)-C(20)	116.8(4)
N(2)-C(21)-P(2)	113.4(3)
C(20)-C(21)-P(2)	129.7(3)
N(1)-C(22)-C(23)	117.1(4)
N(1)-C(22)-P(2)	113.7(3)
C(23)-C(22)-P(2)	129.2(3)
C(24)-C(23)-C(28)	117.0(4)
C(24)-C(23)-C(22)	121.4(4)
C(28)-C(23)-C(22)	121.5(4)
C(25)-C(24)-C(23)	121.3(4)
C(25)-C(24)-H(24)	119.3
C(23)-C(24)-H(24)	119.3

C(26)-C(25)-C(24)	120.6(5)
C(26)-C(25)-H(25)	119.7
C(24)-C(25)-H(25)	119.7
C(25)-C(26)-C(27)	119.0(5)
C(25)-C(26)-H(26)	120.5
C(27)-C(26)-H(26)	120.5
C(28)-C(27)-C(26)	120.4(5)
C(28)-C(27)-H(27)	119.8
C(26)-C(27)-H(27)	119.8
C(27)-C(28)-C(23)	121.6(4)
C(27)-C(28)-H(28)	119.2
C(23)-C(28)-H(28)	119.2
C(22)-N(1)-N(2)	112.8(3)
C(22)-N(1)-Bi(1)	134.5(3)
N(2)-N(1)-Bi(1)	107.7(2)
C(21)-N(2)-N(1)	113.4(3)
C(21)-N(2)-Bi(1)#1	135.4(3)
N(1)-N(2)-Bi(1)#1	108.7(2)
C(7)-N(3)-N(4)	112.6(3)
C(7)-N(3)-Bi(1)	135.4(3)
N(4)-N(3)-Bi(1)	109.3(2)
C(8)-N(4)-N(3)	113.0(3)
C(8)-N(4)-Bi(1)#1	138.4(3)
N(3)-N(4)-Bi(1)#1	107.0(2)
C(7)-P(1)-C(8)	86.68(19)
C(21)-P(2)-C(22)	86.7(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+2

Table 4. Anisotropic displacement parameters (Aˆ2 x 10ˆ3) for **6**.
The anisotropic displacement factor exponent takes the form:
-2 piˆ2 [hˆ2 a*ˆ2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Bi(1)	37(1)	34(1)	19(1)	0(1)	1(1)	1(1)
C(1)	43(3)	65(4)	42(3)	12(3)	3(2)	17(3)
C(2)	69(4)	92(4)	38(3)	10(3)	21(3)	25(3)
C(3)	65(4)	92(4)	28(3)	2(3)	2(3)	15(3)

C(4)	52(3)	83(4)	37(3)	-5(3)	-7(2)	16(3)
C(5)	47(3)	56(3)	38(3)	-5(2)	0(2)	17(2)
C(6)	46(3)	26(2)	32(2)	3(2)	0(2)	3(2)
C(7)	36(3)	32(2)	32(2)	4(2)	-1(2)	5(2)
C(8)	42(3)	29(2)	30(2)	-2(2)	3(2)	-3(2)
C(9)	49(3)	26(2)	37(2)	-2(2)	-1(2)	-8(2)
C(10)	52(3)	38(3)	39(3)	-7(2)	-8(2)	-3(2)
C(11)	73(4)	45(3)	38(3)	2(2)	-15(3)	-14(3)
C(12)	84(4)	75(4)	28(2)	-10(3)	7(3)	-36(4)
C(13)	66(4)	80(4)	46(3)	-14(3)	26(3)	-11(3)
C(14)	51(3)	56(3)	43(3)	-8(2)	3(2)	0(3)
C(15)	55(4)	93(5)	68(4)	-29(3)	12(3)	-26(3)
C(16)	59(4)	142(7)	82(5)	-66(5)	9(4)	-28(4)
C(17)	48(4)	191(9)	48(4)	-44(5)	-1(3)	-3(5)
C(18)	46(4)	148(7)	40(3)	1(4)	-2(3)	12(4)
C(19)	33(3)	92(4)	42(3)	-6(3)	0(2)	11(3)
C(20)	29(3)	71(4)	42(3)	-15(3)	5(2)	-8(2)
C(21)	35(3)	45(3)	37(3)	-1(2)	-1(2)	-1(2)
C(22)	34(3)	40(3)	35(2)	2(2)	10(2)	0(2)
C(23)	31(3)	44(3)	37(3)	3(2)	16(2)	1(2)
C(24)	57(3)	51(3)	45(3)	-2(2)	14(2)	-13(3)
C(25)	70(4)	73(4)	47(3)	17(3)	16(3)	-8(3)
C(26)	65(4)	86(4)	37(3)	-1(3)	4(3)	-6(3)
C(27)	66(3)	62(4)	47(3)	-14(3)	14(3)	-8(3)
C(28)	52(3)	48(3)	46(3)	2(2)	19(2)	3(2)
N(1)	38(2)	44(2)	26(2)	1(2)	2(2)	-6(2)
N(2)	39(2)	51(2)	26(2)	0(2)	5(2)	-4(2)
N(3)	44(2)	31(2)	25(2)	-3(2)	-2(2)	4(2)
N(4)	46(2)	33(2)	24(2)	-1(2)	-1(2)	3(2)
P(1)	67(1)	37(1)	35(1)	-3(1)	-6(1)	16(1)
P(2)	45(1)	65(1)	45(1)	-4(1)	10(1)	-18(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **6**.

	x	y	z	U(eq)
H(1)	98	6230	7616	60
H(2)	-479	6167	5922	78

H(3)	-2673	6519	5193	74
H(4)	-4297	6905	6169	70
H(5)	-3767	6955	7862	57
H(10)	1123	6354	12173	53
H(11)	1426	6545	13854	64
H(12)	-234	7130	14580	75
H(13)	-2241	7518	13620	75
H(14)	-2563	7315	11931	60
H(15)	4505	6794	11417	86
H(16)	4997	7019	13090	113
H(17)	4816	6207	14229	115
H(18)	4129	5162	13735	95
H(19)	3669	4926	12055	67
H(24)	3536	6341	7288	61
H(25)	3048	6236	5596	75
H(26)	1983	5296	4908	76
H(27)	1503	4439	5933	69
H(28)	2042	4529	7617	57

Table 6. Torsion angles [deg] for **6**.

C(6)-C(1)-C(2)-C(3)	1.3(8)
C(1)-C(2)-C(3)-C(4)	-0.8(9)
C(2)-C(3)-C(4)-C(5)	0.1(9)
C(3)-C(4)-C(5)-C(6)	0.0(8)
C(4)-C(5)-C(6)-C(1)	0.5(7)
C(4)-C(5)-C(6)-C(7)	-177.6(4)
C(2)-C(1)-C(6)-C(5)	-1.2(7)
C(2)-C(1)-C(6)-C(7)	177.0(4)
C(5)-C(6)-C(7)-N(3)	138.6(4)
C(1)-C(6)-C(7)-N(3)	-39.5(6)
C(5)-C(6)-C(7)-P(1)	-42.8(6)
C(1)-C(6)-C(7)-P(1)	139.1(4)
N(4)-C(8)-C(9)-C(14)	-148.4(4)
P(1)-C(8)-C(9)-C(14)	32.9(6)
N(4)-C(8)-C(9)-C(10)	31.8(6)
P(1)-C(8)-C(9)-C(10)	-146.8(4)
C(14)-C(9)-C(10)-C(11)	0.7(7)
C(8)-C(9)-C(10)-C(11)	-179.5(4)
C(9)-C(10)-C(11)-C(12)	-0.8(7)
C(10)-C(11)-C(12)-C(13)	0.4(7)

C(11)-C(12)-C(13)-C(14)	0.0(8)
C(10)-C(9)-C(14)-C(13)	-0.3(7)
C(8)-C(9)-C(14)-C(13)	179.9(4)
C(12)-C(13)-C(14)-C(9)	-0.1(8)
C(20)-C(15)-C(16)-C(17)	0.0(9)
C(15)-C(16)-C(17)-C(18)	-0.1(10)
C(16)-C(17)-C(18)-C(19)	0.7(9)
C(17)-C(18)-C(19)-C(20)	-1.2(8)
C(16)-C(15)-C(20)-C(19)	-0.5(7)
C(16)-C(15)-C(20)-C(21)	176.2(5)
C(18)-C(19)-C(20)-C(15)	1.1(7)
C(18)-C(19)-C(20)-C(21)	-175.7(4)
C(15)-C(20)-C(21)-N(2)	-135.1(5)
C(19)-C(20)-C(21)-N(2)	41.6(6)
C(15)-C(20)-C(21)-P(2)	44.0(7)
C(19)-C(20)-C(21)-P(2)	-139.3(4)
N(1)-C(22)-C(23)-C(24)	144.4(4)
P(2)-C(22)-C(23)-C(24)	-36.4(6)
N(1)-C(22)-C(23)-C(28)	-32.8(6)
P(2)-C(22)-C(23)-C(28)	146.3(4)
C(28)-C(23)-C(24)-C(25)	0.9(7)
C(22)-C(23)-C(24)-C(25)	-176.5(4)
C(23)-C(24)-C(25)-C(26)	0.8(8)
C(24)-C(25)-C(26)-C(27)	-1.6(8)
C(25)-C(26)-C(27)-C(28)	0.7(8)
C(26)-C(27)-C(28)-C(23)	1.0(7)
C(24)-C(23)-C(28)-C(27)	-1.8(6)
C(22)-C(23)-C(28)-C(27)	175.6(4)
C(23)-C(22)-N(1)-N(2)	-179.8(3)
P(2)-C(22)-N(1)-N(2)	0.9(5)
C(23)-C(22)-N(1)-Bi(1)	-28.8(6)
P(2)-C(22)-N(1)-Bi(1)	151.9(2)
N(3)-Bi(1)-N(1)-C(22)	-84.5(4)
N(4)#1-Bi(1)-N(1)-C(22)	129.8(4)
N(2)#1-Bi(1)-N(1)-C(22)	-161.0(3)
Bi(1)#1-Bi(1)-N(1)-C(22)	-156.8(4)
N(3)-Bi(1)-N(1)-N(2)	67.5(3)
N(4)#1-Bi(1)-N(1)-N(2)	-78.2(3)
N(2)#1-Bi(1)-N(1)-N(2)	-8.9(4)
Bi(1)#1-Bi(1)-N(1)-N(2)	-4.7(2)
C(20)-C(21)-N(2)-N(1)	179.3(4)
P(2)-C(21)-N(2)-N(1)	0.1(5)
C(20)-C(21)-N(2)-Bi(1)#1	19.8(6)
P(2)-C(21)-N(2)-Bi(1)#1	-159.5(2)

C(22)-N(1)-N(2)-C(21)	-0.6(5)
Bi(1)-N(1)-N(2)-C(21)	-159.4(3)
C(22)-N(1)-N(2)-Bi(1)#1	164.4(3)
Bi(1)-N(1)-N(2)-Bi(1)#1	5.6(3)
C(6)-C(7)-N(3)-N(4)	179.5(3)
P(1)-C(7)-N(3)-N(4)	0.7(5)
C(6)-C(7)-N(3)-Bi(1)	-21.6(6)
P(1)-C(7)-N(3)-Bi(1)	159.6(2)
N(1)-Bi(1)-N(3)-C(7)	124.2(4)
N(4)#1-Bi(1)-N(3)-C(7)	-165.1(3)
N(2)#1-Bi(1)-N(3)-C(7)	-91.5(4)
Bi(1)#1-Bi(1)-N(3)-C(7)	-162.4(4)
N(1)-Bi(1)-N(3)-N(4)	-76.4(2)
N(4)#1-Bi(1)-N(3)-N(4)	-5.7(4)
N(2)#1-Bi(1)-N(3)-N(4)	68.0(2)
Bi(1)#1-Bi(1)-N(3)-N(4)	-3.0(2)
C(9)-C(8)-N(4)-N(3)	-179.5(3)
P(1)-C(8)-N(4)-N(3)	-0.7(5)
C(9)-C(8)-N(4)-Bi(1)#1	17.9(6)
P(1)-C(8)-N(4)-Bi(1)#1	-163.3(2)
C(7)-N(3)-N(4)-C(8)	0.0(5)
Bi(1)-N(3)-N(4)-C(8)	-164.5(3)
C(7)-N(3)-N(4)-Bi(1)#1	168.0(3)
Bi(1)-N(3)-N(4)-Bi(1)#1	3.5(3)
N(3)-C(7)-P(1)-C(8)	-0.9(3)
C(6)-C(7)-P(1)-C(8)	-179.5(4)
N(4)-C(8)-P(1)-C(7)	0.8(3)
C(9)-C(8)-P(1)-C(7)	179.6(4)
N(2)-C(21)-P(2)-C(22)	0.3(4)
C(20)-C(21)-P(2)-C(22)	-178.8(4)
N(1)-C(22)-P(2)-C(21)	-0.7(3)
C(23)-C(22)-P(2)-C(21)	-179.9(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z+2

4. Theoretically computed data of **4**, **5**, and **6**

Cartesian Coordinates of the Optimized Geometries of Compound **4**, **5**, and **6** by theB3LYP method in combination of 6-31G(d) basis set for C, N, P and H atoms, and L-anl2dz basis set and psuedopotential for Bi atoms. All calculations were performed using Gaussian 09 package.[3]

Compound **4**:

Bi	-0.00043600	0.00010300	-1.39825500
Bi	-0.00025700	-0.00014300	1.39551900
P	-3.31974100	-3.56650100	0.00122100
P	3.56656700	-3.31900400	0.00266900
P	-3.56624900	3.31997000	0.00078600
P	3.32016200	3.56537300	0.00291400
N	-1.78721800	-1.56461100	-0.64324200
N	-1.42954500	-1.89646000	0.64087800
N	1.89585800	-1.42920300	0.64167900
N	1.56463100	-1.78686400	-0.64260300
N	-1.56437200	1.78731100	-0.64330700
N	-1.89669600	1.42941000	0.64062200
N	1.42917000	1.89584500	0.64133700
N	1.78741900	1.56396600	-0.64262900
C	-2.77754000	-2.32306600	-1.13366200
C	-2.11578900	-2.93691700	1.13369200
C	-1.78024400	-3.55844900	2.49327800
C	-1.75383400	-2.51238900	3.62756500
C	-2.83222900	-4.62431100	2.86625200
C	-0.39945600	-4.24867300	2.38372700
C	-3.42259300	-2.03449500	-2.49306300
C	-4.41652600	-3.15658000	-2.86034400
C	-2.38237500	-1.94246100	-3.62923800
C	-4.20332200	-0.70255600	-2.38703700
C	2.93645300	-2.11505600	1.13483700
C	2.32345700	-2.77701500	-1.13269100
C	2.03551600	-3.42207500	-2.49221900
C	3.15742400	-4.41650100	-2.85870100
C	1.94473000	-2.38182100	-3.62845900
C	0.70317100	-4.20222100	-2.38706200
C	3.55811100	-1.77901500	2.49424700
C	4.62199000	-2.83247300	2.86877700

C	4.25088100	-0.39961800	2.38302900
C	2.51197300	-1.74916300	3.62834200
C	-2.32240000	2.77797100	-1.13373800
C	-2.93734700	2.11553700	1.13315000
C	-3.55985500	1.77922900	2.49211300
C	-4.25021500	0.39861900	2.38111900
C	-2.51466100	1.75180400	3.62716000
C	-4.62581100	2.83114200	2.86502100
C	-2.03320000	3.42335100	-2.49285900
C	-3.15480500	4.41784400	-2.86008900
C	-1.94129900	2.38348000	-3.62936800
C	-0.70099300	4.20355100	-2.38628200
C	2.11519000	2.93630100	1.13452900
C	2.77839800	2.32198600	-1.13231600
C	3.42505100	2.03299300	-2.49087700
C	4.41523000	3.15787500	-2.85982300
C	4.21039900	0.70397500	-2.38154900
C	2.38610000	1.93466400	-3.62761300
C	1.77829600	3.55862800	2.49343900
C	2.83009900	4.62448500	2.86696400
C	1.75034600	2.51333000	3.62838100
C	0.39779700	4.24911400	2.38191300
H	-0.96559000	-1.76557800	3.49032000
H	-1.55938900	-3.00837400	4.58585900
H	-2.71117600	-1.98686500	3.70694500
H	-2.57118500	-5.08006100	3.82855100
H	-2.87977300	-5.42471700	2.12042200
H	-3.83280200	-4.18765800	2.95862000
H	0.38133900	-3.54052000	2.09201800
H	-0.42299100	-5.04391700	1.63078600
H	-0.12030600	-4.69810000	3.34519200
H	-3.91434800	-4.12618800	-2.95012300
H	-4.89032200	-2.92988100	-3.82265200
H	-5.21075300	-3.25483700	-2.11285600
H	-1.68858500	-1.10679800	-3.49465500
H	-2.89143100	-1.78328800	-4.58716700
H	-1.79546000	-2.86353100	-3.70702300
H	-4.99323900	-0.77578700	-1.63168300
H	-4.67301400	-0.45820200	-3.34829900
H	-3.54818600	0.12501700	-2.10064200
H	4.12728400	-3.91472400	-2.94800700
H	2.93108900	-4.89036100	-3.82106300
H	3.25494200	-5.21064700	-2.11102800
H	1.10913300	-1.68782100	-3.49456300

H	1.78625600	-2.89079000	-4.58655000
H	2.86603200	-1.79515100	-3.70541200
H	0.77560400	-4.99224000	-1.63173600
H	0.45917200	-4.67171700	-3.34851100
H	-0.12427400	-3.54674100	-2.10108000
H	4.18348400	-3.83213000	2.96226600
H	5.07798800	-2.57105900	3.83085900
H	5.42250100	-2.88240800	2.12322100
H	5.04632500	-0.42563200	1.63038300
H	4.70048200	-0.11993800	3.34426000
H	3.54419900	0.38202100	2.09000300
H	1.76689700	-0.95945400	3.49015500
H	3.00826900	-1.55466300	4.58645800
H	1.98442900	-2.70530000	3.70878700
H	-5.04482000	0.42276200	1.62752100
H	-4.70049500	0.11893600	3.34202900
H	-3.54192300	-0.38210400	2.08952900
H	-3.01141300	1.55675500	4.58493200
H	-1.98900900	2.70898000	3.70764000
H	-1.76792600	0.96349600	3.48989800
H	-5.42565300	2.87933400	2.11862800
H	-4.18904800	3.83157500	2.95839300
H	-5.08232600	2.56952500	3.82680200
H	-4.12458400	3.91607500	-2.95028900
H	-2.92767000	4.89188300	-3.82217500
H	-3.25294100	5.21184800	-2.11234800
H	-1.10593800	1.68931800	-3.49483100
H	-1.78170300	2.89280100	-4.58708800
H	-2.86257900	1.79695400	-3.70757600
H	-0.77412800	4.99332900	-1.63077300
H	-0.45619800	4.67337200	-3.34737000
H	0.12626500	3.54805700	-2.09978600
H	3.90958700	4.12545300	-2.95201000
H	4.89058700	2.93082600	-3.82128000
H	5.20856200	3.26063300	-2.11199200
H	4.68161000	0.45929700	-3.34199300
H	3.55784200	-0.12525600	-2.09397100
H	4.99954600	0.78148400	-1.62581700
H	1.79495800	2.85287800	-3.70716100
H	1.69629000	1.09582500	-3.49249700
H	2.89663800	1.77657000	-4.58492700
H	3.83046900	4.18766400	2.96072500
H	2.56807000	5.08086100	3.82869800
H	2.87866700	5.42443700	2.12071500

H	2.70749300	1.98769800	3.70927700
H	0.96211600	1.76658300	3.49071800
H	1.55483900	3.01000000	4.58610100
H	0.11761800	4.69910700	3.34281300
H	-0.38281300	3.54097900	2.08966400
H	0.42240600	5.04395200	1.62857900

Compound **5**:

Bi	-0.000283000	-0.000200000	-1.430550000
Bi	0.000306000	0.000189000	1.430400000
P	-3.305306000	3.550147000	0.000386000
P	-3.550241000	-3.305179000	0.001432000
P	3.550119000	3.305348000	-0.001417000
P	3.305328000	-3.550107000	-0.000410000
N	-1.554953000	1.744040000	-0.680229000
N	-1.629802000	1.674144000	0.680219000
N	-1.673661000	-1.630083000	0.680688000
N	-1.744465000	-1.554681000	-0.679694000
N	1.744015000	1.554612000	-0.681008000
N	1.674199000	1.630142000	0.679409000
N	1.630493000	-1.673650000	0.679842000
N	1.554301000	-1.744467000	-0.680497000
C	-2.357305000	2.670297000	-1.210460000
C	-2.495485000	2.541242000	1.210762000
C	-2.720407000	2.547384000	2.708273000
C	-2.606492000	3.961575000	3.304004000
C	-4.075973000	1.905398000	3.066347000
C	-2.346668000	2.896278000	-2.707860000
C	-3.765430000	2.891457000	-3.303464000
C	-1.603043000	4.199190000	-3.064655000
C	-2.540513000	-2.495874000	1.211461000
C	-2.671189000	-2.356705000	-1.209622000
C	-2.898205000	-2.345465000	-2.706866000
C	-2.893116000	-3.763955000	-3.303128000
C	-4.201705000	-1.602291000	-3.062457000
C	-2.545667000	-2.721417000	2.708881000
C	-3.959417000	-2.607426000	3.305658000
C	-1.903750000	-4.077278000	3.065932000
C	2.670384000	2.356542000	-1.211703000
C	2.541385000	2.496031000	1.209448000
C	2.547514000	2.721819000	2.706828000
C	1.905309000	4.077490000	3.064104000
C	3.961725000	2.608482000	3.302624000

C	2.896373000	2.345069000	-2.709097000
C	2.891101000	3.763485000	-3.305527000
C	4.199520000	1.601652000	-3.065485000
C	2.496631000	-2.540462000	1.210104000
C	2.356062000	-2.671152000	-1.210900000
C	2.343953000	-2.898172000	-2.708133000
C	3.762092000	-2.892994000	-3.305224000
C	1.600653000	-4.201718000	-3.063292000
C	2.723066000	-2.545613000	2.707394000
C	2.609205000	-3.959333000	3.304259000
C	4.079236000	-1.903893000	3.063651000
H	-2.736000000	3.930476000	4.392189000
H	-3.377148000	4.623099000	2.891848000
H	-1.630835000	4.409211000	3.086432000
H	-4.153711000	0.891737000	2.658464000
H	-4.903953000	2.495019000	2.656991000
H	-4.200916000	1.851075000	4.154439000
H	-4.286340000	1.952645000	-3.086948000
H	-3.724702000	3.019496000	-4.391472000
H	-4.365933000	3.710025000	-2.890247000
H	-2.127696000	5.069348000	-2.654396000
H	-1.539333000	4.320694000	-4.152656000
H	-0.586415000	4.198775000	-2.656730000
H	-1.953906000	-4.284516000	-3.087510000
H	-3.021931000	-3.722782000	-4.391029000
H	-3.711108000	-4.365038000	-2.889615000
H	-5.071350000	-2.127562000	-2.651902000
H	-4.323940000	-1.538102000	-4.150347000
H	-4.201508000	-0.585863000	-2.654030000
H	-4.406962000	-1.631555000	3.088863000
H	-3.927590000	-2.737454000	4.393760000
H	-4.621419000	-3.377722000	2.893601000
H	-2.493917000	-4.904960000	2.656759000
H	-1.848572000	-4.202627000	4.153935000
H	-0.890446000	-4.155119000	2.657191000
H	2.494838000	4.905329000	2.654327000
H	1.850887000	4.203033000	4.152122000
H	0.891664000	4.154847000	2.656107000
H	4.623133000	3.378982000	2.889992000
H	4.409504000	1.632757000	3.085657000
H	3.930611000	2.738661000	4.390729000
H	1.952133000	4.284229000	-3.089303000
H	3.019141000	3.722157000	-4.393513000
H	3.709486000	4.364484000	-2.892668000

H	5.069515000	2.126821000	-2.655544000
H	4.321029000	1.537356000	-4.153451000
H	4.199443000	0.585260000	-2.656975000
H	4.282718000	-1.953749000	-3.089917000
H	3.720288000	-3.021821000	-4.393099000
H	4.363469000	-3.710944000	-2.892055000
H	1.535843000	-4.323953000	-4.151146000
H	0.584464000	-4.201581000	-2.654278000
H	2.126213000	-5.071334000	-2.653045000
H	1.633128000	-4.406714000	3.088074000
H	2.739910000	-3.927509000	4.392281000
H	3.379135000	-4.621469000	2.891735000
H	4.205227000	-1.848703000	4.151579000
H	4.156989000	-0.890608000	2.654839000
H	4.906596000	-2.494192000	2.654016000
H	-1.925101000	-1.930044000	3.156117000
H	-1.928699000	1.927324000	3.155618000
H	1.927571000	1.930277000	3.154624000
H	1.932053000	-1.924911000	3.155073000
H	-2.062515000	-1.787094000	-3.155479000
H	1.785266000	-2.062520000	-3.156427000
H	2.060287000	1.786784000	-3.157085000
H	-1.788896000	2.060023000	-3.156170000

Compound **6**:

Bi	-1.434350000	0.000903000	-0.001179000
C	-3.472658000	3.076677000	0.751111000
C	-4.860149000	3.218510000	0.742168000
C	-5.478792000	4.009950000	-0.228621000
C	-4.699606000	4.663552000	-1.187269000
C	-3.312448000	4.518393000	-1.184369000
C	-2.679526000	3.715326000	-0.219767000
C	-1.211993000	3.552781000	-0.222301000
C	1.212109000	3.551766000	-0.219078000
C	2.679723000	3.713670000	-0.212159000
C	3.469937000	3.074172000	0.760615000
C	4.857397000	3.216259000	0.756312000
C	5.479029000	4.008758000	-0.211706000
C	4.702814000	4.662946000	-1.172323000
C	3.315675000	4.517607000	-1.173998000
N	-0.679172000	2.346226000	0.022022000
N	0.677438000	2.345610000	0.023674000
P	0.001004000	4.820001000	-0.470176000
H	-2.997154000	2.498063000	1.537262000

H	-5.451624000	2.717846000	1.503695000
H	-6.559301000	4.125885000	-0.232160000
H	-5.172500000	5.285623000	-1.942477000
H	-2.711274000	5.015161000	-1.940624000
H	2.992077000	2.494758000	1.544753000
H	5.446549000	2.715140000	1.519337000
H	6.559530000	4.124925000	-0.211581000
H	5.178013000	5.285640000	-1.925546000
H	2.716943000	5.014734000	-1.931971000
C	3.314694000	1.178821000	4.514324000
C	4.701854000	1.180366000	4.659201000
C	5.480094000	0.221376000	4.004973000
C	4.860456000	-0.748316000	3.213001000
C	3.472935000	-0.755845000	3.071316000
C	2.680726000	0.215226000	3.710862000
C	1.213159000	0.218948000	3.549042000
C	-1.210908000	0.220110000	3.549867000
C	-2.678360000	0.216856000	3.712966000
C	-3.311512000	1.180540000	4.516949000
C	-4.698534000	1.182234000	4.663108000
C	-5.477472000	0.223229000	4.009732000
C	-4.858628000	-0.746663000	3.217358000
C	-3.471244000	-0.754354000	3.074448000
N	-0.677810000	-0.022699000	2.343170000
N	0.678823000	-0.024404000	2.342821000
P	0.001692000	0.467442000	4.817487000
H	2.714312000	1.935431000	5.011539000
H	5.175549000	1.934752000	5.281640000
H	6.560641000	0.223955000	4.120718000
H	5.451112000	-1.510030000	2.711687000
H	2.996691000	-1.541130000	2.492155000
H	-2.710637000	1.937188000	5.013495000
H	-5.171552000	1.936780000	5.285869000
H	-6.557901000	0.225898000	4.126449000
H	-5.449822000	-1.508636000	2.717033000
H	-2.995600000	-1.540020000	2.495262000
Bi	1.434212000	0.001238000	-0.000973000
C	3.470943000	-3.075272000	-0.756676000
C	4.858224000	-3.219202000	-0.752183000
C	5.478628000	-4.012864000	0.215650000
C	4.701301000	-4.666356000	1.175906000
C	3.314409000	-4.519033000	1.177454000
C	2.679619000	-3.713918000	0.215747000
C	1.212360000	-3.550153000	0.222225000

C	-1.211732000	-3.549185000	0.224647000
C	-2.679298000	-3.711452000	0.221951000
C	-3.472272000	-3.073790000	-0.749799000
C	-4.859647000	-3.216450000	-0.741681000
C	-5.478480000	-4.007681000	0.229183000
C	-4.699515000	-4.660082000	1.188781000
C	-3.312461000	-4.514171000	1.186640000
N	0.678813000	-2.343944000	-0.022667000
N	-0.677745000	-2.343521000	-0.021555000
P	0.000010000	-4.816897000	0.475421000
H	2.994041000	-2.495335000	-1.540966000
H	5.448075000	-2.718498000	-1.514949000
H	6.558949000	-4.130578000	0.215708000
H	5.175503000	-5.290126000	1.928896000
H	2.714923000	-5.015503000	1.935252000
H	-2.996599000	-2.495709000	-1.536266000
H	-5.450970000	-2.716877000	-1.504044000
H	-6.558914000	-4.124416000	0.231885000
H	-5.172497000	-5.281725000	1.944260000
H	-2.711588000	-5.009733000	1.943955000
C	-3.315580000	-1.186335000	-4.512452000
C	-4.702904000	-1.188480000	-4.655804000
C	-5.480627000	-0.227981000	-4.003178000
C	-4.860305000	0.743893000	-3.214388000
C	-3.472632000	0.752030000	-3.074283000
C	-2.680960000	-0.220675000	-3.712088000
C	-1.213237000	-0.223535000	-3.551191000
C	1.210765000	-0.222063000	-3.552375000
C	2.678248000	-0.217126000	-3.715254000
C	3.312901000	-1.180357000	-4.518550000
C	4.699984000	-1.180262000	-4.664316000
C	5.477432000	-0.219924000	-4.011128000
C	4.857097000	0.749464000	-3.219281000
C	3.469685000	0.755378000	-3.076837000
N	0.677625000	0.021156000	-2.345729000
N	-0.678940000	0.020129000	-2.344981000
P	-0.001769000	-0.471215000	-4.819659000
H	-2.715536000	-1.943972000	-5.008513000
H	-5.177131000	-1.944507000	-5.275842000
H	-6.561297000	-0.231085000	-4.117761000
H	-5.450557000	1.506821000	-2.714403000
H	-2.995791000	1.538904000	-2.497683000
H	2.713170000	-1.938090000	-5.014824000
H	5.174193000	-1.934446000	-5.286615000

H	6.557911000	-0.221248000	-4.127414000
H	5.447193000	1.512269000	-2.718950000
H	2.992740000	1.540518000	-2.497943000

Comparison of selected bond distances (Å), bond angles (°) and torsion angles (°) of **4**

	Experimental value	Calculated value		Experimental value	Calculated value
Bi(1)-Bi(2)	2.7964(4)	2.79377	Bi(1)-Bi(2)-N(2)-N(1)	-26.2(4)	-21.410
Bi(1)-N(1)	2.472(7)	2.49260	Bi(1)-Bi(2)-N(3)-N(4)	-22.8(4)	-21.367
Bi(1)-N(4)	2.483(6)	2.49273	Bi(1)-Bi(2)-N(6)-N(5)	-24.3(4)	-21.382
Bi(1)-N(5)	2.480(6)	2.49218	Bi(1)-Bi(2)-N(7)-N(8)	-27.1(4)	-21.410
Bi(1)-N(8)	2.500(6)	2.49198	Bi-Bi-N-$N_{(avg)}$	-25.0(7)	-21.397
Bi(2)-N(2)	2.499(7)	2.49135	N(1)-N(2)	1.374(8)	1.37368
Bi(2)-N(3)	2.454(6)	2.49198	N(3)-N(4)	1.368(8)	1.37369
Bi(2)-N(6)	2.475(5)	2.49166	N(5)-N(6)	1.352(8)	1.37369
Bi(2)-N(7)	2.492(7)	2.49113	N(7)-N(8)	1.377(8)	1.37370
Bi-$N_{(avg)}$	2.481(8)	2.492	N-$N_{(avg)}$	1.367(8)	1.37369
N(1)-Bi(1)-N(5)	83.4(2)	84.741	P(1)-C(2)	1.746(8)	1.76874
N(1)-Bi(1)-N(4)	85.2(2)	84.742	P(1)-C(1)	1.753(8)	1.76863
N(4)-Bi(1)-N(8)	82.3(2)	84.694	P(2)-C(12)	1.748(7)	1.76872
N(5)-Bi(1)-N(8)	86.5(2)	84.753	P(2)-C(11)	1.753(8)	1.76864
N(6)-Bi(2)-N(2)	84.5(2)	84.743	P(3)-C(21)	1.743(8)	1.76871
N(3)-Bi(2)-N(2)	83.8(2)	84.739	P(3)-C(22)	1.756(7)	1.76865
N(3)-Bi(2)-N(7)	84.6(2)	84.734	P(4)-C(32)	1.743(8)	1.76868
N(6)-Bi(2)-N(7)	84.8(2)	84.736	P(4)-C(31)	1.765(8)	1.76869
N-Bi-$N_{(avg)}$	84.3(8)	84.735	P-$C_{(avg)}$	1.750(8)	1.76868
Bi(2)-Bi(1)-N(8)-N(7)	-26.8(4)	-21.423	C(2)-P(1)-C(1)	87.2(4)	87.245
Bi(2)-Bi(1)-N(1)-N(2)	-26.7(4)	-21.414	C(12)-P(2)-C(11)	87.3(4)	87.244
Bi(2)-Bi(1)-N(4)-N(3)	-22.7(4)	-21.379	C(21)-P(3)-C(22)	87.0(4)	87.245
Bi(2)-Bi(1)-N(5)-N(6)	-24.0(4)	-21.388	C(32)-P(4)-C(31)	86.7(4)	87.244

5. References

[1] J.-W. Wang, L.-Y. Ding, B.-Q. Wang, Y.-Y. He, Y. Guo, X.-F. Jia, W. Zheng, *J. Mol. Struct.* **2014**, *1058,* 62–70;

[2] W. Zheng, G.-Z. Zhang, K.-N. Fan, *Organometallics* **2006**, *25*, 1548–1550;

[3] M. J. Frisch, et. al, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford CT, 2010.