Electronic Supplementary Information

Paddlewheel 1,2,4-Diazaphospholide Distibines with the Shortest Antimony-Antimony Single Bonds

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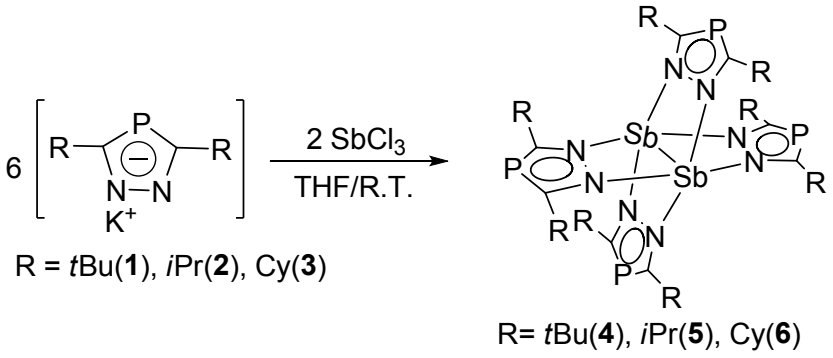
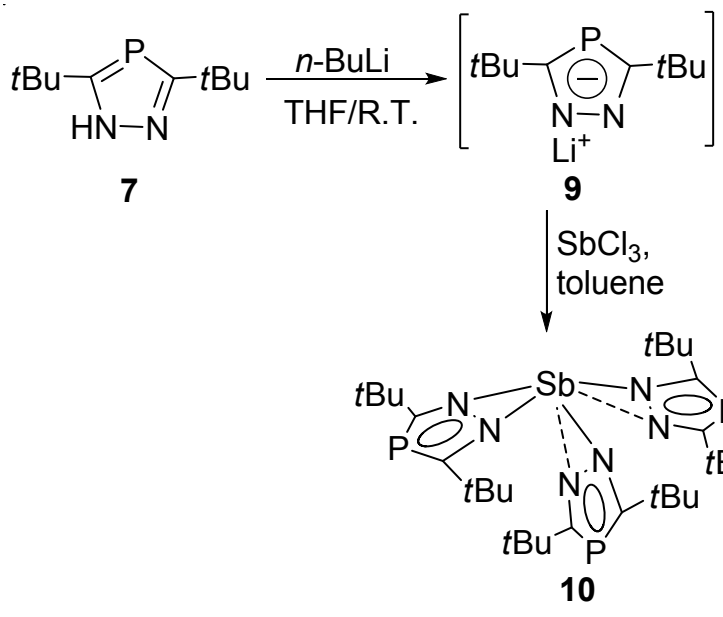
All manipulations were carried out in a nitrogen atmosphere under anaerobic conditions using standard Schlenk, vacuum line and glove box techniques. The solvents were thoroughly dried, deoxygenated and distilled in a nitrogen atmosphere prior to use. THF-d_8 and C_6D_6 were dried with metallic potassium before the use. DMSO-d_6 was dried over 4Å molecular sieve before the use. $CDCl_3$ was dried with CaH_2 before the use. The ^1H NMR, $^{13}C\{^1H\}$ NMR and $^{31}P\{^1H\}$ NMR spectra were recorded with a BrukerDRX-600 spectrometer. IR measurements were carried out on a NICOLET 360 FT-IR spectrometer from Nujol mulls prepared in a dry box. Melting points were measured in sealed argon-filled capillaries without temperature correction with an apparatus XT4-100A (Electronic and Optical Instruments, Beijing). $SbCl_3$ were purchased from Aldrich. K[3,5-tBu_2dp] and K[3,5-iPr_2dp] were prepared according to the literatures.





1. Synthetic Procedures, Spectral Data, and Analytical Data for **H[3,5-Cy_2dp]**, **3**, **4**, **5**, **6**, **9** and **10**

Preparation of 1*H*-3,5-di-cyclohexyl-1,2,4-diazaphospholeH[3,5-Cy_2dp]: H[3,5-Cy_2dp] was prepared according to the previously published procedure[1] using N,N-dimethylcyclohexanecarboxamide as the

starting material. M.p.:90°C. ^{1}H NMR (600 MHz,$CDCl_3$, 23°C):δ = 2.88–2.87 (m, overlapped, 2 H, C*H* for Cy), 2.09–2.07 (d, $^{1}J_{H–H}$ = 12.6 Hz, 4 H, CH_2 for Cy),1.86–1.84 (d, $^{1}J_{H–H}$ = 13.2 Hz, 4 H, CH_2 for Cy),1.76–1.74 (d, $^{1}J_{H–H}$ = 13.2 Hz, 2 H, CH_2 for Cy),1.55–1.51 (m , overlapped, 4 H, CH_2 for Cy), 1.48–1.41 (m , overlapped, 4 H, CH_2 for Cy), 1.39–1.29 (m , overlapped, 2 H, CH_2 for Cy)ppm; ^{13}C{^{1}H} NMR (150 MHz,$CDCl_3$, 23°C): δ = 185.54, 185.23 (d, $^{1}J_{C–P}$ = 46.5 Hz, P*C*N), 40.43, 40.33 (d, $^{2}J_{C–P}$ = 15 Hz, *C*H for Cy), 35.10, 35.05 (d, $^{3}J_{C–P}$ = 7.5 Hz, *C*H_2 for Cy), 26.39, 25.93 (2s, *C*H_2 for Cy) ppm; ^{31}P{^{1}H} NMR (243 MHz,$CDCl_3$, 23°C): δ = 67.30 (s) ppm; IR(Nujol mull, cm–1):3181(w), 2958(s), 2923(vs), 2852(s), 1459(m), 1376(w), 1261(s), 1091(s), 1020(s), 863(vw), 798(s), 701(vw); Anal. calcd for $C_{14}H_{23}N_2P$: C 67.17, H 9.26, N 11.19; Found: C 67.07, H 9.18, N 11.13.

Preparation of K[3,5-Cy$_2$dp] (3): To a mixture of 1*H*-3,5-di-cyclohexyl-1,2,4-diazaphosphole(H[3,5-Cy$_2$dp]) (0.75 g, 3.0 mmol)[1]and KH (0.160 g, 4.0 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 at high vacuum (0.01 mmHg) to yield **3** as off-white pure solids (0.66 g, 76 %).M.p.: >250°C decomp..^{1}H NMR (600 MHz,DMSO-d_6, 23°C):δ = 2.66–2.64 (m, 2 H, C*H* for Cy), 1.89–1.87 (d, $^{1}J_{H–H}$ = 12.0 Hz, 4 H, CH_2 for Cy),1.72–1.70 (d, $^{1}J_{H–H}$ = 12.6 Hz, 4 H, CH_2 for Cy),1.65–1.63 (m, 2 H, CH_2 for Cy),1.35–1.28 (m, 8 H, CH_2 for Cy), 1.18–1.16 (m, 2 H, CH_2 for Cy)ppm; ^{13}C{^{1}H} NMR (150 MHz,DMSO-d_6, 23°C): δ = 184.15, 183.84 (d, $^{1}J_{C–P}$ = 46.5 Hz, P*C*N), 42.40, 42.26 (d, $^{2}J_{C–P}$ = 21.0 Hz, *C*H for Cy), 36.78, 36.74 (d, $^{3}J_{C–P}$ = 6.0 Hz, *C*H_2 for Cy), 27.15, 26.73 (*C*H_2 for Cy) ppm; ^{31}P{^{1}H} NMR (243 MHz,DMSO-d_6, 23°C): δ = 47.94 (s) ppm.IR(Nujol mull, cm–1):2960(s), 2923(vs), 2854(s), 1461(m), 1376(m), 1261(s), 1091(s), 1020(s), 863(vw), 798(s); Anal. calcd for $C_{14}H_{22}KN_2P$: C 58.30, H 7.69, N 9.71; Found: C 58.18, H 7.63, N 9.62.

Preparation of {η^1,η^1-3,5-*t*Bu$_2$dp}$_2$(Sb-Sb){η^1,η^1-3,5-*t*Bu$_2$dp}$_2$ (4): To a mixture of $SbCl_3$ (0.228 g, 1.0 mmol) and K[3,5-*t*Bu$_2$dp][1] (**1**, 0.709 g, 3.0 mmol) was added30 mL tetrahydrofuran (THF) via syringe. After the mixture was stirred for 72 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (4 × 10 mL) and the solution was filtered through Celite. The filtrate was concentrated under the reduced pressure to about 20 mL to give **4**ascolorless 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] (0.08 g, 13.4%)at –20°C.Thetotal yield of **4**is 0.24 g (46 %). M.p.: 120°C, turn black, >250°C decomp..^{1}H NMR (600 MHz,THF-d_8, 23°C): δ = 1.361 (s, 72 H, –CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz,THF-d_8, 23°C): δ = 188.47, 188.11 (d, $^{1}J_{C–P}$ = 54.0 Hz, P*C*N), 34.92, 34.81 (d, $^{2}J_{C–P}$ = 16.5 Hz, *C*CH_3), 31.91, 31.88 (d, $^{3}J_{C–P}$ = 4.5 Hz, *C*H_3) ppm; ^{31}P{^{1}H} NMR (243 MHz,THF-d_8, 23°C): 87.93 ppm; ^{1}H NMR (600 MHz, C_6D_6, 23°C): δ = 1.31 (s, 72 H, –CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 23°C): δ = ~190 (d, not observed after 10240 scans for P*C*N) ppm, 32.56, 32.51 (d, $^{2}J_{C–P}$ = 7.5 Hz, *C*CH_3), 31.51, 31.06 (2d, overlapped, *C*H_3); ^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 23°C): 88.62(s) ppm; IR(Nujol mull, cm^{-1}):2960(s), 2923(vs), 2854(s), 1461(m), 1376(w), 1261(vs), 1095(vs),1020(vs), 863(w), 798(vs), 682(w); Anal. calcd for $C_{40}H_{72}Sb_2P_4N_8$: C 46.53, H 7.03, N 10.85; Found: C 46.41, H 6.95, N 10.74.

Preparation of {η^1,η^1-3,5-*i*Pr$_2$dp}$_2$(Sb-Sb){η^1,η^1-3,5-*i*Pr$_2$dp}$_2$(5α, 5β): To a mixture of $SbCl_3$ (0.23 g, 1.0 mmol) and K[3,5-*i*Pr$_2$dp][2](0.63 g, 3.0 mmol) was added THF (20 mL) via syringe. After the mixture was stirred for 72 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (3 × 10 mL). The solution was filtered through Celite and the filtrate was concentrated to about 10 mL to give **5** as colorless crystals at –20 °C. The mother liquor was further concentrated to afford another portion of **5**andsmall amount of colorless crystals H[3,5-*i*Pr$_2$dp]at –30°C.

The total yield of **5** was 0.19 g (42 %). M.p.: 220 °C, turn black, 248–250°C decomp.. ^{1}H NMR (600 MHz, C_6D_6, 23°C): δ = 3.25–3.19 (m, slightly overlapped, 8H, C*H*for *i*Pr), 1.31, 1.29 (d, $^{3}J_{P-H}$ = 7.2 Hz, 48 H, CH_3) ppm; ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 23°C): δ = 192.43, 192.03 (d, $^{1}J_{C-P}$ = 60.0 Hz, P*C*N),33.49, 33.37 (d, $^{2}J_{P-C}$ = 18.0 Hz, *C*H), 25.57, 25.52 (d, $^{3}J_{P-C}$ = 7.5 Hz, *C*H_3) ppm; ^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 23°C): δ = 73.09 (s) ppm; IR(Nujol mull, cm^{-1}):2923(vs), 2854(s), 1459(m), 1376(m), 1259(m), 1081(m), 1020(m), 798(m), 721(w), 682(w); Anal. calcd for $C_{32}H_{56}Sb_2P_4N_8$: C 41.77, H 6.13, N 12.18; Found: C 41.65, H 6.04, N 12.09.

Preparation of{η^{1},η^{1}-3,5-Cy$_2$dp}$_2$(Sb-Sb){η^{1},η^{1}-3,5-Cy$_2$dp}$_2$(6):To a mixture of $SbCl_3$ (0.228 g, 1.0 mmol) and K[3,5-Cy$_2$dp] (**3**, 0.865 g, 3.0 mmol) was added THF (40 mL) via syringe. After the mixture was stirred for 72 hours the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (4 × 10 mL) and the solution was filtered through Celite. The filtrate was concentrated to about 15 mL to give **6** as colorless crystals at –15°C. The mother liquor was further concentrated to afford another portion of **6** and small amount of colorless crystals H[3,5-Cy$_2$dp] at –30°C. The total yield of **6** was 0.235 g (38%). M.p.154–156 °C. ^{1}H NMR (600 MHz, C_6D_6, 23°C): δ = 8.04, 8.03 (d, 16 H,C*H*), 7.74–7.22 (t, 16 H,C*H*), 7.09–7.07 (t, 8H, C*H*) ppm; ^{13}C{^{1}H} NMR (150 MHz, C_6D_6, 23°C): δ = 190.75, 190.35 (d, $^{1}J_{C-P}$ = 60 Hz, P*C*N), 43.64, 43.54 (d, $^{2}J_{C-P}$ = 15 Hz, *C*H for Cy), 36.42, 36.37 (d, $^{3}J_{C-P}$ = 7.5 Hz, *C*H_2 for Cy), 26.67, 25.75 (*C*H_2 for Cy) ppm; ^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 23°C): 75.22 (s) ppm; IR(Nujol mull, cm^{-1}): 2960(s), 2923(vs), 2852(s), 1461(m), 1411(w), 1376(m), 1261(vs), 1093(vs), 1020(vs), 863(m), 800(vs), 701(m), 657(w); Anal. calcd for $C_{56}H_{88}Sb_2P_4N_8$: C 54.21, H 7.15, N 9.03; Found: C 54.11, H 7.06, N 8.95.

Preparation of Li[3,5-*t*Bu$_2$dp] (9):

To a mixture of H[3,5-*t*Bu$_2$dp] (0.594 g, 3 mmol) in THF (20 mL) at 0 °C, *n*-BuLi (1.2 mL, 3 mmol) was added *via* syringe. After the solution was stirred for 10 h at room temperature the volatile components were removed under the reduced pressure. The resultant residue was extracted by toluene (3 × 8 mL) and the solution was filtered through Celite. The filtrate was concentrated to about 10 mL to give **9** as colorless crystals at –20°C. The total yield of **9** was 0.58 g (70%). M.p. 191–193°C. ^{1}H NMR (600 MHz, DMSO-d_6, 23°C):δ = 3.61 (m, 4 H, -CH_2-O- for THF), 1.76 (m, 4 H, -CH_2- for THF), 1.29,1.27 (2s, 18 H,CH_3 for *t*Bu) ppm; ^{13}C{^{1}H} NMR (150 MHz, DMSO-d_6, 23°C): δ=188.18, 187.85 (2d, overlapped, $^{1}J_{C-P}$, P*C*N), 67.49 (s, -*C*H_2-O- for THF), 35.67, 35.53 (d, $^{2}J_{C-P}$ = 21.0 Hz, *C*CH_3), 33.66, 33.62 (d, $^{3}J_{C-P}$ = 6.0 Hz, *C*H_3),25.61(s, -*C*H_2- for THF) ppm; ^{31}P{^{1}H}NMR (243 MHz, DMSO-d_6,23°C): δ = 47.68(t) ppm. ^{7}Li{^{1}H}NMR (233 MHz, DMSO-d_6,23°C): δ = –0.95(s) ppm. IR(Nujol mull, cm^{-1}): 2927(vs), 2923(vs), 2854(vs), 1461(s), 1376(m), 1261(s), 1099(s), 1037(s), 1020(s), 865(w), 798(s), 700(w); Anal. calcd for $C_{14}H_{26}LiN_2OP$: C 60.86, H 9.49, N 10.14; Found: C 60.73, H 9.39, N 10.02.

Preparation of Sb[3,5-*t*Bu$_2$dp]$_3$ (10):

To a mixture of Li[3,5-*t*Bu$_2$dp]·THF (**9**, 1.136 g, 4.08 mmol) and $SbCl_3$ (0.31 g, 1.36 mmol) 30 mL of toluene was added via syringe. After the solution stirred for 72 h at room temperature the mixture was filtered by Celite. The filtrate was concentrated in vacuum to about 20 mL and then kept at –10 °C to afford **4** (0.246 g, 35%)**.** The mother liquor was further concentrated in vacuum to about 8 mL and then kept at –20 °C to afford X-ray quality blocks of **10** (0.117 g, 12.1%)**.** M.p. 180–181°C. ^{1}H NMR (600 MHz, C_6D_6, 23 °C): δ = 1.34 (s, 54 H, CH_3 for *t*Bu) ppm. ^{13}C{^{1}H}NMR (150 MHz, C_6D_6,23 °C): δ = 193.34, 192.93 (P*C*N), 35.60, 35.50 (*C*CH_3), 32.57, 32.52 (*C*H_3) ppm; ^{31}P{^{1}H}NMR (243 MHz, C_6D_6,23 °C): δ = 85.47 ppm;

IR(Nujol mull,cm^{-1}): 2726(m), 1461(vs), 1376(vs), 1303(w), 1261(m), 1153(vw), 1091(m), 1018(m), 890(vw), 800(m), 723(s), 684(w); Anal. calcd for $C_{30}H_{54}SbN_6P_3$: C 50.50, H 7.63, N 11.78; Found: C 50.38, H 7.54, N 11.69.

2. ^{1}H, $^{31}P\{^{1}H\}$, $^{13}C\{^{1}H\}$ NMR data for **H[3,5-Cy$_2$dp]**, **3**, **4**, **5** , **6**, **9** and **10**

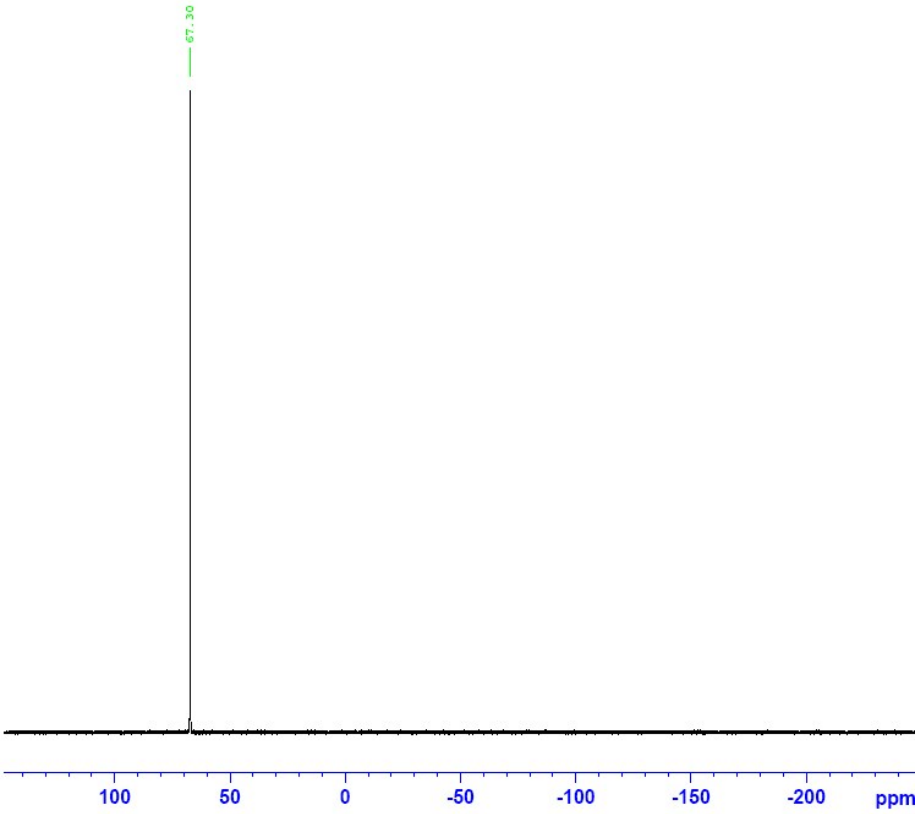


Figure 1. The $^{31}P\{^{1}H\}$ NMR spectrum of **H[3,5-Cy$_2$dp]** in $CDCl_3$

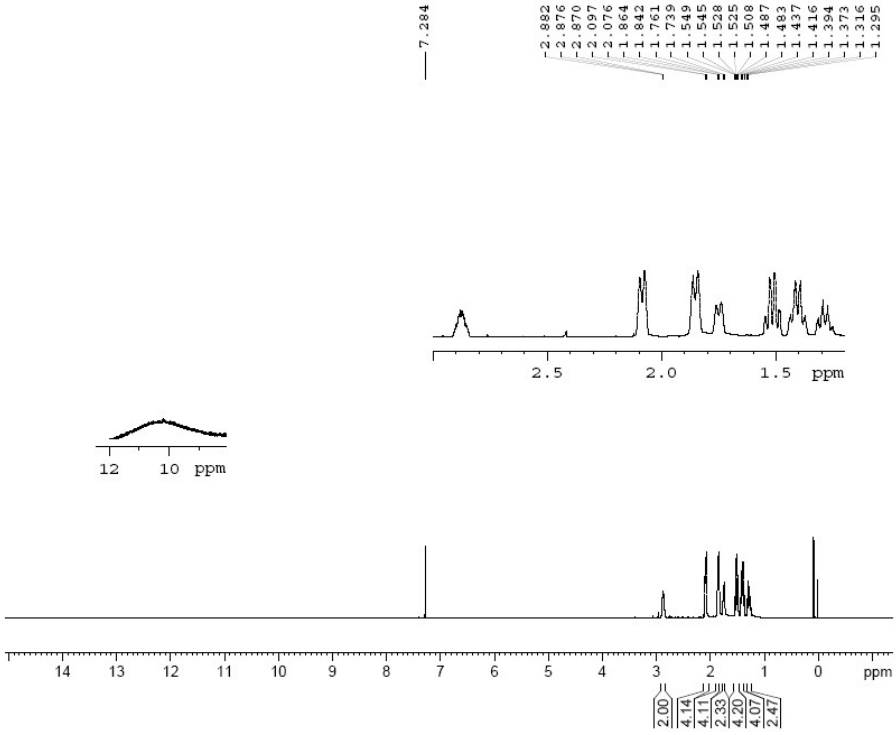


Figure 2. The ^{1}H NMR spectrum of **H[3,5-Cy$_2$dp]** in $CDCl_3$

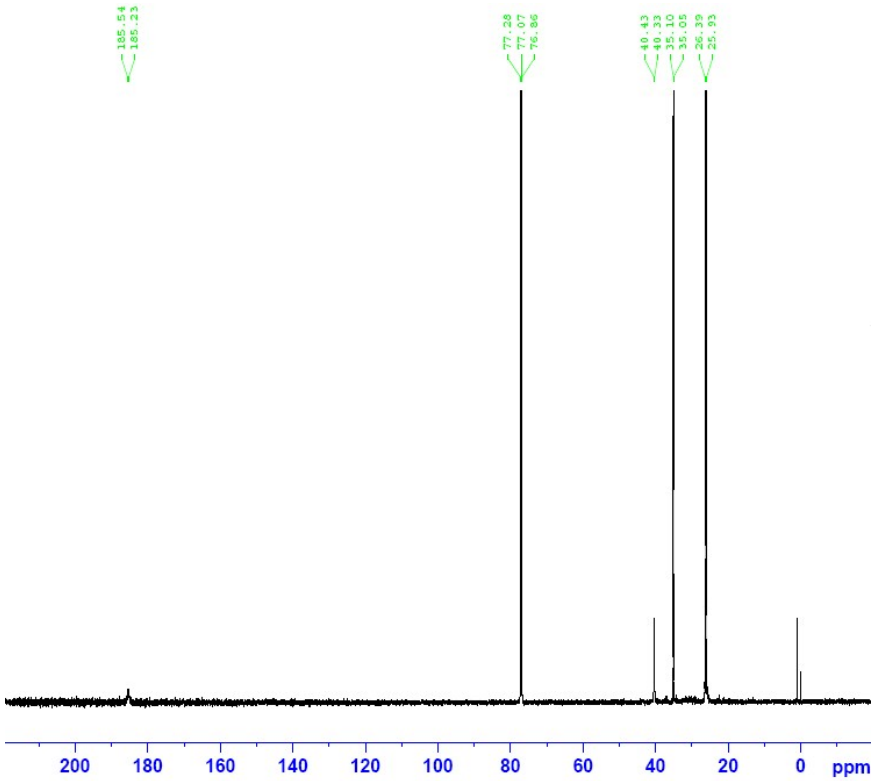


Figure 3. The $^{13}C\{^{1}H\}$ NMR spectrum of **H[3,5-Cy$_2$dp]**in $CDCl_3$

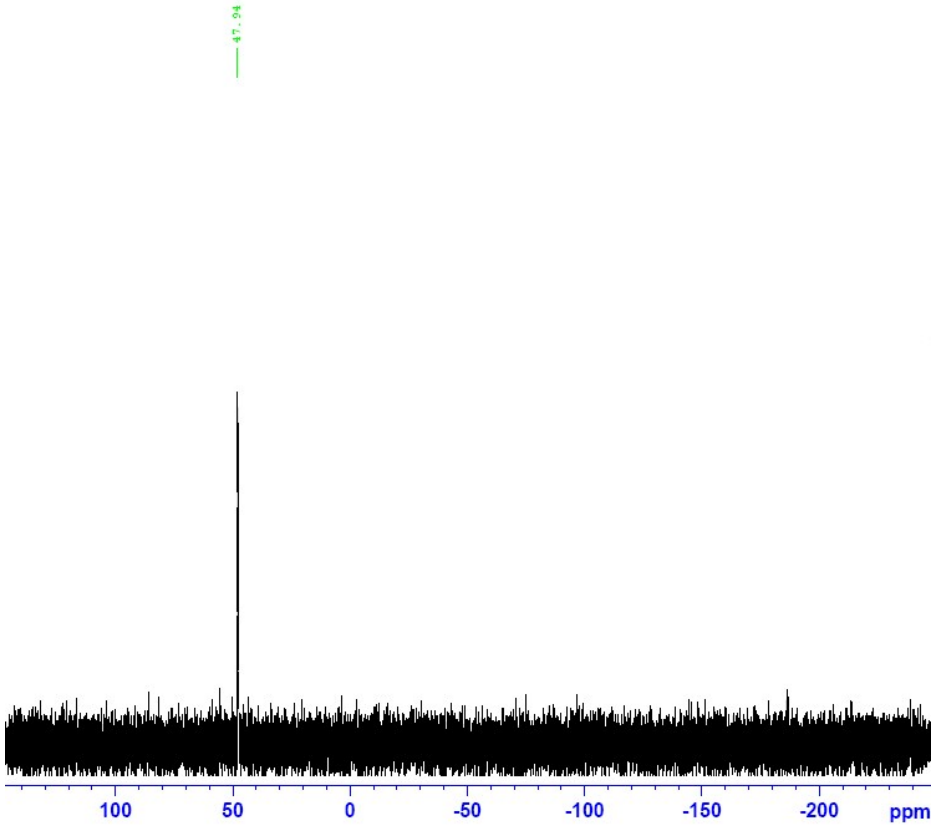


Figure 4. The $^{31}P\{^{1}H\}$ NMR spectrum of compound**3** in DMSO-d_6

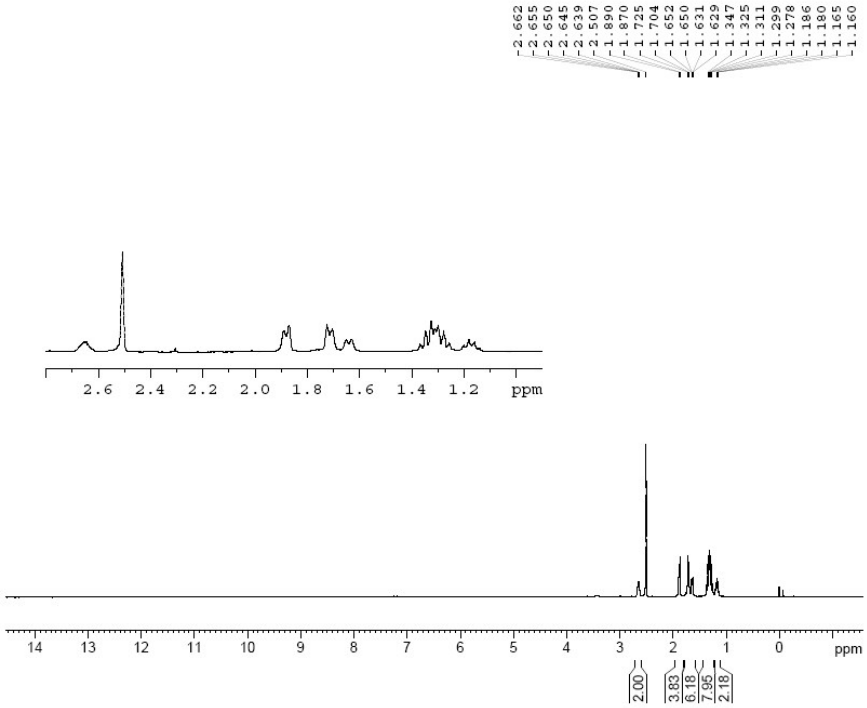


Figure 5. The ^{1}H NMR spectrum of compound**3** in DMSO-d_6

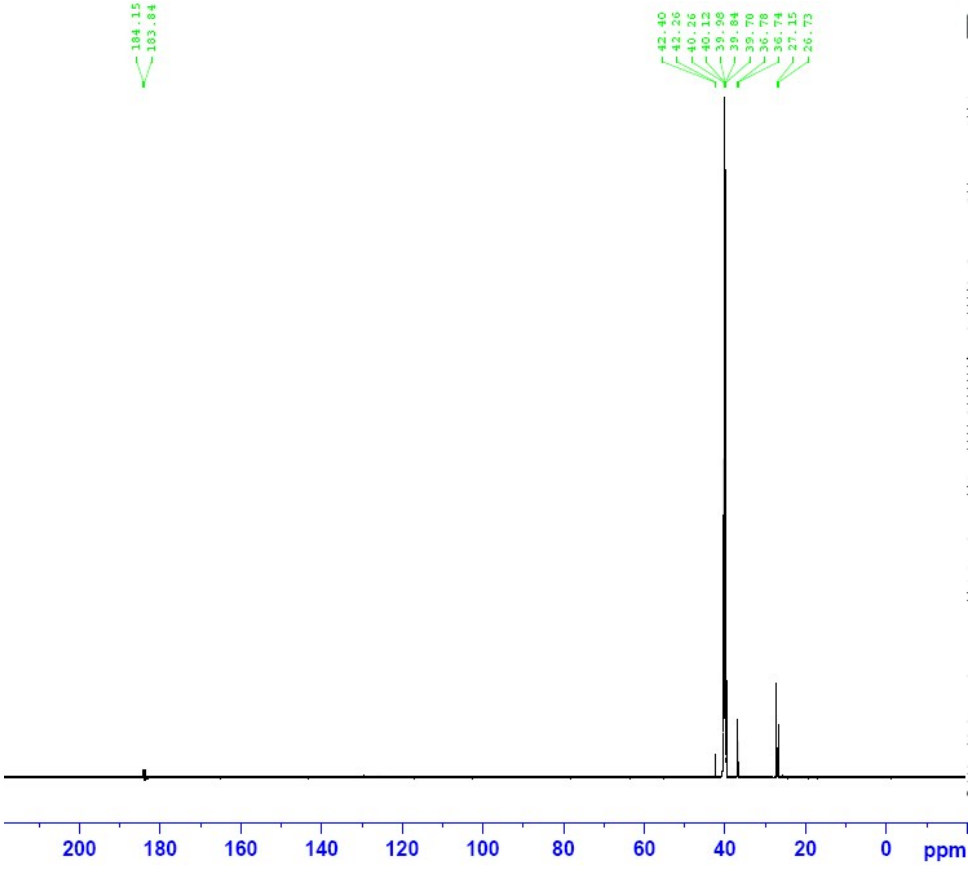


Figure 6. The ^{13}C{^{1}H} NMR spectrum of compound **3** in DMSO-d_6

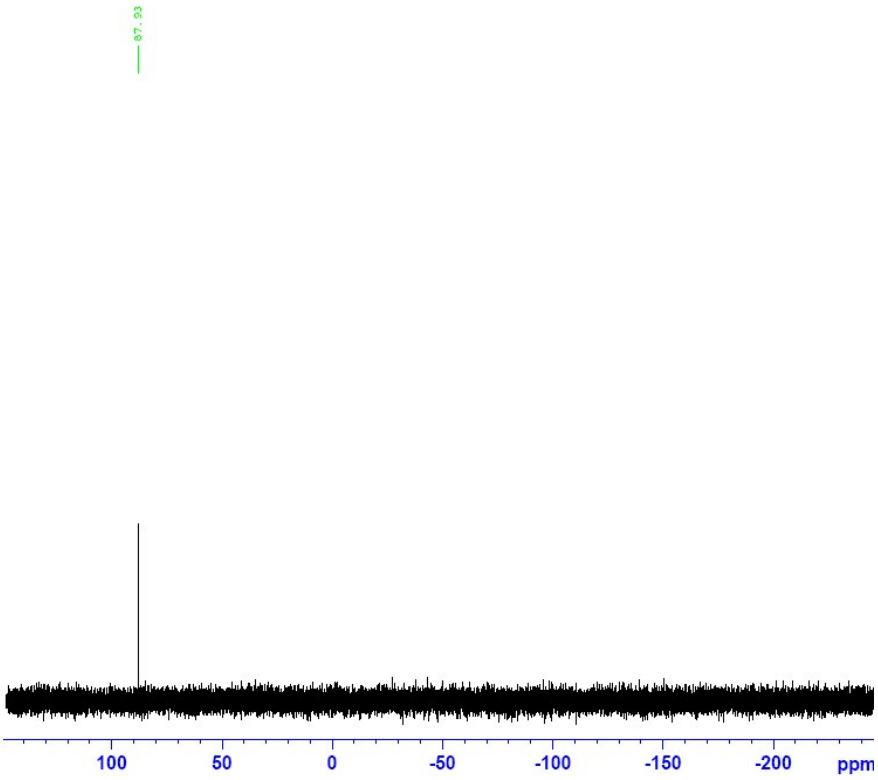


Figure 7. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **4** in THF-d_8

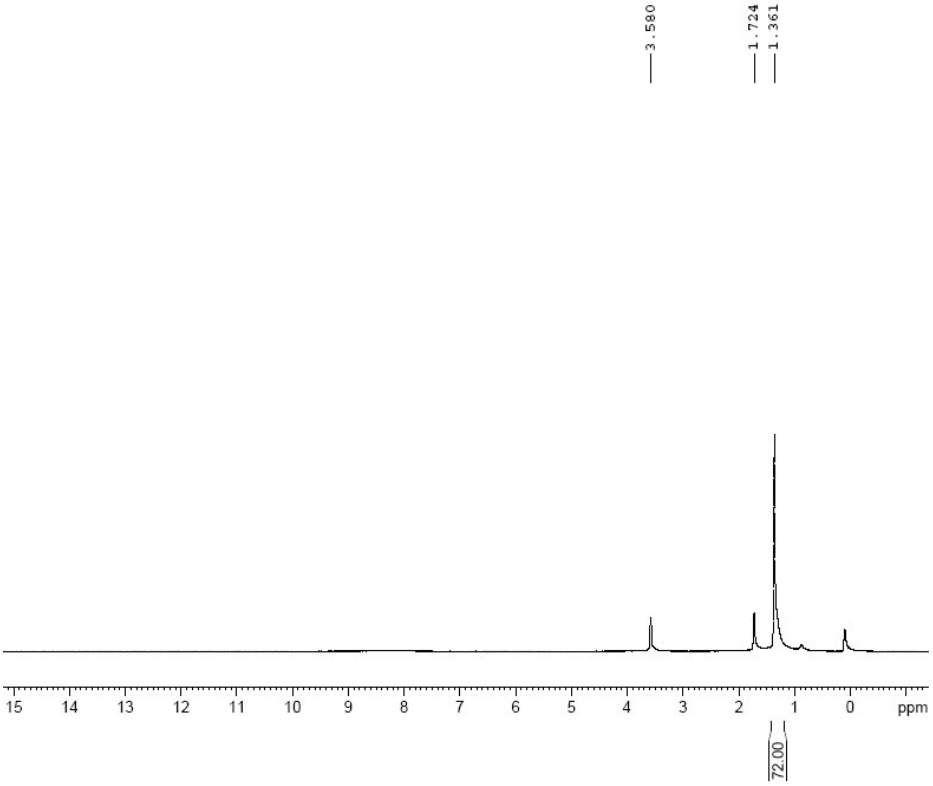


Figure 8. The ^{1}H NMR spectrum of compound **4** in THF-d_8

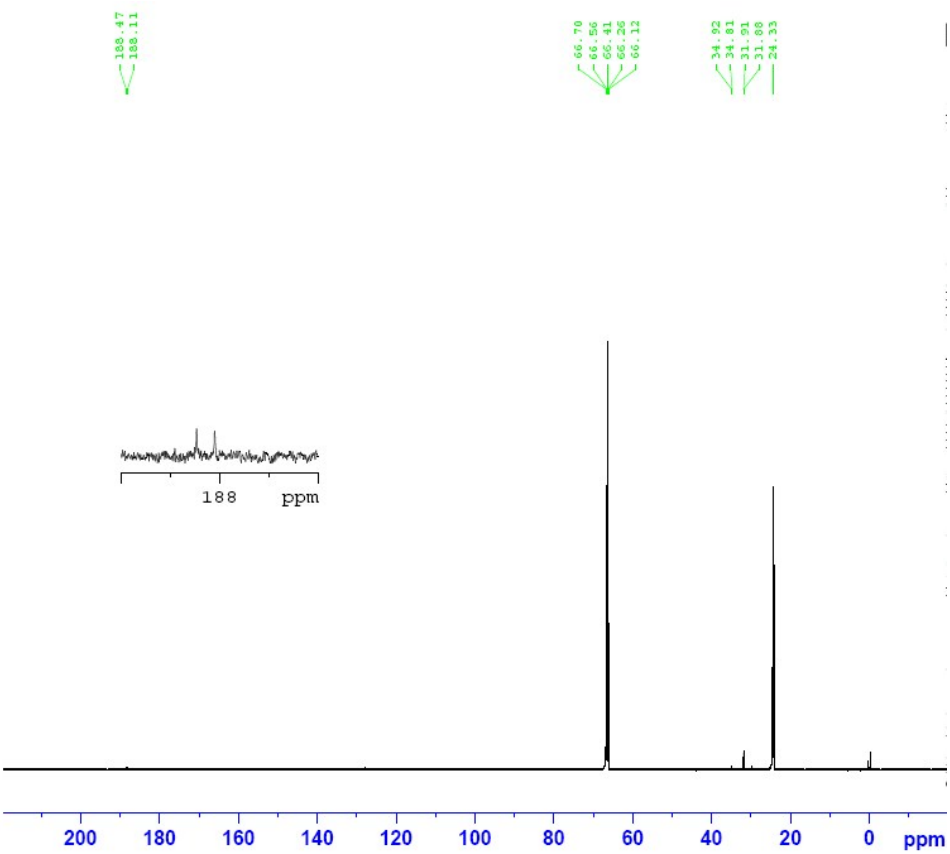


Figure 9. The $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** in THF-d_8

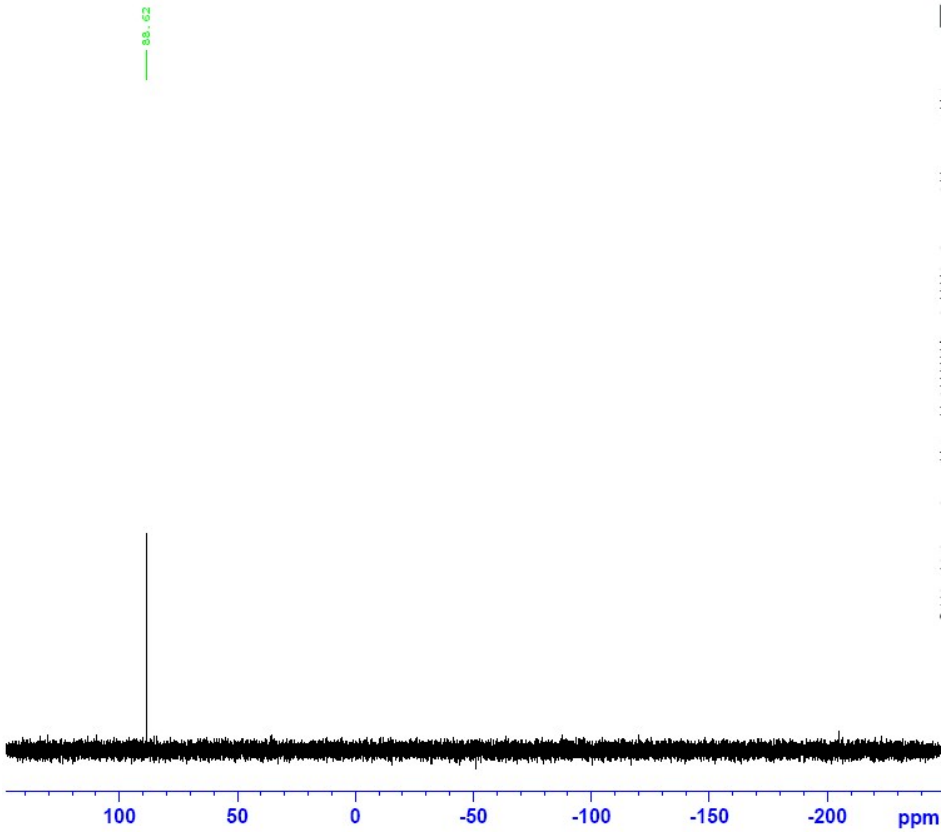


Figure 10. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **4** in C_6D_6

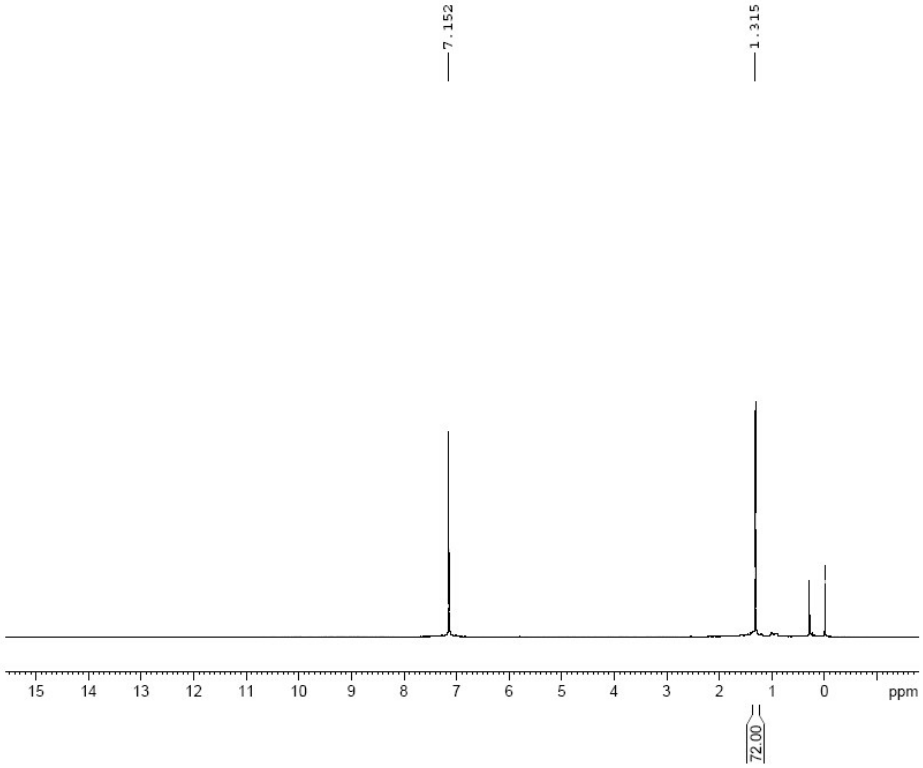


Figure 11. The ^{1}H NMR spectrum of compound **4** in C_6D_6

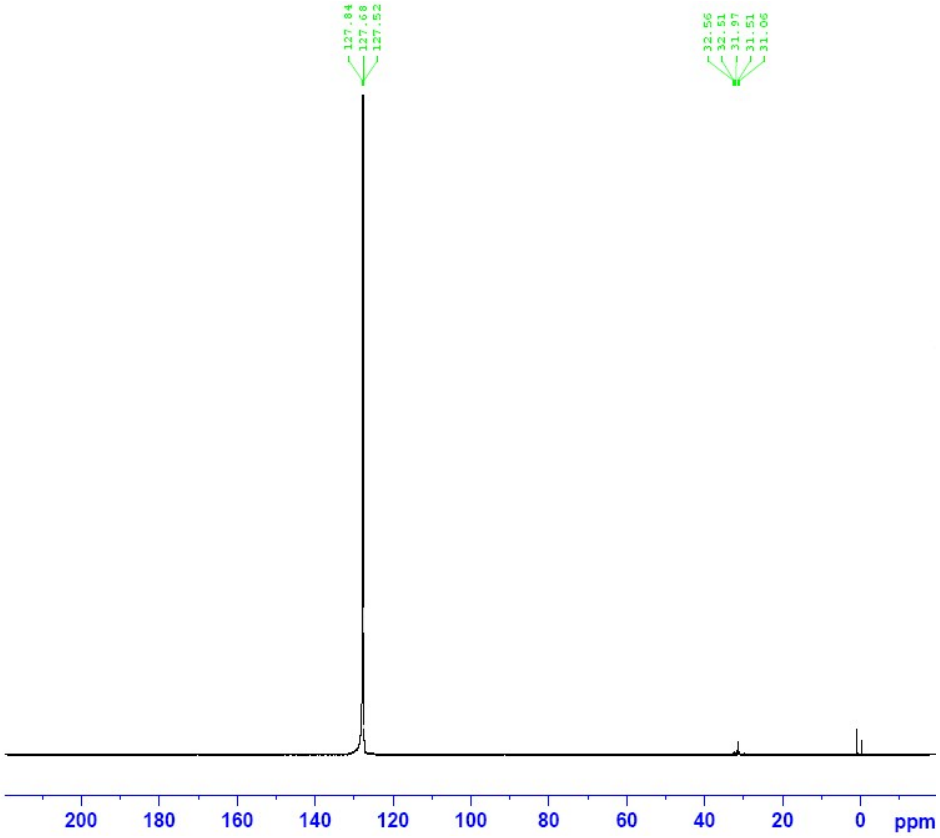


Figure12. The $^{13}C\{^{1}H\}$ NMR spectrum of compound **4** in C_6D_6

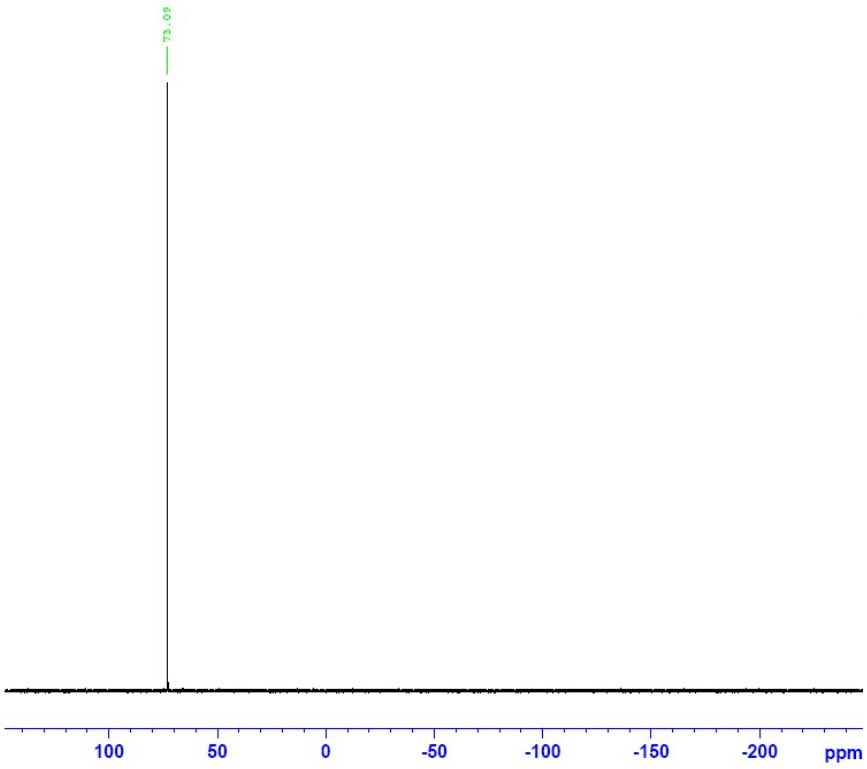


Figure 13. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **5** in C_6D_6

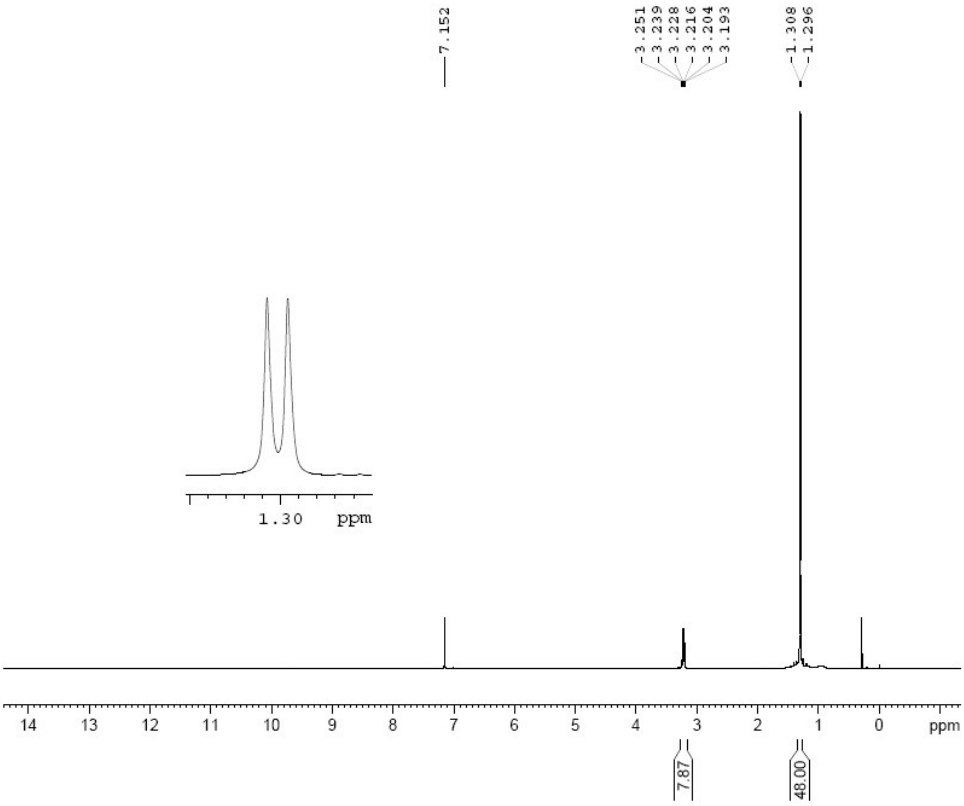


Figure 14. The ^{1}H NMR spectrum of compound **5** in C_6D_6

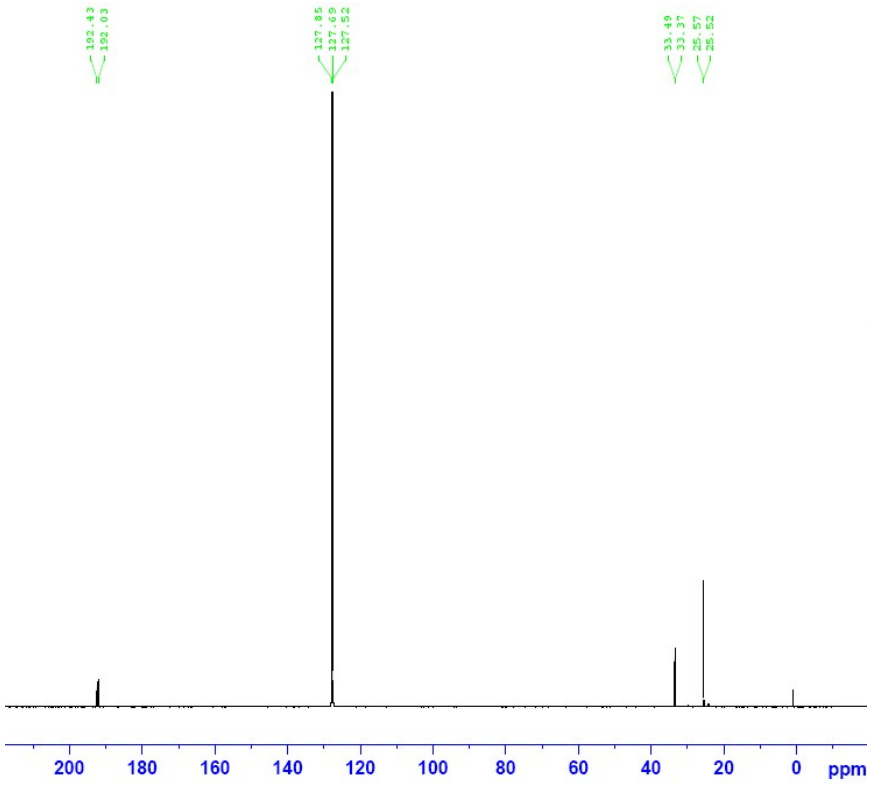


Figure15. The $^{13}C\{^{1}H\}$ NMR spectrum of compound **5** in C_6D_6

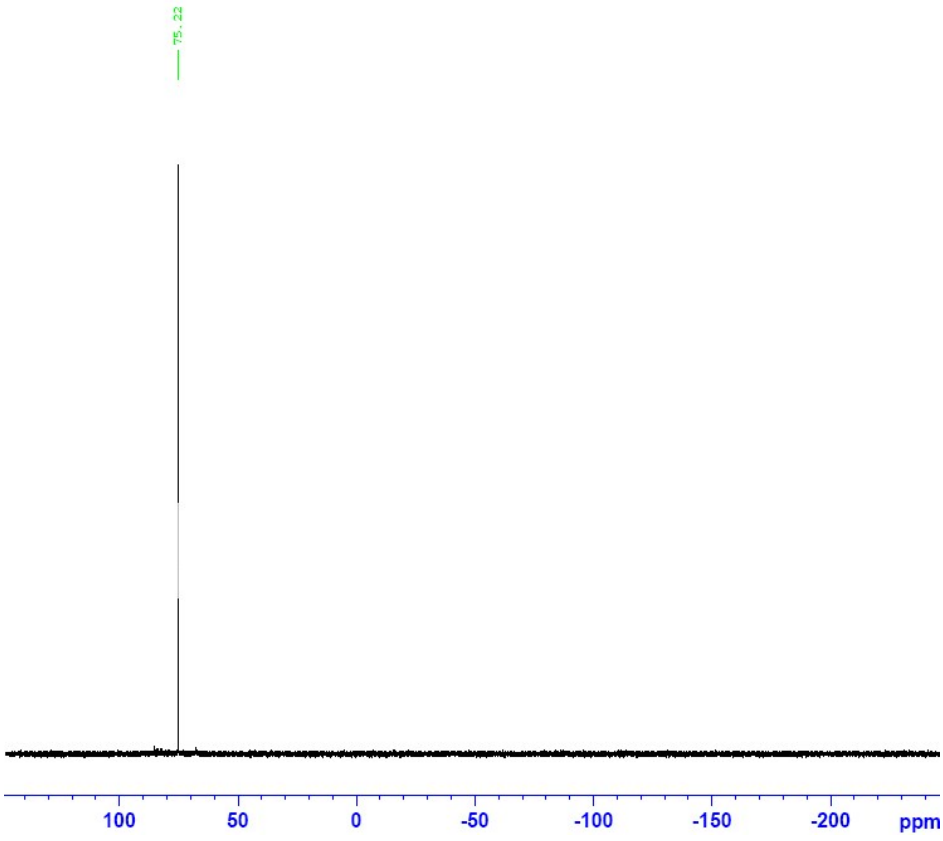


Figure 16. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **6** in C_6D_6

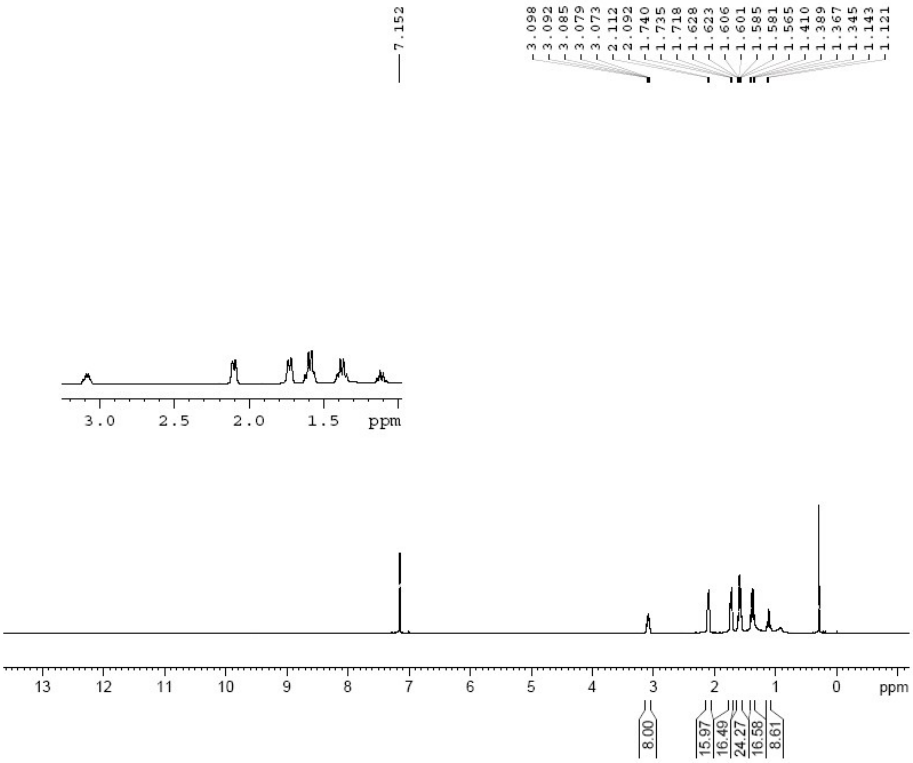


Figure 17. The ^{1}H NMR spectrum of compound **6** in C_6D_6

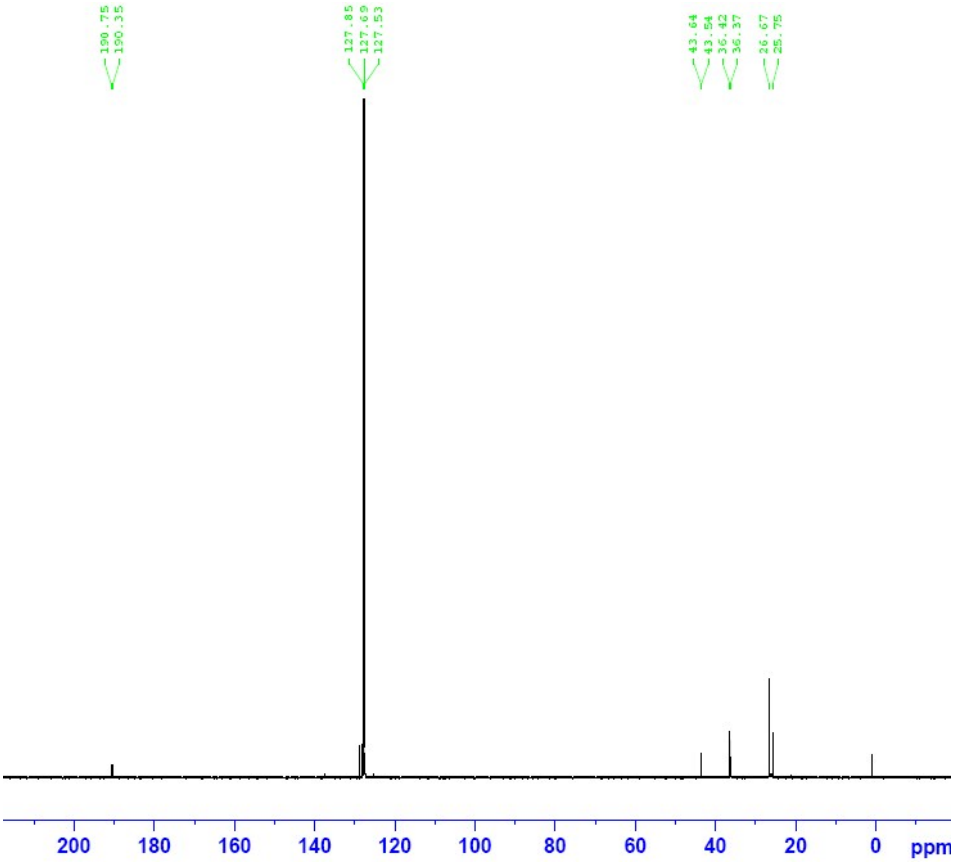


Figure 18. The $^{13}C\{^{1}H\}$ NMR spectrum of compound **6** in C_6D_6

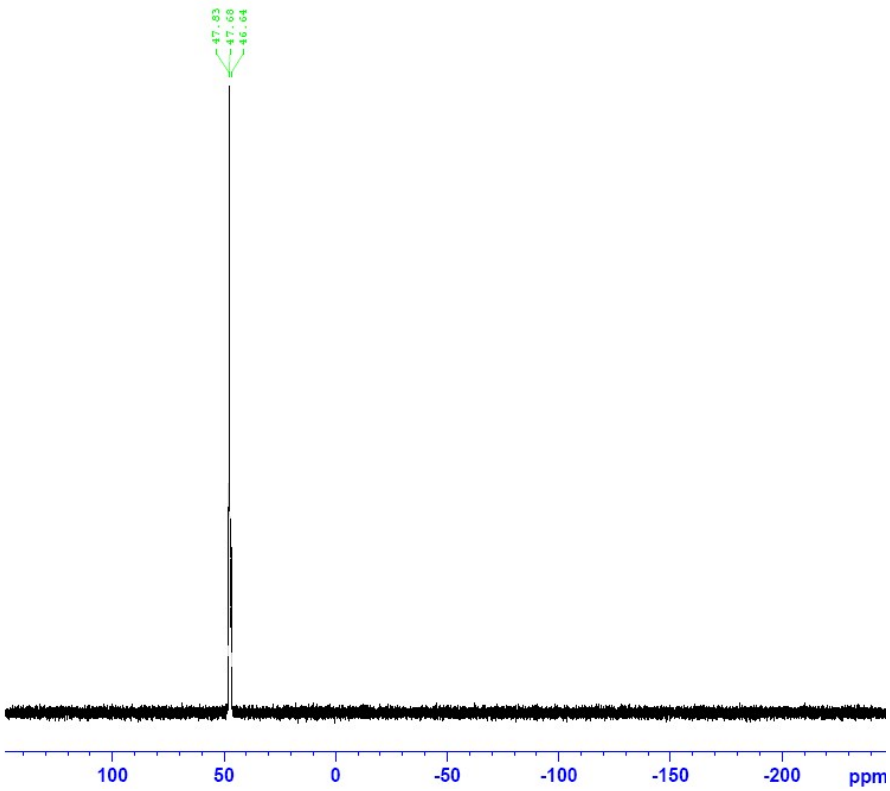


Figure 19. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **9** in DMSO-d_6

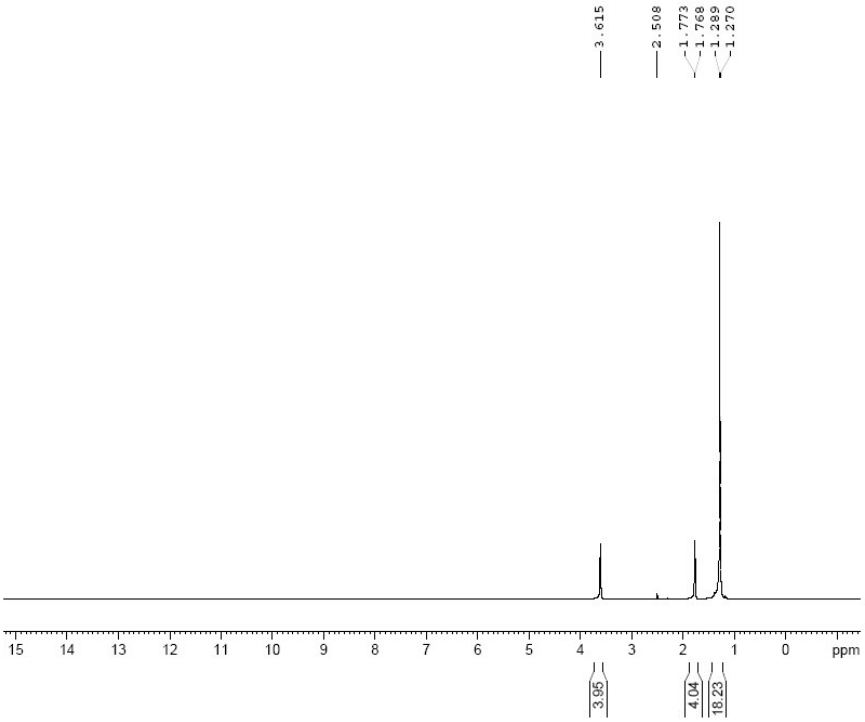


Figure 20. The ^{1}H NMR spectrum of compound **9** in DMSO-d_6

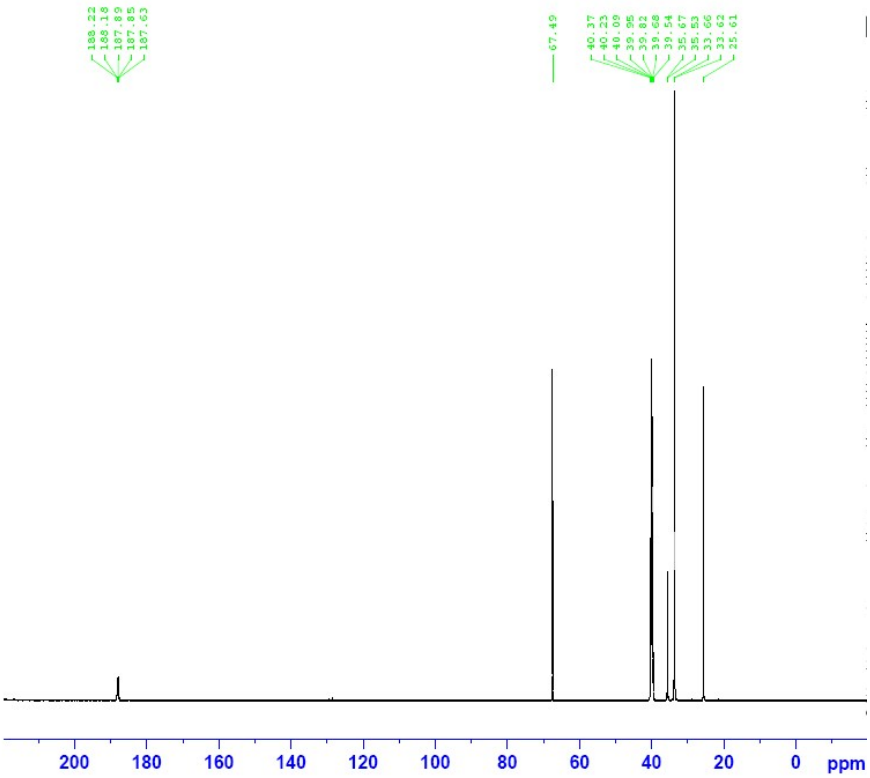


Figure 21. The $^{13}C\{^{1}H\}$ NMR spectrum of compound **9** in DMSO-d_6

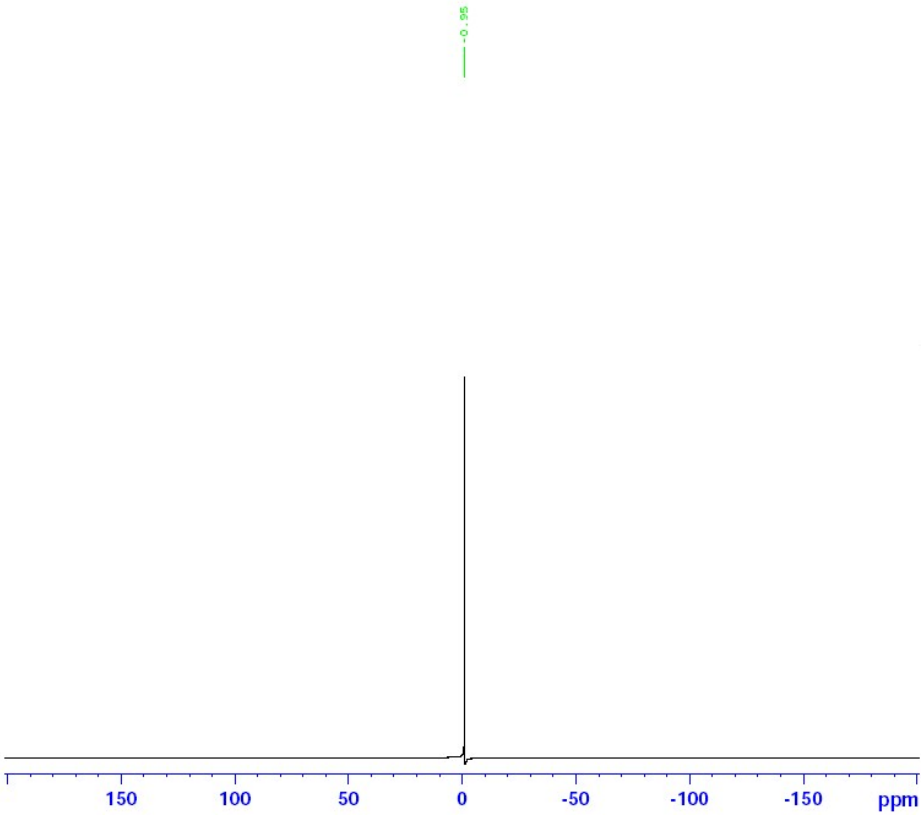


Figure 22. The $^{7}Li\{^{1}H\}$ NMR spectrum of compound **9** in DMSO-d_6

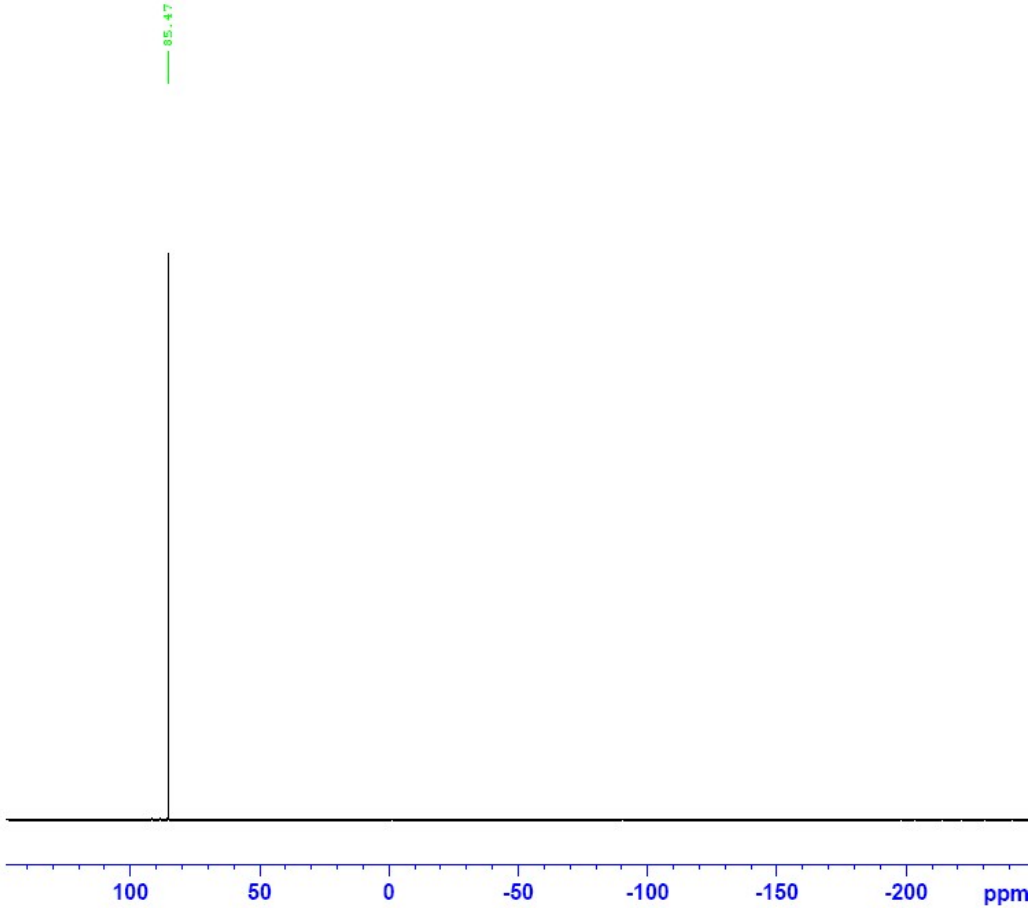


Figure 23. The $^{31}P\{^{1}H\}$ NMR spectrum of compound **10** in C_6D_6

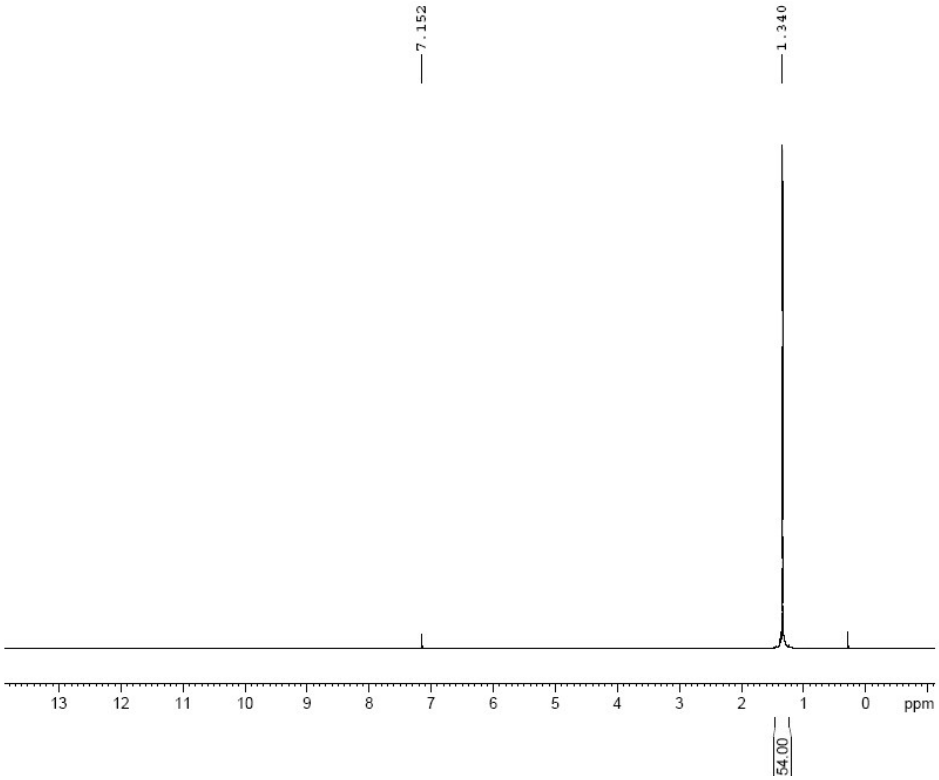


Figure 24. The ^{1}H NMR spectra of compound **10** in C_6D_6

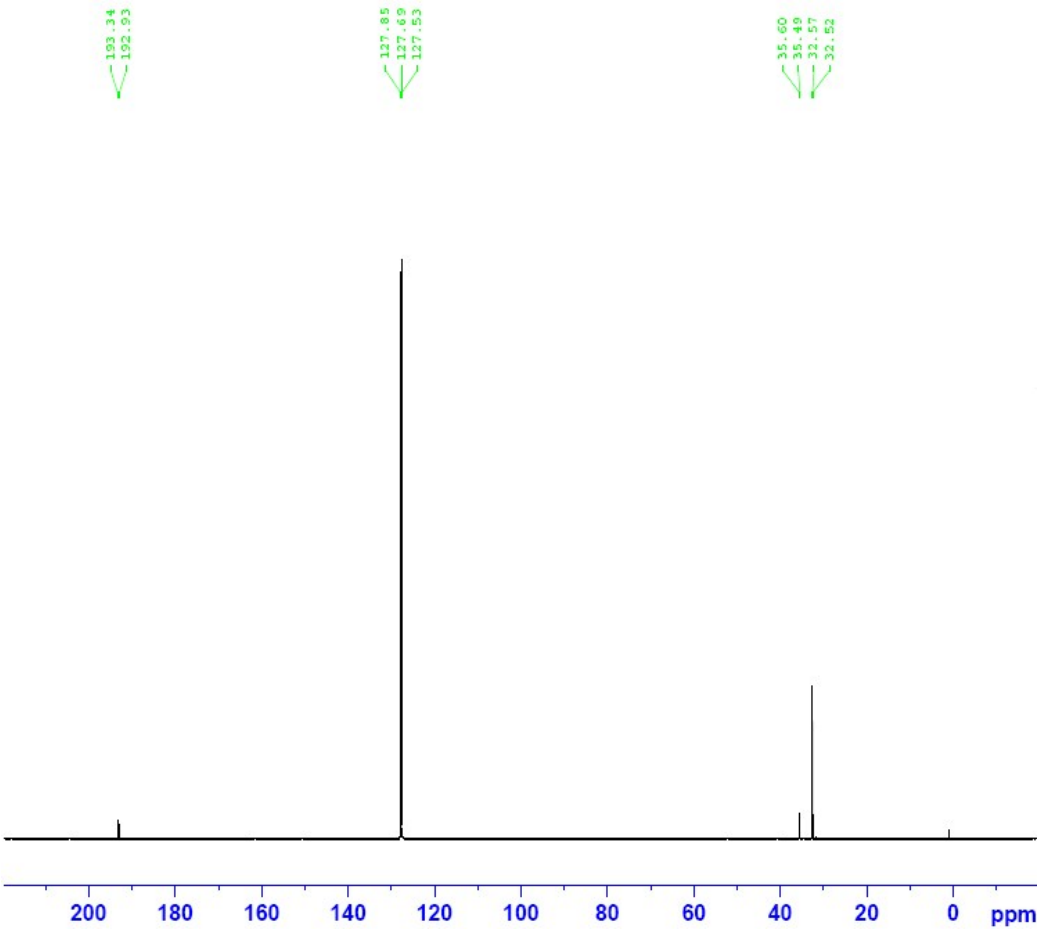


Figure 25. The ^{13}C NMR spectra of compound **10** in C_6D_6

3. Crystal structural analysis data for **4**, **5**, **6**, **9**and **10**

3.1 Crystal structural analysis data for **4**

Table 1. Crystal data and structure refinement for 11.

Identification code	11
Empirical formula	C40 H72 N8 P4 Sb2
Formula weight	1032.44
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 23.2715(12) A alpha = 90 deg.
	b = 10.7778(4) A beta = 114.457(7) deg.
	c = 21.6431(14) A gamma = 90 deg.
Volume	4941.3(4) A^3
Z, Calculated density	4, 1.388 Mg/m^3
Absorption coefficient	1.258 mm^-1
F(000)	2120
Crystal size	0.17 x 0.10 x 0.07 mm
Theta range for data collection	2.80 to 25.68 deg.
Limiting indices	-25<=h<=28, -10<=k<=13, -21<=l<=26
Reflections collected / unique	28867 / 9379 [R(int) = 0.1018]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.58624
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9379 / 0 / 511
Goodness-of-fit on F^2	1.000
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1349
R indices (all data)	R1 = 0.1455, wR2 = 0.1673
Largest diff. peak and hole	1.480 and -1.294 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 11.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	1850(4)	5121(9)	2840(5)	75(3)
C(2)	1761(4)	4783(9)	3930(5)	67(3)
C(3)	2727(3)	4078(9)	3812(5)	68(3)
C(4)	2006(4)	4224(8)	3442(4)	43(2)
C(5)	1701(3)	2949(7)	3191(4)	34(2)
C(6)	1094(3)	1091(8)	2863(4)	36(2)
C(7)	612(3)	38(8)	2624(4)	39(2)
C(8)	909(4)	-1267(8)	2809(6)	82(4)
C(9)	269(4)	151(10)	1862(5)	83(4)
C(10)	148(4)	203(10)	2943(6)	84(4)
C(11)	883(4)	-1883(9)	-90(5)	75(3)
C(12)	1139(5)	-2316(8)	1129(5)	70(3)
C(13)	1998(4)	-2033(8)	725(5)	69(3)
C(14)	1353(4)	-1632(8)	653(4)	42(2)
C(15)	1364(3)	-235(7)	776(4)	40(2)
C(16)	1349(3)	2009(8)	821(4)	37(2)
C(17)	1228(4)	3376(8)	753(4)	44(2)
C(18)	854(4)	3712(9)	1170(5)	65(3)
C(19)	837(5)	3744(9)	13(5)	84(4)
C(20)	1834(4)	4136(8)	1019(5)	68(3)
C(21)	4192(4)	3508(9)	3581(5)	78(4)
C(22)	4974(4)	2621(9)	4637(4)	66(3)
C(23)	4740(4)	1506(9)	3550(5)	63(3)

C(24)	4458(3)	2297(8)	3949(4)	39(2)
C(25)	3958(3)	1471(8)	4026(4)	38(2)
C(26)	3291(3)	33(7)	4302(4)	30(2)
C(27)	2951(4)	-834(8)	4593(4)	42(2)
C(28)	3324(4)	-982(10)	5353(4)	73(3)
C(29)	2869(6)	-2105(9)	4272(6)	104(5)
C(30)	2321(4)	-247(11)	4463(5)	91(4)
C(31)	2969(4)	1756(10)	684(5)	79(4)
C(32)	4059(5)	1198(10)	863(5)	85(4)
C(33)	3898(5)	2716(9)	1648(6)	82(4)
C(34)	3640(4)	1552(9)	1238(4)	50(2)
C(35)	3613(3)	467(7)	1672(4)	37(2)
C(36)	3617(3)	-1425(8)	2265(4)	35(2)
C(37)	3728(4)	-2636(8)	2649(4)	43(2)
C(38)	3120(5)	-3307(9)	2521(7)	100(4)
C(39)	4132(5)	-3490(10)	2415(5)	79(3)
C(40)	4091(5)	-2378(9)	3406(5)	87(4)
N(1)	1948(3)	2144(6)	2895(3)	34(2)
N(2)	1610(3)	1057(6)	2730(3)	33(2)
N(3)	1761(3)	1492(6)	1397(3)	36(2)
N(4)	1757(3)	232(6)	1384(3)	34(2)
N(5)	3237(3)	506(6)	1984(3)	38(2)
N(6)	3226(3)	-560(6)	2326(3)	32(2)
N(7)	3414(3)	1213(6)	3498(3)	33(2)
N(8)	3058(3)	346(6)	3657(3)	34(2)
P(1)	1012(1)	2454(2)	3243(1)	41(1)
P(2)	949(1)	906(2)	197(1)	45(1)
P(3)	4010(1)	-933(2)	1772(1)	49(1)
P(4)	4029(1)	739(2)	4776(1)	43(1)
Sb(1)	2698(1)	1935(1)	2407(1)	38(1)

Sb(2)	2309(1)	-326(1)	2563(1)	38(1)

Table 3. Bond lengths [A] and angles [deg] for 11.

C(1)-C(4)	1.539(12)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(4)	1.518(11)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-C(4)	1.538(10)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-C(5)	1.539(10)
C(5)-N(1)	1.341(9)
C(5)-P(1)	1.738(7)
C(6)-N(2)	1.346(8)
C(6)-C(7)	1.528(10)
C(6)-P(1)	1.733(8)
C(7)-C(9)	1.511(11)
C(7)-C(10)	1.514(10)
C(7)-C(8)	1.545(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(14)	1.548(11)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-C(14)	1.509(12)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-C(14)	1.507(10)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-C(15)	1.528(10)
C(15)-N(4)	1.350(9)
C(15)-P(2)	1.736(8)
C(16)-N(3)	1.339(9)
C(16)-C(17)	1.496(11)
C(16)-P(2)	1.750(8)
C(17)-C(20)	1.522(11)
C(17)-C(19)	1.531(11)
C(17)-C(18)	1.534(11)
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(24)	1.521(11)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(24)	1.517(10)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(24)	1.541(11)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(25)	1.527(10)
C(25)-N(7)	1.336(8)
C(25)-P(4)	1.751(8)
C(26)-N(8)	1.316(8)
C(26)-C(27)	1.520(10)
C(26)-P(4)	1.767(7)
C(27)-C(30)	1.511(11)
C(27)-C(29)	1.512(12)
C(27)-C(28)	1.518(10)
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(34)	1.540(11)
C(31)-H(31A)	0.9600
C(31)-H(31B)	0.9600
C(31)-H(31C)	0.9600
C(32)-C(34)	1.552(12)
C(32)-H(32A)	0.9600
C(32)-H(32B)	0.9600
C(32)-H(32C)	0.9600
C(33)-C(34)	1.510(12)
C(33)-H(33A)	0.9600
C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600
C(34)-C(35)	1.518(10)
C(35)-N(5)	1.309(9)
C(35)-P(3)	1.736(8)
C(36)-N(6)	1.346(9)
C(36)-C(37)	1.512(10)
C(36)-P(3)	1.751(8)
C(37)-C(38)	1.509(11)
C(37)-C(40)	1.526(12)
C(37)-C(39)	1.543(12)
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)-N(2)	1.372(8)
N(1)-Sb(1)	2.395(6)
N(2)-Sb(2)	2.341(6)
N(3)-N(4)	1.359(8)
N(3)-Sb(1)	2.411(6)
N(4)-Sb(2)	2.411(6)
N(5)-N(6)	1.372(8)
N(5)-Sb(1)	2.395(6)
N(6)-Sb(2)	2.407(5)
N(7)-N(8)	1.383(8)
N(7)-Sb(1)	2.388(6)
N(8)-Sb(2)	2.398(6)
Sb(1)-Sb(2)	2.6691(8)

C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5

C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-C(3)	108.7(7)
C(2)-C(4)-C(5)	110.4(7)
C(3)-C(4)-C(5)	109.6(7)
C(2)-C(4)-C(1)	108.4(8)
C(3)-C(4)-C(1)	109.2(7)
C(5)-C(4)-C(1)	110.5(7)
N(1)-C(5)-C(4)	121.4(7)
N(1)-C(5)-P(1)	115.0(6)
C(4)-C(5)-P(1)	123.7(6)
N(2)-C(6)-C(7)	120.2(7)
N(2)-C(6)-P(1)	114.1(6)
C(7)-C(6)-P(1)	125.5(6)
C(9)-C(7)-C(10)	109.6(8)
C(9)-C(7)-C(6)	106.9(7)
C(10)-C(7)-C(6)	108.7(7)
C(9)-C(7)-C(8)	109.5(8)
C(10)-C(7)-C(8)	108.4(8)
C(6)-C(7)-C(8)	113.7(6)
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
C(14)-C(11)-H(11A)	109.5
C(14)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(14)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(14)-C(12)-H(12A)	109.5
C(14)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(14)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(13)-C(14)-C(12)	112.7(8)

C(13)-C(14)-C(15)	108.7(7)
C(12)-C(14)-C(15)	110.4(7)
C(13)-C(14)-C(11)	107.7(7)
C(12)-C(14)-C(11)	109.4(8)
C(15)-C(14)-C(11)	107.9(7)
N(4)-C(15)-C(14)	119.5(7)
N(4)-C(15)-P(2)	112.9(6)
C(14)-C(15)-P(2)	127.5(6)
N(3)-C(16)-C(17)	122.3(7)
N(3)-C(16)-P(2)	112.5(6)
C(17)-C(16)-P(2)	125.1(6)
C(16)-C(17)-C(20)	112.7(7)
C(16)-C(17)-C(19)	111.3(7)
C(20)-C(17)-C(19)	108.2(8)
C(16)-C(17)-C(18)	107.7(7)
C(20)-C(17)-C(18)	108.3(7)
C(19)-C(17)-C(18)	108.5(8)
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
C(24)-C(21)-H(21A)	109.5
C(24)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(24)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(24)-C(22)-H(22A)	109.5
C(24)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(24)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-H(23A)	109.5
C(24)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(24)-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)-C(21)	107.6(7)
C(22)-C(24)-C(25)	110.9(7)
C(21)-C(24)-C(25)	113.2(6)
C(22)-C(24)-C(23)	109.2(7)
C(21)-C(24)-C(23)	110.9(8)
C(25)-C(24)-C(23)	105.0(7)
N(7)-C(25)-C(24)	121.6(7)

N(7)-C(25)-P(4)	113.0(5)
C(24)-C(25)-P(4)	125.4(5)
N(8)-C(26)-C(27)	122.8(6)
N(8)-C(26)-P(4)	112.3(5)
C(27)-C(26)-P(4)	124.9(5)
C(30)-C(27)-C(29)	111.5(8)
C(30)-C(27)-C(28)	108.8(8)
C(29)-C(27)-C(28)	108.0(8)
C(30)-C(27)-C(26)	107.2(7)
C(29)-C(27)-C(26)	110.7(7)
C(28)-C(27)-C(26)	110.6(7)
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
C(34)-C(31)-H(31A)	109.5

C(34)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(34)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(34)-C(32)-H(32A)	109.5
C(34)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(34)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-H(33A)	109.5
C(34)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(34)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(33)-C(34)-C(35)	112.6(7)
C(33)-C(34)-C(31)	111.6(8)
C(35)-C(34)-C(31)	107.7(7)
C(33)-C(34)-C(32)	109.2(8)
C(35)-C(34)-C(32)	109.3(7)
C(31)-C(34)-C(32)	106.4(8)
N(5)-C(35)-C(34)	120.2(7)
N(5)-C(35)-P(3)	113.5(6)
C(34)-C(35)-P(3)	126.2(6)
N(6)-C(36)-C(37)	120.8(7)
N(6)-C(36)-P(3)	113.3(6)
C(37)-C(36)-P(3)	125.7(6)
C(38)-C(37)-C(36)	112.3(7)

C(38)-C(37)-C(40)	110.1(8)
C(36)-C(37)-C(40)	109.0(7)
C(38)-C(37)-C(39)	107.8(8)
C(36)-C(37)-C(39)	108.9(7)
C(40)-C(37)-C(39)	108.7(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
C(5)-N(1)-N(2)	111.3(6)
C(5)-N(1)-Sb(1)	143.7(5)
N(2)-N(1)-Sb(1)	104.4(4)
C(6)-N(2)-N(1)	112.8(6)
C(6)-N(2)-Sb(2)	142.0(5)
N(1)-N(2)-Sb(2)	102.9(4)
C(16)-N(3)-N(4)	113.6(6)

C(16)-N(3)-Sb(1)	142.3(5)
N(4)-N(3)-Sb(1)	102.2(4)
C(15)-N(4)-N(3)	112.8(6)
C(15)-N(4)-Sb(2)	142.0(5)
N(3)-N(4)-Sb(2)	103.4(4)
C(35)-N(5)-N(6)	114.7(6)
C(35)-N(5)-Sb(1)	141.8(6)
N(6)-N(5)-Sb(1)	101.7(4)
C(36)-N(6)-N(5)	111.2(6)
C(36)-N(6)-Sb(2)	142.1(5)
N(5)-N(6)-Sb(2)	104.1(4)
C(25)-N(7)-N(8)	112.4(6)
C(25)-N(7)-Sb(1)	143.5(5)
N(8)-N(7)-Sb(1)	102.8(4)
C(26)-N(8)-N(7)	114.3(6)
C(26)-N(8)-Sb(2)	141.4(5)
N(7)-N(8)-Sb(2)	103.0(4)
C(6)-P(1)-C(5)	86.7(3)
C(15)-P(2)-C(16)	88.0(4)
C(35)-P(3)-C(36)	87.3(4)
C(25)-P(4)-C(26)	87.7(3)
N(7)-Sb(1)-N(1)	86.1(2)
N(7)-Sb(1)-N(5)	84.6(2)
N(1)-Sb(1)-N(5)	145.2(2)
N(7)-Sb(1)-N(3)	146.2(2)
N(1)-Sb(1)-N(3)	82.4(2)
N(5)-Sb(1)-N(3)	87.0(2)
N(7)-Sb(1)-Sb(2)	73.26(15)
N(1)-Sb(1)-Sb(2)	71.51(15)
N(5)-Sb(1)-Sb(2)	73.74(14)

N(3)-Sb(1)-Sb(2)	72.99(15)
N(2)-Sb(2)-N(8)	85.6(2)
N(2)-Sb(2)-N(6)	146.5(2)
N(8)-Sb(2)-N(6)	84.0(2)
N(2)-Sb(2)-N(4)	84.6(2)
N(8)-Sb(2)-N(4)	145.2(2)
N(6)-Sb(2)-N(4)	86.0(2)
N(2)-Sb(2)-Sb(1)	74.44(15)
N(8)-Sb(2)-Sb(1)	72.74(15)
N(6)-Sb(2)-Sb(1)	72.04(15)
N(4)-Sb(2)-Sb(1)	72.42(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 11.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	75(7)	54(7)	84(8)	-28(6)	22(6)	-33(6)
C(2)	57(6)	57(7)	99(8)	-45(6)	45(6)	-31(5)
C(3)	22(5)	59(7)	107(8)	-45(6)	9(4)	-8(4)
C(4)	39(5)	35(6)	56(6)	-16(5)	20(4)	-9(4)
C(5)	28(4)	36(5)	44(5)	-13(4)	20(3)	2(4)
C(6)	21(4)	41(6)	42(5)	-4(4)	10(3)	-1(3)
C(7)	32(5)	37(6)	49(5)	-2(4)	19(4)	-9(4)
C(8)	42(6)	40(7)	160(11)	3(7)	39(6)	-19(5)
C(9)	70(7)	86(9)	74(8)	0(7)	10(5)	-44(6)
C(10)	68(7)	89(9)	128(10)	-40(8)	73(7)	-44(6)
C(11)	74(8)	51(7)	74(7)	-14(6)	3(5)	4(5)
C(12)	100(8)	16(5)	110(9)	-4(6)	58(7)	-10(5)
C(13)	65(7)	42(7)	99(8)	-13(6)	34(6)	20(5)
C(14)	39(5)	30(5)	56(6)	-7(4)	17(4)	5(4)
C(15)	33(5)	25(5)	50(5)	-13(4)	8(4)	2(4)
C(16)	37(5)	33(5)	39(5)	-7(4)	14(4)	-2(4)
C(17)	48(5)	40(6)	36(5)	-2(4)	10(4)	-4(4)
C(18)	57(6)	47(7)	101(8)	-3(6)	43(6)	6(5)
C(19)	114(9)	45(7)	71(7)	23(6)	17(6)	11(6)
C(20)	64(7)	28(6)	107(8)	-3(6)	31(6)	3(5)
C(21)	34(6)	55(7)	125(9)	27(7)	12(5)	-12(5)

C(22)	42(6)	81(8)	62(6)	4(6)	9(4)	-28(5)
C(23)	53(6)	74(8)	75(7)	-9(6)	40(5)	-9(5)
C(24)	22(4)	40(6)	53(5)	6(4)	13(4)	-1(4)
C(25)	15(4)	54(6)	40(5)	-4(4)	7(3)	-7(4)
C(26)	30(4)	32(5)	31(4)	11(4)	14(3)	1(3)
C(27)	41(5)	37(6)	43(5)	5(4)	13(4)	-3(4)
C(28)	66(7)	98(9)	46(6)	16(6)	13(5)	-24(6)
C(29)	194(14)	33(7)	127(11)	-7(7)	107(10)	-43(8)
C(30)	53(7)	129(11)	104(9)	58(8)	45(6)	0(7)
C(31)	71(7)	91(9)	74(7)	47(7)	29(6)	7(6)
C(32)	100(8)	100(10)	84(8)	40(7)	68(7)	25(7)
C(33)	98(9)	53(8)	110(9)	20(7)	58(7)	-20(6)
C(34)	51(6)	59(7)	50(6)	22(5)	30(4)	4(5)
C(35)	43(5)	34(5)	39(5)	4(4)	22(4)	-3(4)
C(36)	38(5)	32(5)	29(4)	7(4)	6(3)	4(4)
C(37)	40(5)	42(6)	52(6)	19(4)	23(4)	13(4)
C(38)	62(8)	48(8)	194(14)	32(8)	58(8)	12(6)
C(39)	88(8)	70(8)	92(8)	25(7)	50(6)	29(6)
C(40)	143(11)	53(8)	56(7)	20(6)	30(6)	30(7)
N(1)	26(4)	29(4)	51(4)	10(3)	20(3)	7(3)
N(2)	28(4)	22(4)	53(4)	-15(3)	20(3)	-10(3)
N(3)	38(4)	31(4)	39(4)	1(3)	15(3)	-4(3)
N(4)	35(4)	19(4)	41(4)	1(3)	10(3)	-8(3)
N(5)	34(4)	38(5)	55(4)	2(3)	32(3)	-11(3)
N(6)	36(4)	28(4)	43(4)	-7(3)	26(3)	-7(3)
N(7)	23(3)	32(4)	39(4)	10(3)	7(3)	1(3)
N(8)	25(3)	40(4)	33(4)	2(3)	9(3)	-7(3)
P(1)	33(1)	36(1)	64(2)	-7(1)	28(1)	-2(1)
P(2)	44(1)	37(2)	41(1)	-2(1)	3(1)	6(1)
P(3)	47(1)	49(2)	66(2)	12(1)	37(1)	14(1)

P(4)	35(1)	48(2)	38(1)	6(1)	7(1)	-7(1)
Sb(1)	39(1)	28(1)	48(1)	2(1)	19(1)	-5(1)
Sb(2)	36(1)	27(1)	54(1)	2(1)	21(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 11.

	x	y	z	U(eq)
H(1A)	1401	5169	2589	112
H(1B)	2039	4823	2549	112
H(1C)	2014	5929	3007	112
H(2A)	1309	4828	3714	100
H(2B)	1932	5602	4057	100
H(2C)	1888	4273	4328	100
H(3A)	2907	4832	4049	103
H(3B)	2898	3904	3487	103
H(3C)	2824	3406	4131	103
H(8A)	580	-1880	2678	122
H(8B)	1157	-1314	3290	122
H(8C)	1173	-1419	2575	122
H(9A)	62	942	1748	124
H(9B)	-39	-499	1691	124
H(9C)	567	80	1661	124
H(10A)	-66	983	2803	126
H(10B)	371	189	3429	126
H(10C)	-155	-459	2800	126
H(11A)	472	-1586	-159	113
H(11B)	863	-2758	-178	113
H(11C)	1022	-1459	-393	113
H(12A)	1469	-2295	1580	105
H(12B)	1046	-3162	983	105
H(12C)	768	-1925	1126	105
H(13A)	2121	-1546	428	103

H(13B)	1987	-2894	607	103
H(13C)	2298	-1915	1186	103
H(18A)	440	3353	962	98
H(18B)	819	4598	1186	98
H(18C)	1069	3395	1623	98
H(19A)	1072	3563	-251	126
H(19B)	746	4616	-11	126
H(19C)	449	3283	-162	126
H(20A)	2053	4021	1501	102
H(20B)	1733	4999	923	102
H(20C)	2098	3869	801	102
H(21A)	3915	3335	3118	117
H(21B)	4532	4027	3594	117
H(21C)	3962	3925	3799	117
H(22A)	4805	3149	4878	99
H(22B)	5310	3043	4577	99
H(22C)	5134	1874	4893	99
H(23A)	4919	761	3800	94
H(23B)	5064	1970	3487	94
H(23C)	4414	1293	3116	94
H(28A)	3722	-1368	5442	110
H(28B)	3091	-1490	5533	110
H(28C)	3395	-181	5566	110
H(29A)	2682	-2023	3787	157
H(29B)	2601	-2600	4411	157
H(29C)	3274	-2499	4414	157
H(30A)	2389	535	4694	137
H(30B)	2087	-786	4628	137
H(30C)	2088	-120	3984	137
H(31A)	2699	2045	889	118

H(31B)	2809	988	452	118
H(31C)	2982	2363	365	118
H(32A)	4060	1867	570	127
H(32B)	3893	464	597	127
H(32C)	4482	1044	1189	127
H(33A)	3598	3029	1809	123
H(33B)	3972	3330	1368	123
H(33C)	4287	2528	2028	123
H(38A)	2836	-2754	2602	150
H(38B)	3207	-4008	2820	150
H(38C)	2931	-3588	2058	150
H(39A)	3889	-3744	1954	118
H(39B)	4259	-4208	2702	118
H(39C)	4500	-3048	2442	118
H(40A)	4496	-2031	3488	131
H(40B)	4147	-3139	3655	131
H(40C)	3857	-1801	3551	131

Table 6. Torsion angles [deg] for 11.

C(2)-C(4)-C(5)-N(1)	-163.4(7)
C(3)-C(4)-C(5)-N(1)	-43.7(11)
C(1)-C(4)-C(5)-N(1)	76.8(9)
C(2)-C(4)-C(5)-P(1)	18.5(10)
C(3)-C(4)-C(5)-P(1)	138.3(7)
C(1)-C(4)-C(5)-P(1)	-101.3(8)
N(2)-C(6)-C(7)-C(9)	-71.5(9)
P(1)-C(6)-C(7)-C(9)	102.6(8)
N(2)-C(6)-C(7)-C(10)	170.3(8)
P(1)-C(6)-C(7)-C(10)	-15.7(10)
N(2)-C(6)-C(7)-C(8)	49.5(11)
P(1)-C(6)-C(7)-C(8)	-136.4(8)
C(13)-C(14)-C(15)-N(4)	-61.2(10)
C(12)-C(14)-C(15)-N(4)	62.8(10)
C(11)-C(14)-C(15)-N(4)	-177.7(8)
C(13)-C(14)-C(15)-P(2)	114.9(8)
C(12)-C(14)-C(15)-P(2)	-121.1(8)
C(11)-C(14)-C(15)-P(2)	-1.6(11)
N(3)-C(16)-C(17)-C(20)	47.5(11)
P(2)-C(16)-C(17)-C(20)	-136.7(7)
N(3)-C(16)-C(17)-C(19)	169.2(8)
P(2)-C(16)-C(17)-C(19)	-14.9(11)
N(3)-C(16)-C(17)-C(18)	-71.9(10)
P(2)-C(16)-C(17)-C(18)	104.0(8)
C(22)-C(24)-C(25)-N(7)	170.3(8)
C(21)-C(24)-C(25)-N(7)	49.3(11)
C(23)-C(24)-C(25)-N(7)	-71.8(10)

C(22)-C(24)-C(25)-P(4)	-11.5(11)
C(21)-C(24)-C(25)-P(4)	-132.5(8)
C(23)-C(24)-C(25)-P(4)	106.4(8)
N(8)-C(26)-C(27)-C(30)	-59.5(10)
P(4)-C(26)-C(27)-C(30)	120.1(8)
N(8)-C(26)-C(27)-C(29)	62.3(11)
P(4)-C(26)-C(27)-C(29)	-118.1(8)
N(8)-C(26)-C(27)-C(28)	-178.0(8)
P(4)-C(26)-C(27)-C(28)	1.6(10)
C(33)-C(34)-C(35)-N(5)	65.1(10)
C(31)-C(34)-C(35)-N(5)	-58.3(10)
C(32)-C(34)-C(35)-N(5)	-173.4(8)
C(33)-C(34)-C(35)-P(3)	-118.9(8)
C(31)-C(34)-C(35)-P(3)	117.7(8)
C(32)-C(34)-C(35)-P(3)	2.6(11)
N(6)-C(36)-C(37)-C(38)	54.2(11)
P(3)-C(36)-C(37)-C(38)	-131.5(8)
N(6)-C(36)-C(37)-C(40)	-68.1(9)
P(3)-C(36)-C(37)-C(40)	106.2(8)
N(6)-C(36)-C(37)-C(39)	173.5(7)
P(3)-C(36)-C(37)-C(39)	-12.2(10)
C(4)-C(5)-N(1)-N(2)	178.3(7)
P(1)-C(5)-N(1)-N(2)	-3.5(8)
C(4)-C(5)-N(1)-Sb(1)	-12.4(13)
P(1)-C(5)-N(1)-Sb(1)	165.8(5)
C(7)-C(6)-N(2)-N(1)	171.6(6)
P(1)-C(6)-N(2)-N(1)	-3.1(8)
C(7)-C(6)-N(2)-Sb(2)	-29.7(12)
P(1)-C(6)-N(2)-Sb(2)	155.6(5)
C(5)-N(1)-N(2)-C(6)	4.2(9)

Sb(1)-N(1)-N(2)-C(6)	-169.3(5)
C(5)-N(1)-N(2)-Sb(2)	-162.6(5)
Sb(1)-N(1)-N(2)-Sb(2)	24.0(4)
C(17)-C(16)-N(3)-N(4)	173.5(7)
P(2)-C(16)-N(3)-N(4)	-2.9(9)
C(17)-C(16)-N(3)-Sb(1)	-25.6(14)
P(2)-C(16)-N(3)-Sb(1)	158.0(5)
C(14)-C(15)-N(4)-N(3)	173.9(7)
P(2)-C(15)-N(4)-N(3)	-2.7(9)
C(14)-C(15)-N(4)-Sb(2)	-25.1(13)
P(2)-C(15)-N(4)-Sb(2)	158.3(5)
C(16)-N(3)-N(4)-C(15)	3.6(10)
Sb(1)-N(3)-N(4)-C(15)	-164.6(5)
C(16)-N(3)-N(4)-Sb(2)	-164.5(5)
Sb(1)-N(3)-N(4)-Sb(2)	27.3(4)
C(34)-C(35)-N(5)-N(6)	176.1(7)
P(3)-C(35)-N(5)-N(6)	-0.4(9)
C(34)-C(35)-N(5)-Sb(1)	-23.0(13)
P(3)-C(35)-N(5)-Sb(1)	160.5(5)
C(37)-C(36)-N(6)-N(5)	174.6(6)
P(3)-C(36)-N(6)-N(5)	-0.4(8)
C(37)-C(36)-N(6)-Sb(2)	-28.0(12)
P(3)-C(36)-N(6)-Sb(2)	157.0(5)
C(35)-N(5)-N(6)-C(36)	0.5(9)
Sb(1)-N(5)-N(6)-C(36)	-167.6(5)
C(35)-N(5)-N(6)-Sb(2)	-165.4(5)
Sb(1)-N(5)-N(6)-Sb(2)	26.5(4)
C(24)-C(25)-N(7)-N(8)	173.4(7)
P(4)-C(25)-N(7)-N(8)	-5.0(8)
C(24)-C(25)-N(7)-Sb(1)	-23.2(14)

P(4)-C(25)-N(7)-Sb(1)	158.3(5)
C(27)-C(26)-N(8)-N(7)	175.5(7)
P(4)-C(26)-N(8)-N(7)	-4.1(8)
C(27)-C(26)-N(8)-Sb(2)	-20.6(13)
P(4)-C(26)-N(8)-Sb(2)	159.7(5)
C(25)-N(7)-N(8)-C(26)	6.0(9)
Sb(1)-N(7)-N(8)-C(26)	-164.0(5)
C(25)-N(7)-N(8)-Sb(2)	-163.8(5)
Sb(1)-N(7)-N(8)-Sb(2)	26.3(4)
N(2)-C(6)-P(1)-C(5)	1.0(6)
C(7)-C(6)-P(1)-C(5)	-173.4(7)
N(1)-C(5)-P(1)-C(6)	1.5(6)
C(4)-C(5)-P(1)-C(6)	179.6(7)
N(4)-C(15)-P(2)-C(16)	0.9(6)
C(14)-C(15)-P(2)-C(16)	-175.4(8)
N(3)-C(16)-P(2)-C(15)	1.1(6)
C(17)-C(16)-P(2)-C(15)	-175.1(8)
N(5)-C(35)-P(3)-C(36)	0.1(6)
C(34)-C(35)-P(3)-C(36)	-176.1(7)
N(6)-C(36)-P(3)-C(35)	0.1(6)
C(37)-C(36)-P(3)-C(35)	-174.5(7)
N(7)-C(25)-P(4)-C(26)	2.3(6)
C(24)-C(25)-P(4)-C(26)	-176.0(8)
N(8)-C(26)-P(4)-C(25)	1.1(6)
C(27)-C(26)-P(4)-C(25)	-178.6(7)
C(25)-N(7)-Sb(1)-N(1)	-116.3(9)
N(8)-N(7)-Sb(1)-N(1)	48.0(4)
C(25)-N(7)-Sb(1)-N(5)	97.2(9)
N(8)-N(7)-Sb(1)-N(5)	-98.5(4)
C(25)-N(7)-Sb(1)-N(3)	173.5(8)

N(8)-N(7)-Sb(1)-N(3)	-22.2(6)
C(25)-N(7)-Sb(1)-Sb(2)	171.8(9)
N(8)-N(7)-Sb(1)-Sb(2)	-23.9(4)
C(5)-N(1)-Sb(1)-N(7)	95.2(9)
N(2)-N(1)-Sb(1)-N(7)	-95.1(4)
C(5)-N(1)-Sb(1)-N(5)	170.0(8)
N(2)-N(1)-Sb(1)-N(5)	-20.3(6)
C(5)-N(1)-Sb(1)-N(3)	-116.6(9)
N(2)-N(1)-Sb(1)-N(3)	53.1(4)
C(5)-N(1)-Sb(1)-Sb(2)	168.9(9)
N(2)-N(1)-Sb(1)-Sb(2)	-21.5(4)
C(35)-N(5)-Sb(1)-N(7)	-112.2(9)
N(6)-N(5)-Sb(1)-N(7)	50.1(4)
C(35)-N(5)-Sb(1)-N(1)	172.6(8)
N(6)-N(5)-Sb(1)-N(1)	-25.1(6)
C(35)-N(5)-Sb(1)-N(3)	100.5(9)
N(6)-N(5)-Sb(1)-N(3)	-97.1(4)
C(35)-N(5)-Sb(1)-Sb(2)	173.7(9)
N(6)-N(5)-Sb(1)-Sb(2)	-24.0(4)
C(16)-N(3)-Sb(1)-N(7)	171.2(8)
N(4)-N(3)-Sb(1)-N(7)	-26.7(7)
C(16)-N(3)-Sb(1)-N(1)	100.0(9)
N(4)-N(3)-Sb(1)-N(1)	-97.9(5)
C(16)-N(3)-Sb(1)-N(5)	-113.2(9)
N(4)-N(3)-Sb(1)-N(5)	49.0(4)
C(16)-N(3)-Sb(1)-Sb(2)	172.9(9)
N(4)-N(3)-Sb(1)-Sb(2)	-25.0(4)
C(6)-N(2)-Sb(2)-N(8)	-108.1(8)
N(1)-N(2)-Sb(2)-N(8)	51.8(4)
C(6)-N(2)-Sb(2)-N(6)	179.7(7)

N(1)-N(2)-Sb(2)-N(6)	-20.3(6)
C(6)-N(2)-Sb(2)-N(4)	105.4(8)
N(1)-N(2)-Sb(2)-N(4)	-94.7(4)
C(6)-N(2)-Sb(2)-Sb(1)	178.6(8)
N(1)-N(2)-Sb(2)-Sb(1)	-21.5(4)
C(26)-N(8)-Sb(2)-N(2)	96.1(8)
N(7)-N(8)-Sb(2)-N(2)	-98.9(4)
C(26)-N(8)-Sb(2)-N(6)	-115.8(8)
N(7)-N(8)-Sb(2)-N(6)	49.1(4)
C(26)-N(8)-Sb(2)-N(4)	170.1(7)
N(7)-N(8)-Sb(2)-N(4)	-25.0(6)
C(26)-N(8)-Sb(2)-Sb(1)	171.2(8)
N(7)-N(8)-Sb(2)-Sb(1)	-23.9(4)
C(36)-N(6)-Sb(2)-N(2)	176.2(7)
N(5)-N(6)-Sb(2)-N(2)	-25.5(6)
C(36)-N(6)-Sb(2)-N(8)	103.6(8)
N(5)-N(6)-Sb(2)-N(8)	-98.1(4)
C(36)-N(6)-Sb(2)-N(4)	-109.9(8)
N(5)-N(6)-Sb(2)-N(4)	48.5(4)
C(36)-N(6)-Sb(2)-Sb(1)	177.3(8)
N(5)-N(6)-Sb(2)-Sb(1)	-24.3(4)
C(15)-N(4)-Sb(2)-N(2)	-111.8(8)
N(3)-N(4)-Sb(2)-N(2)	50.2(4)
C(15)-N(4)-Sb(2)-N(8)	174.0(7)
N(3)-N(4)-Sb(2)-N(8)	-24.1(6)
C(15)-N(4)-Sb(2)-N(6)	100.5(8)
N(3)-N(4)-Sb(2)-N(6)	-97.6(4)
C(15)-N(4)-Sb(2)-Sb(1)	172.9(9)
N(3)-N(4)-Sb(2)-Sb(1)	-25.2(4)
N(7)-Sb(1)-Sb(2)-N(2)	104.0(2)

N(1)-Sb(1)-Sb(2)-N(2)	12.5(2)
N(5)-Sb(1)-Sb(2)-N(2)	-166.9(2)
N(3)-Sb(1)-Sb(2)-N(2)	-75.1(2)
N(7)-Sb(1)-Sb(2)-N(8)	13.8(2)
N(1)-Sb(1)-Sb(2)-N(8)	-77.7(2)
N(5)-Sb(1)-Sb(2)-N(8)	103.0(2)
N(3)-Sb(1)-Sb(2)-N(8)	-165.2(2)
N(7)-Sb(1)-Sb(2)-N(6)	-75.4(2)
N(1)-Sb(1)-Sb(2)-N(6)	-166.9(2)
N(5)-Sb(1)-Sb(2)-N(6)	13.8(2)
N(3)-Sb(1)-Sb(2)-N(6)	105.6(2)
N(7)-Sb(1)-Sb(2)-N(4)	-166.9(2)
N(1)-Sb(1)-Sb(2)-N(4)	101.6(2)
N(5)-Sb(1)-Sb(2)-N(4)	-77.7(2)
N(3)-Sb(1)-Sb(2)-N(4)	14.1(2)

Symmetry transformations used to generate equivalent atoms:

3.2 Crystal structural analysis data for **5**

Table 1. Crystal data and structure refinement for 150708-1.

Identification code	150708-1
Empirical formula	C64 H112 N16 P8 Sb4
Formula weight	1840.46
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.4526(6) A alpha = 90.444(5) deg.
	b = 13.8011(9) A beta = 100.987(5) deg.
	c = 15.2389(10) A gamma = 94.207(5) deg.
Volume	2151.7(2) A^3
Z, Calculated density	1, 1.420 Mg/m^3
Absorption coefficient	1.435 mm^-1
F(000)	932
Crystal size	0.18 x 0.14 x 0.07 mm
Theta range for data collection	2.92 to 25.68 deg.
Limiting indices	-12<=h<=12, -16<=k<=16, -18<=l<=18
Reflections collected / unique	20849 / 8167 [R(int) = 0.0425]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.53061
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8167 / 1 / 431
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0575, wR2 = 0.1425
R indices (all data)	R1 = 0.0862, wR2 = 0.1660
Largest diff. peak and hole	1.814 and -0.947 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 150708-1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6768(11)	7793(6)	-1884(5)	91(3)
C(2)	6551(7)	7342(5)	-1016(5)	52(2)
C(3)	7164(10)	6379(6)	-915(6)	86(3)
C(4)	7087(6)	8030(5)	-246(4)	46(2)
C(5)	8186(6)	9077(5)	995(5)	49(2)
C(6)	9014(7)	9671(6)	1755(5)	60(2)
C(7)	9317(10)	9062(8)	2584(6)	96(3)
C(8)	10293(8)	10080(7)	1494(7)	87(3)
C(9)	5630(11)	9241(9)	3123(7)	117(4)
C(10)	3371(13)	8979(10)	3434(6)	129(5)
C(11)	4215(9)	9330(6)	2779(5)	70(2)
C(12)	3781(7)	8809(4)	1885(4)	46(2)
C(13)	3055(6)	7835(5)	533(4)	43(1)
C(14)	2522(7)	7163(5)	-266(4)	49(2)
C(15)	2080(12)	6161(6)	22(7)	106(4)
C(16)	1438(9)	7591(6)	-888(5)	72(2)
C(17)	5772(13)	5643(8)	1312(6)	110(4)
C(18)	5743(8)	5817(6)	2285(5)	65(2)
C(19)	6664(13)	6655(7)	2636(7)	109(4)
C(20)	6025(7)	4932(5)	2820(4)	49(2)
C(21)	6622(7)	3459(5)	3579(5)	56(2)
C(22)	7046(11)	2489(6)	3969(6)	85(3)
C(23)	5930(17)	1894(8)	4230(10)	162(7)

C(24)	7598(10)	1917(7)	3290(8)	99(3)
C(25)	9204(15)	3789(8)	6450(8)	140(6)
C(26)	8592(8)	4456(6)	7006(6)	67(2)
C(27)	9505(10)	4676(7)	7875(6)	89(3)
C(28)	8200(7)	5336(5)	6489(5)	54(2)
C(29)	7808(7)	6819(5)	5688(5)	55(2)
C(30)	7738(9)	7790(5)	5254(5)	69(2)
C(31)	7746(19)	8582(7)	5917(8)	165(7)
C(32)	8842(13)	7996(9)	4755(8)	125(4)
N(1)	3750(5)	8657(4)	418(3)	43(1)
N(2)	4156(5)	9217(4)	1184(3)	46(1)
N(3)	7065(5)	9404(4)	593(3)	47(1)
N(4)	6436(5)	8798(4)	-126(3)	45(1)
N(5)	5718(5)	4881(4)	3636(4)	49(1)
N(6)	6062(6)	4043(4)	4070(4)	52(1)
N(7)	6844(5)	6138(4)	5461(4)	49(1)
N(8)	7073(5)	5287(4)	5914(4)	48(1)
P(1)	6778(2)	3921(2)	2541(1)	68(1)
P(2)	2858(2)	7690(1)	1629(1)	62(1)
P(3)	8552(2)	7983(2)	527(2)	62(1)
P(4)	9091(2)	6456(2)	6516(2)	78(1)
Sb(1)	4505(1)	9386(1)	-716(1)	43(1)
Sb(2)	4692(1)	5798(1)	4496(1)	48(1)

Table 3. Bond lengths [A] and angles [deg] for 150708-1.

C(1)-C(2)	1.515(11)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(4)	1.500(9)
C(2)-C(3)	1.514(10)
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(4)	1.330(8)
C(4)-P(3)	1.750(7)
C(5)-N(3)	1.327(8)
C(5)-C(6)	1.503(10)
C(5)-P(3)	1.764(7)
C(6)-C(7)	1.519(11)
C(6)-C(8)	1.535(12)
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(11)	1.486(13)
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600

C(10)-C(11)	1.514(14)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-C(12)	1.510(9)
C(11)-H(11)	0.9800
C(12)-N(2)	1.323(8)
C(12)-P(2)	1.759(7)
C(13)-N(1)	1.333(8)
C(13)-C(14)	1.517(9)
C(13)-P(2)	1.733(6)
C(14)-C(16)	1.493(10)
C(14)-C(15)	1.520(10)
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)	1.507(12)
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-C(19)	1.477(13)
C(18)-C(20)	1.490(10)
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(5)	1.343(8)
C(20)-P(1)	1.740(7)
C(21)-N(6)	1.332(9)
C(21)-C(22)	1.531(11)
C(21)-P(1)	1.742(8)
C(22)-C(23)	1.495(16)
C(22)-C(24)	1.519(13)
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)	1.502(14)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-C(27)	1.492(11)
C(26)-C(28)	1.493(10)
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(8)	1.324(8)
C(28)-P(4)	1.741(8)
C(29)-N(7)	1.319(9)
C(29)-C(30)	1.500(10)
C(29)-P(4)	1.762(7)
C(30)-C(31)	1.480(13)

C(30)-C(32)	1.510(14)
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(2)	1.373(7)
N(1)-Sb(1)	2.248(5)
N(2)-Sb(1)#1	2.488(5)
N(3)-N(4)	1.401(7)
N(3)-Sb(1)#1	2.456(5)
N(4)-Sb(1)	2.258(5)
N(5)-N(6)	1.374(7)
N(5)-Sb(2)	2.275(5)
N(6)-Sb(2)#2	2.474(6)
N(7)-N(8)	1.380(7)
N(7)-Sb(2)	2.453(5)
N(8)-Sb(2)#2	2.276(5)
Sb(1)-N(3)#1	2.456(5)
Sb(1)-N(2)#1	2.488(5)
Sb(1)-Sb(1)#1	2.7451(8)
Sb(2)-N(8)#2	2.276(5)
Sb(2)-N(6)#2	2.474(6)
Sb(2)-Sb(2)#2	2.7407(8)

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(4)-C(2)-C(3)	112.3(6)
C(4)-C(2)-C(1)	110.0(6)
C(3)-C(2)-C(1)	109.1(7)
C(4)-C(2)-H(2)	108.4
C(3)-C(2)-H(2)	108.4
C(1)-C(2)-H(2)	108.4
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(4)-C(4)-C(2)	118.9(6)
N(4)-C(4)-P(3)	113.5(5)
C(2)-C(4)-P(3)	127.5(5)
N(3)-C(5)-C(6)	118.5(6)
N(3)-C(5)-P(3)	114.0(5)
C(6)-C(5)-P(3)	127.4(5)
C(5)-C(6)-C(7)	110.6(7)
C(5)-C(6)-C(8)	110.6(7)
C(7)-C(6)-C(8)	109.7(7)
C(5)-C(6)-H(6)	108.6
C(7)-C(6)-H(6)	108.6
C(8)-C(6)-H(6)	108.6
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(11)-C(9)-H(9A)	109.5
C(11)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(11)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(11)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-C(12)	110.7(7)
C(9)-C(11)-C(10)	112.6(8)
C(12)-C(11)-C(10)	110.9(8)
C(9)-C(11)-H(11)	107.5
C(12)-C(11)-H(11)	107.5
C(10)-C(11)-H(11)	107.5
N(2)-C(12)-C(11)	117.5(6)
N(2)-C(12)-P(2)	113.4(5)
C(11)-C(12)-P(2)	129.1(5)

N(1)-C(13)-C(14)	119.3(6)
N(1)-C(13)-P(2)	112.7(5)
C(14)-C(13)-P(2)	127.9(5)
C(16)-C(14)-C(13)	111.2(6)
C(16)-C(14)-C(15)	110.8(7)
C(13)-C(14)-C(15)	111.6(6)
C(16)-C(14)-H(14)	107.7
C(13)-C(14)-H(14)	107.7
C(15)-C(14)-H(14)	107.7
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(20)	111.7(7)
C(19)-C(18)-C(17)	109.5(8)
C(20)-C(18)-C(17)	111.8(7)

C(19)-C(18)-H(18)	107.9
C(20)-C(18)-H(18)	107.9
C(17)-C(18)-H(18)	107.9
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(5)-C(20)-C(18)	119.0(6)
N(5)-C(20)-P(1)	113.0(5)
C(18)-C(20)-P(1)	128.0(5)
N(6)-C(21)-C(22)	118.4(7)
N(6)-C(21)-P(1)	113.9(5)
C(22)-C(21)-P(1)	127.7(6)
C(23)-C(22)-C(24)	109.2(9)
C(23)-C(22)-C(21)	111.5(8)
C(24)-C(22)-C(21)	110.0(8)
C(23)-C(22)-H(22)	108.7
C(24)-C(22)-H(22)	108.7
C(21)-C(22)-H(22)	108.7
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(27)-C(26)-C(28)	113.9(7)
C(27)-C(26)-C(25)	109.2(8)
C(28)-C(26)-C(25)	110.0(8)
C(27)-C(26)-H(26)	107.9
C(28)-C(26)-H(26)	107.9
C(25)-C(26)-H(26)	107.9
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(8)-C(28)-C(26)	118.9(7)
N(8)-C(28)-P(4)	113.6(5)
C(26)-C(28)-P(4)	127.4(6)
N(7)-C(29)-C(30)	120.2(7)
N(7)-C(29)-P(4)	113.4(5)
C(30)-C(29)-P(4)	126.4(6)
C(31)-C(30)-C(29)	111.5(7)
C(31)-C(30)-C(32)	109.8(10)
C(29)-C(30)-C(32)	111.6(8)

C(31)-C(30)-H(30)	108.0
C(29)-C(30)-H(30)	108.0
C(32)-C(30)-H(30)	108.0
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(13)-N(1)-N(2)	114.1(5)
C(13)-N(1)-Sb(1)	136.6(4)
N(2)-N(1)-Sb(1)	109.2(4)
C(12)-N(2)-N(1)	112.2(5)
C(12)-N(2)-Sb(1)#1	143.3(4)
N(1)-N(2)-Sb(1)#1	104.4(4)
C(5)-N(3)-N(4)	111.9(5)
C(5)-N(3)-Sb(1)#1	143.4(4)
N(4)-N(3)-Sb(1)#1	104.3(3)
C(4)-N(4)-N(3)	113.3(5)
C(4)-N(4)-Sb(1)	137.8(4)
N(3)-N(4)-Sb(1)	108.7(4)
C(20)-N(5)-N(6)	113.2(5)
C(20)-N(5)-Sb(2)	136.9(4)
N(6)-N(5)-Sb(2)	109.8(4)

C(21)-N(6)-N(5)	112.3(6)
C(21)-N(6)-Sb(2)#2	144.0(5)
N(5)-N(6)-Sb(2)#2	103.6(4)
C(29)-N(7)-N(8)	112.7(6)
C(29)-N(7)-Sb(2)	143.0(5)
N(8)-N(7)-Sb(2)	104.3(4)
C(28)-N(8)-N(7)	113.2(6)
C(28)-N(8)-Sb(2)#2	137.6(5)
N(7)-N(8)-Sb(2)#2	109.1(4)
C(20)-P(1)-C(21)	87.6(3)
C(13)-P(2)-C(12)	87.6(3)
C(4)-P(3)-C(5)	87.2(3)
C(28)-P(4)-C(29)	87.0(3)
N(1)-Sb(1)-N(4)	85.88(19)
N(1)-Sb(1)-N(3)#1	85.17(19)
N(4)-Sb(1)-N(3)#1	146.85(17)
N(1)-Sb(1)-N(2)#1	146.41(16)
N(4)-Sb(1)-N(2)#1	85.56(19)
N(3)#1-Sb(1)-N(2)#1	84.49(18)
N(1)-Sb(1)-Sb(1)#1	76.80(12)
N(4)-Sb(1)-Sb(1)#1	76.27(13)
N(3)#1-Sb(1)-Sb(1)#1	70.62(12)
N(2)#1-Sb(1)-Sb(1)#1	69.62(11)
N(5)-Sb(2)-N(8)#2	86.4(2)
N(5)-Sb(2)-N(7)	86.47(19)
N(8)#2-Sb(2)-N(7)	146.54(17)
N(5)-Sb(2)-N(6)#2	146.55(18)
N(8)#2-Sb(2)-N(6)#2	85.9(2)
N(7)-Sb(2)-N(6)#2	82.32(19)
N(5)-Sb(2)-Sb(2)#2	75.71(14)

N(8)#2-Sb(2)-Sb(2)#2	75.63(13)
N(7)-Sb(2)-Sb(2)#2	70.93(13)
N(6)#2-Sb(2)-Sb(2)#2	70.84(12)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 150708-1.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	159(10)	58(5)	55(5)	-11(4)	21(6)	-4(6)
C(2)	65(4)	39(4)	56(4)	-5(3)	21(3)	3(3)
C(3)	121(8)	51(5)	84(6)	-15(4)	14(6)	14(5)
C(4)	52(4)	40(4)	48(4)	4(3)	18(3)	3(3)
C(5)	43(4)	51(4)	52(4)	3(3)	5(3)	1(3)
C(6)	61(5)	60(5)	53(4)	-8(3)	0(3)	-1(4)
C(7)	110(8)	110(8)	58(5)	14(5)	-3(5)	-20(6)
C(8)	70(6)	87(7)	92(7)	0(5)	-3(5)	-19(5)
C(9)	120(9)	152(11)	66(6)	-36(7)	-17(6)	12(8)
C(10)	160(11)	177(13)	55(6)	-29(7)	40(7)	0(10)
C(11)	123(8)	43(4)	42(4)	-5(3)	4(4)	15(4)
C(12)	64(4)	34(3)	41(3)	1(3)	12(3)	10(3)
C(13)	48(4)	37(3)	43(3)	-2(3)	8(3)	3(3)
C(14)	59(4)	39(4)	49(4)	-12(3)	12(3)	-9(3)
C(15)	164(11)	46(5)	93(7)	2(5)	-2(7)	-29(6)
C(16)	84(6)	60(5)	66(5)	-16(4)	5(4)	1(4)
C(17)	171(11)	100(8)	62(6)	16(5)	33(7)	-4(8)
C(18)	79(5)	63(5)	59(5)	12(4)	29(4)	14(4)
C(19)	169(11)	64(6)	87(7)	10(5)	12(7)	-5(7)
C(20)	58(4)	48(4)	43(4)	-2(3)	14(3)	-2(3)
C(21)	62(4)	50(4)	55(4)	-13(3)	6(3)	9(3)
C(22)	129(8)	54(5)	67(5)	-14(4)	-8(5)	37(5)
C(23)	290(18)	72(8)	175(13)	46(8)	153(14)	53(9)
C(24)	109(8)	55(6)	135(9)	-16(6)	28(7)	12(5)

C(25)	201(14)	91(9)	115(9)	0(7)	-20(9)	69(9)
C(26)	58(5)	57(5)	78(5)	8(4)	-5(4)	6(4)
C(27)	100(7)	91(7)	70(6)	14(5)	-2(5)	1(6)
C(28)	51(4)	54(4)	56(4)	3(3)	3(3)	4(3)
C(29)	64(4)	45(4)	50(4)	-6(3)	8(3)	-11(3)
C(30)	89(6)	47(4)	62(5)	2(4)	1(4)	-10(4)
C(31)	360(20)	50(6)	102(9)	9(6)	85(12)	24(10)
C(32)	165(12)	110(9)	98(8)	36(7)	33(8)	-19(8)
N(1)	58(3)	32(3)	35(3)	-5(2)	6(2)	-5(2)
N(2)	62(3)	38(3)	34(3)	-3(2)	5(2)	-7(3)
N(3)	51(3)	43(3)	43(3)	-5(2)	4(2)	4(3)
N(4)	49(3)	42(3)	44(3)	-6(2)	8(2)	4(2)
N(5)	59(4)	41(3)	46(3)	-5(2)	10(3)	6(3)
N(6)	73(4)	38(3)	44(3)	0(2)	9(3)	9(3)
N(7)	56(3)	41(3)	47(3)	-1(2)	4(3)	6(3)
N(8)	49(3)	41(3)	50(3)	4(2)	0(3)	0(2)
P(1)	87(2)	69(1)	52(1)	-9(1)	20(1)	17(1)
P(2)	94(2)	44(1)	50(1)	3(1)	24(1)	-9(1)
P(3)	60(1)	54(1)	72(1)	-3(1)	6(1)	16(1)
P(4)	70(1)	62(1)	85(2)	10(1)	-15(1)	-17(1)
Sb(1)	54(1)	38(1)	35(1)	-8(1)	5(1)	-3(1)
Sb(2)	60(1)	36(1)	46(1)	4(1)	8(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 150708-1.

	x	y	z	U(eq)
H(1A)	6301	8368	-1983	137
H(1B)	6457	7337	-2370	137
H(1C)	7685	7961	-1849	137
H(2)	5608	7219	-1046	63
H(3A)	8086	6484	-902	129
H(3B)	6774	5955	-1412	129
H(3C)	7023	6087	-369	129
H(6)	8528	10216	1891	72
H(7A)	8519	8856	2776	144
H(7B)	9881	9443	3053	144
H(7C)	9744	8502	2449	144
H(8A)	10722	9559	1282	130
H(8B)	10853	10390	2007	130
H(8C)	10103	10545	1031	130
H(9A)	5754	8603	3357	176
H(9B)	5946	9719	3590	176
H(9C)	6103	9342	2646	176
H(10A)	2469	9045	3179	193
H(10B)	3612	9360	3978	193
H(10C)	3497	8308	3560	193
H(11)	4094	10022	2684	84
H(14)	3232	7086	-593	59
H(15A)	2782	5907	435	159
H(15B)	1839	5735	-493	159
H(15C)	1342	6209	305	159

H(16A)	714	7651	-591	108
H(16B)	1166	7177	-1409	108
H(16C)	1737	8222	-1062	108
H(17A)	6659	5602	1240	165
H(17B)	5404	6170	969	165
H(17C)	5271	5046	1106	165
H(18)	4861	5983	2328	78
H(19A)	6637	6770	3254	163
H(19B)	6420	7221	2301	163
H(19C)	7533	6519	2581	163
H(22)	7730	2619	4502	103
H(23A)	5737	2163	4769	243
H(23B)	6160	1238	4329	243
H(23C)	5175	1900	3760	243
H(24A)	7957	1347	3564	148
H(24B)	8272	2314	3088	148
H(24C)	6913	1728	2791	148
H(25A)	8652	3688	5872	209
H(25B)	9308	3177	6740	209
H(25C)	10044	4076	6383	209
H(26)	7797	4110	7135	80
H(27A)	10278	5039	7769	134
H(27B)	9738	4080	8161	134
H(27C)	9085	5053	8255	134
H(30)	6913	7779	4821	82
H(31A)	6959	8510	6156	247
H(31B)	7794	9198	5631	247
H(31C)	8489	8552	6392	247
H(32A)	9663	7986	5162	187
H(32B)	8774	8625	4492	187

H(32C)	8789	7510	4293	187

Table 6. Torsion angles [deg] for 150708-1.

C(3)-C(2)-C(4)-N(4)	-163.7(7)
C(1)-C(2)-C(4)-N(4)	74.5(9)
C(3)-C(2)-C(4)-P(3)	19.0(9)
C(1)-C(2)-C(4)-P(3)	-102.8(7)
N(3)-C(5)-C(6)-C(7)	125.3(8)
P(3)-C(5)-C(6)-C(7)	-57.2(10)
N(3)-C(5)-C(6)-C(8)	-112.9(8)
P(3)-C(5)-C(6)-C(8)	64.6(9)
C(9)-C(11)-C(12)-N(2)	-73.3(9)
C(10)-C(11)-C(12)-N(2)	161.0(8)
C(9)-C(11)-C(12)-P(2)	104.8(9)
C(10)-C(11)-C(12)-P(2)	-20.9(11)
N(1)-C(13)-C(14)-C(16)	-70.8(8)
P(2)-C(13)-C(14)-C(16)	107.9(7)
N(1)-C(13)-C(14)-C(15)	165.0(7)
P(2)-C(13)-C(14)-C(15)	-16.3(10)
C(19)-C(18)-C(20)-N(5)	73.6(10)
C(17)-C(18)-C(20)-N(5)	-163.3(8)
C(19)-C(18)-C(20)-P(1)	-104.2(9)
C(17)-C(18)-C(20)-P(1)	18.9(11)
N(6)-C(21)-C(22)-C(23)	56.0(11)
P(1)-C(21)-C(22)-C(23)	-124.0(9)
N(6)-C(21)-C(22)-C(24)	177.3(8)
P(1)-C(21)-C(22)-C(24)	-2.7(12)
C(27)-C(26)-C(28)-N(8)	-154.5(8)
C(25)-C(26)-C(28)-N(8)	82.5(10)
C(27)-C(26)-C(28)-P(4)	27.9(11)
C(25)-C(26)-C(28)-P(4)	-95.0(10)

N(7)-C(29)-C(30)-C(31)	118.0(11)
P(4)-C(29)-C(30)-C(31)	-61.6(12)
N(7)-C(29)-C(30)-C(32)	-118.9(9)
P(4)-C(29)-C(30)-C(32)	61.5(10)
C(14)-C(13)-N(1)-N(2)	178.6(5)
P(2)-C(13)-N(1)-N(2)	-0.3(7)
C(14)-C(13)-N(1)-Sb(1)	-3.4(9)
P(2)-C(13)-N(1)-Sb(1)	177.7(4)
C(11)-C(12)-N(2)-N(1)	177.4(6)
P(2)-C(12)-N(2)-N(1)	-1.0(7)
C(11)-C(12)-N(2)-Sb(1)#1	3.5(11)
P(2)-C(12)-N(2)-Sb(1)#1	-174.9(4)
C(13)-N(1)-N(2)-C(12)	0.8(8)
Sb(1)-N(1)-N(2)-C(12)	-177.7(4)
C(13)-N(1)-N(2)-Sb(1)#1	177.1(4)
Sb(1)-N(1)-N(2)-Sb(1)#1	-1.5(4)
C(6)-C(5)-N(3)-N(4)	177.1(6)
P(3)-C(5)-N(3)-N(4)	-0.7(7)
C(6)-C(5)-N(3)-Sb(1)#1	-12.2(11)
P(3)-C(5)-N(3)-Sb(1)#1	170.0(5)
C(2)-C(4)-N(4)-N(3)	-177.6(5)
P(3)-C(4)-N(4)-N(3)	0.0(7)
C(2)-C(4)-N(4)-Sb(1)	6.7(10)
P(3)-C(4)-N(4)-Sb(1)	-175.7(4)
C(5)-N(3)-N(4)-C(4)	0.5(8)
Sb(1)#1-N(3)-N(4)-C(4)	-173.8(4)
C(5)-N(3)-N(4)-Sb(1)	177.4(4)
Sb(1)#1-N(3)-N(4)-Sb(1)	3.1(4)
C(18)-C(20)-N(5)-N(6)	-178.2(6)
P(1)-C(20)-N(5)-N(6)	-0.1(8)

C(18)-C(20)-N(5)-Sb(2)	4.7(11)
P(1)-C(20)-N(5)-Sb(2)	-177.2(4)
C(22)-C(21)-N(6)-N(5)	-179.3(7)
P(1)-C(21)-N(6)-N(5)	0.7(8)
C(22)-C(21)-N(6)-Sb(2)#2	-1.8(13)
P(1)-C(21)-N(6)-Sb(2)#2	178.2(5)
C(20)-N(5)-N(6)-C(21)	-0.4(8)
Sb(2)-N(5)-N(6)-C(21)	177.5(5)
C(20)-N(5)-N(6)-Sb(2)#2	-178.8(5)
Sb(2)-N(5)-N(6)-Sb(2)#2	-1.0(4)
C(30)-C(29)-N(7)-N(8)	179.1(7)
P(4)-C(29)-N(7)-N(8)	-1.2(8)
C(30)-C(29)-N(7)-Sb(2)	-1.1(12)
P(4)-C(29)-N(7)-Sb(2)	178.6(4)
C(26)-C(28)-N(8)-N(7)	-178.2(6)
P(4)-C(28)-N(8)-N(7)	-0.3(8)
C(26)-C(28)-N(8)-Sb(2)#2	6.3(11)
P(4)-C(28)-N(8)-Sb(2)#2	-175.8(4)
C(29)-N(7)-N(8)-C(28)	1.0(8)
Sb(2)-N(7)-N(8)-C(28)	-178.9(5)
C(29)-N(7)-N(8)-Sb(2)#2	177.7(5)
Sb(2)-N(7)-N(8)-Sb(2)#2	-2.1(4)
N(5)-C(20)-P(1)-C(21)	0.4(6)
C(18)-C(20)-P(1)-C(21)	178.3(7)
N(6)-C(21)-P(1)-C(20)	-0.6(6)
C(22)-C(21)-P(1)-C(20)	179.4(8)
N(1)-C(13)-P(2)-C(12)	-0.2(5)
C(14)-C(13)-P(2)-C(12)	-179.0(6)
N(2)-C(12)-P(2)-C(13)	0.7(5)
C(11)-C(12)-P(2)-C(13)	-177.5(7)

N(4)-C(4)-P(3)-C(5)	-0.3(5)
C(2)-C(4)-P(3)-C(5)	177.1(6)
N(3)-C(5)-P(3)-C(4)	0.6(5)
C(6)-C(5)-P(3)-C(4)	-177.0(7)
N(8)-C(28)-P(4)-C(29)	-0.3(6)
C(26)-C(28)-P(4)-C(29)	177.4(8)
N(7)-C(29)-P(4)-C(28)	0.8(6)
C(30)-C(29)-P(4)-C(28)	-179.5(7)
C(13)-N(1)-Sb(1)-N(4)	-99.9(6)
N(2)-N(1)-Sb(1)-N(4)	78.2(4)
C(13)-N(1)-Sb(1)-N(3)#1	112.0(6)
N(2)-N(1)-Sb(1)-N(3)#1	-69.9(4)
C(13)-N(1)-Sb(1)-N(2)#1	-175.5(5)
N(2)-N(1)-Sb(1)-N(2)#1	2.6(7)
C(13)-N(1)-Sb(1)-Sb(1)#1	-176.8(6)
N(2)-N(1)-Sb(1)-Sb(1)#1	1.3(3)
C(4)-N(4)-Sb(1)-N(1)	95.6(7)
N(3)-N(4)-Sb(1)-N(1)	-80.2(4)
C(4)-N(4)-Sb(1)-N(3)#1	170.3(5)
N(3)-N(4)-Sb(1)-N(3)#1	-5.5(7)
C(4)-N(4)-Sb(1)-N(2)#1	-116.9(7)
N(3)-N(4)-Sb(1)-N(2)#1	67.3(4)
C(4)-N(4)-Sb(1)-Sb(1)#1	173.0(7)
N(3)-N(4)-Sb(1)-Sb(1)#1	-2.8(4)
C(20)-N(5)-Sb(2)-N(8)#2	101.9(7)
N(6)-N(5)-Sb(2)-N(8)#2	-75.2(4)
C(20)-N(5)-Sb(2)-N(7)	-110.8(7)
N(6)-N(5)-Sb(2)-N(7)	72.1(4)
C(20)-N(5)-Sb(2)-N(6)#2	178.9(6)
N(6)-N(5)-Sb(2)-N(6)#2	1.7(7)

C(20)-N(5)-Sb(2)-Sb(2)#2	178.0(7)
N(6)-N(5)-Sb(2)-Sb(2)#2	0.9(4)
C(29)-N(7)-Sb(2)-N(5)	105.9(8)
N(8)-N(7)-Sb(2)-N(5)	-74.3(4)
C(29)-N(7)-Sb(2)-N(8)#2	-176.1(7)
N(8)-N(7)-Sb(2)-N(8)#2	3.6(7)
C(29)-N(7)-Sb(2)-N(6)#2	-105.7(8)
N(8)-N(7)-Sb(2)-N(6)#2	74.1(4)
C(29)-N(7)-Sb(2)-Sb(2)#2	-178.0(8)
N(8)-N(7)-Sb(2)-Sb(2)#2	1.8(3)

Symmetry transformations used to generate equivalent atoms:

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

3.3 Crystal structural analysis data for **6**

Table 1. Crystal data and structure refinement for 151203-2a.

Identification code	151203-2a
Empirical formula	C63 H96 N8 P4 Sb2
Formula weight	1332.86
Temperature	298(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.9130(3) A alpha = 102.330(2) deg.
	b = 11.8061(3) A beta = 106.292(2) deg.
	c = 16.0228(4) A gamma = 104.337(2) deg.
Volume	1828.71(8) A^3
Z, Calculated density	1, 1.210 Mg/m^3
Absorption coefficient	0.865 mm^-1
F(000)	692
Crystal size	0.25 x 0.14 x 0.08 mm
Theta range for data collection	2.84 to 25.68 deg.
Limiting indices	-13<=h<=13, -14<=k<=14, -19<=l<=19
Reflections collected / unique	42583 / 6954 [R(int) = 0.0386]
Completeness to theta = 25.68	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.64398
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6954 / 80 / 367
Goodness-of-fit on F^2	1.097
Final R indices [I>2sigma(I)]	R1 = 0.0423, wR2 = 0.1216
R indices (all data)	R1 = 0.0535, wR2 = 0.1307
Largest diff. peak and hole	0.699 and -0.495 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 151203-2a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7852(5)	8062(5)	5823(4)	77(2)
C(2)	7718(6)	8816(7)	6664(5)	98(2)
C(3)	6317(6)	8788(5)	6521(4)	78(2)
C(4)	5346(7)	7508(6)	6176(5)	84(2)
C(5)	5465(5)	6812(5)	5291(4)	75(2)
C(6)	6918(5)	6791(4)	5458(3)	52(1)
C(7)	7065(4)	6081(4)	4608(3)	46(1)
C(8)	7116(4)	5022(4)	3158(3)	47(1)
C(9)	6993(5)	4360(4)	2213(3)	55(1)
C(10)	5941(10)	3133(6)	1852(5)	119(3)
C(11)	5801(12)	2463(7)	876(6)	151(4)
C(12)	5608(8)	3206(9)	243(5)	121(3)
C(13)	6603(8)	4376(7)	599(4)	99(2)
C(14)	6719(8)	5090(6)	1556(4)	84(2)
C(15)	10634(7)	6512(9)	2409(4)	114(3)
C(16)	10606(8)	5917(10)	1443(5)	134(4)
C(17)	11825(9)	6491(11)	1305(5)	134(4)
C(18)	13059(8)	6629(11)	1993(5)	140(4)
C(34)	9045(14)	1212(12)	2(11)	192(12)
C(29)	9501(18)	1823(14)	931(11)	189(7)
C(30)	10814(19)	2635(14)	1369(11)	192(7)
C(31)	11671(15)	2834(13)	878(14)	193(6)
C(32)	11215(16)	2223(15)	-51(14)	193(7)

C(33)	9902(17)	1412(14)	-489(10)	193(7)
C(19)	13084(7)	7287(7)	2966(5)	94(2)
C(20)	11830(6)	6559(5)	3121(3)	68(1)
C(21)	11806(5)	7141(4)	4048(3)	57(1)
C(22)	11803(5)	8275(4)	5487(3)	51(1)
C(23)	11916(5)	9113(4)	6372(3)	56(1)
C(24)	11446(6)	10191(5)	6244(4)	74(1)
C(25)	11575(6)	11034(6)	7154(4)	87(2)
C(26)	13001(7)	11478(6)	7824(5)	90(2)
C(27)	13481(7)	10436(6)	7949(4)	91(2)
C(28)	13362(6)	9602(5)	7049(4)	76(1)
C(35)	7645(16)	305(19)	-464(16)	172(10)
N(1)	11208(3)	7080(3)	5277(2)	43(1)
N(2)	11203(4)	6433(3)	4457(2)	45(1)
N(3)	8071(3)	5626(3)	4688(2)	43(1)
N(4)	8106(3)	5024(3)	3864(2)	46(1)
P(1)	6056(1)	5790(2)	3473(1)	65(1)
P(2)	12442(2)	8697(1)	4669(1)	82(1)
Sb(1)	9974(1)	5616(1)	5819(1)	41(1)

Table 3. Bond lengths [A] and angles [deg] for 151203-2a.

C(1)-C(6)	1.472(7)
C(1)-C(2)	1.515(8)
C(1)-H(1A)	0.9700
C(1)-H(1B)	0.9700
C(2)-C(3)	1.472(8)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.495(8)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.537(8)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
C(5)-C(6)	1.540(7)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-C(7)	1.511(6)
C(6)-H(6)	0.9800
C(7)-N(3)	1.324(5)
C(7)-P(1)	1.750(4)
C(8)-N(4)	1.326(5)
C(8)-C(9)	1.501(6)
C(8)-P(1)	1.751(4)
C(9)-C(10)	1.482(8)
C(9)-C(14)	1.509(7)
C(9)-H(9)	0.9800
C(10)-C(11)	1.539(10)
C(10)-H(10A)	0.9700

C(10)-H(10B)	0.9700
C(11)-C(12)	1.481(13)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.409(11)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.538(8)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(20)	1.451(9)
C(15)-C(16)	1.545(10)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.436(11)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.427(11)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.576(11)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(34)-C(29)	1.3900
C(34)-C(33)	1.3900
C(34)-C(35)	1.499(10)
C(29)-C(30)	1.3900
C(29)-H(29)	0.9300

C(30)-C(31)	1.3900
C(30)-H(30)	0.9300
C(31)-C(32)	1.3900
C(31)-H(31)	0.9300
C(32)-C(33)	1.3900
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(19)-C(20)	1.541(8)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.508(7)
C(20)-H(20)	0.9800
C(21)-N(2)	1.329(6)
C(21)-P(2)	1.746(5)
C(22)-N(1)	1.321(5)
C(22)-C(23)	1.499(6)
C(22)-P(2)	1.753(5)
C(23)-C(24)	1.517(7)
C(23)-C(28)	1.525(7)
C(23)-H(23)	0.9800
C(24)-C(25)	1.527(8)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(26)	1.506(9)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(27)	1.480(9)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-C(28)	1.513(8)

C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
N(1)-N(2)	1.369(4)
N(1)-Sb(1)	2.387(3)
N(2)-Sb(1)#1	2.320(3)
N(3)-N(4)	1.376(4)
N(3)-Sb(1)	2.346(3)
N(4)-Sb(1)#1	2.360(3)
Sb(1)-N(2)#1	2.320(3)
Sb(1)-N(4)#1	2.360(3)
Sb(1)-Sb(1)#1	2.7399(5)

C(6)-C(1)-C(2)	113.8(5)
C(6)-C(1)-H(1A)	108.8
C(2)-C(1)-H(1A)	108.8
C(6)-C(1)-H(1B)	108.8
C(2)-C(1)-H(1B)	108.8
H(1A)-C(1)-H(1B)	107.7
C(3)-C(2)-C(1)	112.2(5)
C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2A)	109.2
C(3)-C(2)-H(2B)	109.2
C(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(2)-C(3)-C(4)	112.2(5)

C(2)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3A)	109.2
C(2)-C(3)-H(3B)	109.2
C(4)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(3)-C(4)-C(5)	109.5(5)
C(3)-C(4)-H(4A)	109.8
C(5)-C(4)-H(4A)	109.8
C(3)-C(4)-H(4B)	109.8
C(5)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.2
C(4)-C(5)-C(6)	110.5(5)
C(4)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
C(6)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	108.1
C(1)-C(6)-C(7)	112.0(4)
C(1)-C(6)-C(5)	108.9(4)
C(7)-C(6)-C(5)	112.1(4)
C(1)-C(6)-H(6)	107.9
C(7)-C(6)-H(6)	107.9
C(5)-C(6)-H(6)	107.9
N(3)-C(7)-C(6)	119.4(4)
N(3)-C(7)-P(1)	113.1(3)
C(6)-C(7)-P(1)	127.5(3)
N(4)-C(8)-C(9)	118.8(4)
N(4)-C(8)-P(1)	113.5(3)
C(9)-C(8)-P(1)	127.7(3)
C(10)-C(9)-C(8)	111.6(5)

C(10)-C(9)-C(14)	110.0(5)
C(8)-C(9)-C(14)	112.5(4)
C(10)-C(9)-H(9)	107.5
C(8)-C(9)-H(9)	107.5
C(14)-C(9)-H(9)	107.5
C(9)-C(10)-C(11)	111.5(6)
C(9)-C(10)-H(10A)	109.3
C(11)-C(10)-H(10A)	109.3
C(9)-C(10)-H(10B)	109.3
C(11)-C(10)-H(10B)	109.3
H(10A)-C(10)-H(10B)	108.0
C(12)-C(11)-C(10)	113.3(7)
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11B)	108.9
C(10)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	111.8(6)
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12B)	109.2
C(11)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(12)-C(13)-C(14)	113.5(6)
C(12)-C(13)-H(13A)	108.9
C(14)-C(13)-H(13A)	108.9
C(12)-C(13)-H(13B)	108.9
C(14)-C(13)-H(13B)	108.9
H(13A)-C(13)-H(13B)	107.7
C(9)-C(14)-C(13)	110.6(5)

C(9)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14A)	109.5
C(9)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	108.1
C(20)-C(15)-C(16)	112.3(6)
C(20)-C(15)-H(15A)	109.1
C(16)-C(15)-H(15A)	109.1
C(20)-C(15)-H(15B)	109.1
C(16)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.9
C(17)-C(16)-C(15)	111.9(7)
C(17)-C(16)-H(16A)	109.2
C(15)-C(16)-H(16A)	109.2
C(17)-C(16)-H(16B)	109.2
C(15)-C(16)-H(16B)	109.2
H(16A)-C(16)-H(16B)	107.9
C(18)-C(17)-C(16)	116.0(8)
C(18)-C(17)-H(17A)	108.3
C(16)-C(17)-H(17A)	108.3
C(18)-C(17)-H(17B)	108.3
C(16)-C(17)-H(17B)	108.3
H(17A)-C(17)-H(17B)	107.4
C(17)-C(18)-C(19)	110.5(7)
C(17)-C(18)-H(18A)	109.6
C(19)-C(18)-H(18A)	109.6
C(17)-C(18)-H(18B)	109.6
C(19)-C(18)-H(18B)	109.6
H(18A)-C(18)-H(18B)	108.1
C(29)-C(34)-C(33)	120.0

C(29)-C(34)-C(35)	120.0
C(33)-C(34)-C(35)	120.0
C(30)-C(29)-C(34)	120.0
C(30)-C(29)-H(29)	120.0
C(34)-C(29)-H(29)	120.0
C(29)-C(30)-C(31)	120.0
C(29)-C(30)-H(30)	120.0
C(31)-C(30)-H(30)	120.0
C(32)-C(31)-C(30)	120.0
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	120.0
C(31)-C(32)-H(32)	120.0
C(33)-C(32)-H(32)	120.0
C(32)-C(33)-C(34)	120.0
C(32)-C(33)-H(33)	120.0
C(34)-C(33)-H(33)	120.0
C(20)-C(19)-C(18)	109.1(6)
C(20)-C(19)-H(19A)	109.9
C(18)-C(19)-H(19A)	109.9
C(20)-C(19)-H(19B)	109.9
C(18)-C(19)-H(19B)	109.9
H(19A)-C(19)-H(19B)	108.3
C(15)-C(20)-C(21)	110.2(5)
C(15)-C(20)-C(19)	108.3(5)
C(21)-C(20)-C(19)	111.5(5)
C(15)-C(20)-H(20)	108.9
C(21)-C(20)-H(20)	108.9
C(19)-C(20)-H(20)	108.9
N(2)-C(21)-C(20)	119.0(4)

N(2)-C(21)-P(2)	113.4(3)
C(20)-C(21)-P(2)	127.6(4)
N(1)-C(22)-C(23)	119.7(4)
N(1)-C(22)-P(2)	113.6(3)
C(23)-C(22)-P(2)	126.7(3)
C(22)-C(23)-C(24)	112.3(4)
C(22)-C(23)-C(28)	111.3(4)
C(24)-C(23)-C(28)	108.8(4)
C(22)-C(23)-H(23)	108.1
C(24)-C(23)-H(23)	108.1
C(28)-C(23)-H(23)	108.1
C(23)-C(24)-C(25)	111.4(5)
C(23)-C(24)-H(24A)	109.4
C(25)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24B)	109.4
C(25)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
C(26)-C(25)-C(24)	111.3(5)
C(26)-C(25)-H(25A)	109.4
C(24)-C(25)-H(25A)	109.4
C(26)-C(25)-H(25B)	109.4
C(24)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0
C(27)-C(26)-C(25)	111.2(5)
C(27)-C(26)-H(26A)	109.4
C(25)-C(26)-H(26A)	109.4
C(27)-C(26)-H(26B)	109.4
C(25)-C(26)-H(26B)	109.4
H(26A)-C(26)-H(26B)	108.0
C(26)-C(27)-C(28)	111.7(6)

C(26)-C(27)-H(27A)	109.3
C(28)-C(27)-H(27A)	109.3
C(26)-C(27)-H(27B)	109.3
C(28)-C(27)-H(27B)	109.3
H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-C(23)	111.6(5)
C(27)-C(28)-H(28A)	109.3
C(23)-C(28)-H(28A)	109.3
C(27)-C(28)-H(28B)	109.3
C(23)-C(28)-H(28B)	109.3
H(28A)-C(28)-H(28B)	108.0
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(22)-N(1)-N(2)	113.0(3)
C(22)-N(1)-Sb(1)	140.7(3)
N(2)-N(1)-Sb(1)	106.1(2)
C(21)-N(2)-N(1)	113.1(3)
C(21)-N(2)-Sb(1)#1	139.1(3)
N(1)-N(2)-Sb(1)#1	107.7(2)
C(7)-N(3)-N(4)	113.5(3)
C(7)-N(3)-Sb(1)	139.8(3)
N(4)-N(3)-Sb(1)	106.5(2)
C(8)-N(4)-N(3)	112.7(3)
C(8)-N(4)-Sb(1)#1	140.1(3)
N(3)-N(4)-Sb(1)#1	107.1(2)
C(7)-P(1)-C(8)	87.2(2)

C(21)-P(2)-C(22)	87.0(2)
N(2)#1-Sb(1)-N(3)	86.25(12)
N(2)#1-Sb(1)-N(4)#1	84.12(12)
N(3)-Sb(1)-N(4)#1	146.31(11)
N(2)#1-Sb(1)-N(1)	146.15(11)
N(3)-Sb(1)-N(1)	84.55(12)
N(4)#1-Sb(1)-N(1)	85.72(12)
N(2)#1-Sb(1)-Sb(1)#1	74.02(8)
N(3)-Sb(1)-Sb(1)#1	73.59(8)
N(4)#1-Sb(1)-Sb(1)#1	72.73(7)
N(1)-Sb(1)-Sb(1)#1	72.13(7)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 151203-2a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	59(3)	78(4)	79(4)	-5(3)	30(3)	16(3)
C(2)	82(4)	96(5)	82(4)	-26(4)	22(3)	25(3)
C(3)	89(4)	66(3)	82(4)	5(3)	42(3)	34(3)
C(4)	96(4)	76(4)	109(5)	23(3)	73(4)	37(3)
C(5)	63(3)	68(3)	90(4)	1(3)	35(3)	24(3)
C(6)	69(3)	58(3)	43(2)	16(2)	26(2)	38(2)
C(7)	55(2)	49(2)	39(2)	10(2)	19(2)	26(2)
C(8)	54(2)	56(3)	31(2)	9(2)	12(2)	26(2)
C(9)	61(3)	68(3)	31(2)	6(2)	10(2)	31(2)
C(10)	196(9)	70(4)	69(4)	-2(3)	65(5)	6(5)
C(11)	228(11)	83(5)	85(6)	-29(4)	65(7)	-11(6)
C(12)	93(5)	176(9)	44(4)	-17(5)	8(3)	20(5)
C(13)	132(6)	131(6)	44(3)	26(4)	35(4)	52(5)
C(14)	124(5)	92(4)	45(3)	21(3)	34(3)	46(4)
C(15)	71(4)	180(8)	65(4)	6(5)	28(3)	18(4)
C(16)	103(6)	204(10)	61(4)	5(5)	23(4)	31(6)
C(17)	118(6)	224(11)	57(4)	39(5)	40(4)	45(7)
C(18)	93(5)	268(13)	74(5)	56(6)	50(4)	60(6)
C(34)	260(30)	140(20)	260(30)	110(20)	100(30)	160(20)
C(29)	206(14)	164(12)	272(18)	111(12)	97(14)	135(11)
C(30)	210(13)	163(12)	274(18)	113(12)	94(13)	133(11)
C(31)	212(13)	163(12)	274(18)	116(12)	96(13)	128(10)
C(32)	215(13)	162(12)	272(18)	117(12)	97(14)	127(11)
C(33)	219(14)	160(12)	274(18)	118(12)	94(14)	133(11)

C(19)	88(3)	118(4)	69(3)	22(3)	35(3)	22(3)
C(20)	92(3)	76(3)	51(2)	26(2)	41(2)	31(2)
C(21)	82(3)	54(2)	48(2)	20(2)	35(2)	28(2)
C(22)	63(2)	39(2)	50(2)	8(2)	25(2)	14(2)
C(23)	67(2)	44(2)	54(2)	6(2)	27(2)	16(2)
C(24)	79(3)	59(2)	72(3)	0(2)	15(2)	32(2)
C(25)	91(3)	67(3)	82(3)	-9(2)	16(2)	36(2)
C(26)	93(3)	67(3)	78(3)	-12(2)	13(3)	23(2)
C(27)	94(3)	79(3)	73(3)	-5(2)	9(3)	28(3)
C(28)	81(3)	70(3)	67(3)	3(2)	16(2)	33(2)
C(35)	107(14)	180(20)	250(30)	100(20)	59(16)	55(14)
N(1)	60(2)	36(2)	36(2)	6(1)	22(2)	15(2)
N(2)	64(2)	42(2)	37(2)	11(2)	26(2)	21(2)
N(3)	55(2)	45(2)	33(2)	7(1)	16(2)	27(2)
N(4)	60(2)	51(2)	28(2)	5(1)	15(2)	29(2)
P(1)	69(1)	90(1)	42(1)	13(1)	14(1)	51(1)
P(2)	127(1)	46(1)	80(1)	18(1)	64(1)	11(1)
Sb(1)	59(1)	41(1)	25(1)	4(1)	16(1)	22(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 151203-2a.

	x	y	z	U(eq)
H(1A)	7690	8461	5351	92
H(1B)	8772	8047	5971	92
H(2A)	8026	8501	7169	117
H(2B)	8295	9659	6829	117
H(3A)	6059	9221	6085	93
H(3B)	6265	9213	7093	93
H(4A)	4432	7527	6060	101
H(4B)	5546	7091	6632	101
H(5A)	5220	7208	4827	90
H(5B)	4844	5978	5070	90
H(6)	7137	6382	5925	62
H(9)	7859	4236	2250	65
H(10A)	5082	3224	1851	143
H(10B)	6175	2643	2248	143
H(11A)	6605	2241	898	181
H(11B)	5036	1710	639	181
H(12A)	5642	2779	-334	145
H(12B)	4722	3299	128	145
H(13A)	6393	4852	187	119
H(13B)	7470	4283	625	119
H(14A)	7446	5868	1774	101
H(14B)	5885	5262	1525	101
H(15A)	10607	7338	2463	137
H(15B)	9836	6046	2494	137
H(16A)	10486	5052	1355	160

H(16B)	9841	5981	993	160
H(17A)	11805	6013	725	161
H(17B)	11829	7297	1258	161
H(18A)	13816	7109	1875	168
H(18B)	13150	5828	1975	168
H(29)	8927	1690	1259	227
H(30)	11119	3044	1990	230
H(31)	12549	3377	1171	231
H(32)	11788	2357	-380	231
H(33)	9596	1003	-1111	232
H(19A)	13899	7327	3432	112
H(19B)	13083	8118	3006	112
H(20)	11842	5721	3075	81
H(23)	11341	8641	6636	67
H(24A)	10510	9889	5838	89
H(24B)	11983	10654	5962	89
H(25A)	11310	11734	7053	104
H(25B)	10969	10594	7406	104
H(26A)	13592	12000	7605	108
H(26B)	13038	11963	8407	108
H(27A)	12953	9968	8232	109
H(27B)	14417	10750	8354	109
H(28A)	13657	8918	7155	92
H(28B)	13952	10052	6791	92
H(35A)	7576	-384	-231	259
H(35B)	7458	29	-1109	259
H(35C)	7003	689	-350	259

Table 6. Torsion angles [deg] for 151203-2a.

C(6)-C(1)-C(2)-C(3)	-53.1(9)
C(1)-C(2)-C(3)-C(4)	53.2(9)
C(2)-C(3)-C(4)-C(5)	-56.5(8)
C(3)-C(4)-C(5)-C(6)	58.5(7)
C(2)-C(1)-C(6)-C(7)	178.8(5)
C(2)-C(1)-C(6)-C(5)	54.3(7)
C(4)-C(5)-C(6)-C(1)	-57.2(6)
C(4)-C(5)-C(6)-C(7)	178.3(5)
C(1)-C(6)-C(7)-N(3)	79.6(6)
C(5)-C(6)-C(7)-N(3)	-157.6(4)
C(1)-C(6)-C(7)-P(1)	-98.9(5)
C(5)-C(6)-C(7)-P(1)	23.9(6)
N(4)-C(8)-C(9)-C(10)	99.7(6)
P(1)-C(8)-C(9)-C(10)	-78.2(7)
N(4)-C(8)-C(9)-C(14)	-136.1(5)
P(1)-C(8)-C(9)-C(14)	46.1(7)
C(8)-C(9)-C(10)-C(11)	179.1(7)
C(14)-C(9)-C(10)-C(11)	53.5(10)
C(9)-C(10)-C(11)-C(12)	-52.0(12)
C(10)-C(11)-C(12)-C(13)	51.7(12)
C(11)-C(12)-C(13)-C(14)	-53.9(10)
C(10)-C(9)-C(14)-C(13)	-55.0(8)
C(8)-C(9)-C(14)-C(13)	179.9(5)
C(12)-C(13)-C(14)-C(9)	56.5(9)
C(20)-C(15)-C(16)-C(17)	-53.1(12)
C(15)-C(16)-C(17)-C(18)	50.3(14)
C(16)-C(17)-C(18)-C(19)	-52.5(13)
C(33)-C(34)-C(29)-C(30)	0.0
C(35)-C(34)-C(29)-C(30)	177.9(14)

C(34)-C(29)-C(30)-C(31)	0.0
C(29)-C(30)-C(31)-C(32)	0.0
C(30)-C(31)-C(32)-C(33)	0.0
C(31)-C(32)-C(33)-C(34)	0.0
C(29)-C(34)-C(33)-C(32)	0.0
C(35)-C(34)-C(33)-C(32)	-177.9(14)
C(17)-C(18)-C(19)-C(20)	55.7(11)
C(16)-C(15)-C(20)-C(21)	-179.7(7)
C(16)-C(15)-C(20)-C(19)	58.1(9)
C(18)-C(19)-C(20)-C(15)	-59.2(8)
C(18)-C(19)-C(20)-C(21)	179.4(6)
C(15)-C(20)-C(21)-N(2)	88.7(7)
C(19)-C(20)-C(21)-N(2)	-151.0(5)
C(15)-C(20)-C(21)-P(2)	-88.8(7)
C(19)-C(20)-C(21)-P(2)	31.5(7)
N(1)-C(22)-C(23)-C(24)	-130.5(5)
P(2)-C(22)-C(23)-C(24)	51.7(6)
N(1)-C(22)-C(23)-C(28)	107.2(5)
P(2)-C(22)-C(23)-C(28)	-70.5(6)
C(22)-C(23)-C(24)-C(25)	-179.8(5)
C(28)-C(23)-C(24)-C(25)	-56.1(7)
C(23)-C(24)-C(25)-C(26)	56.2(8)
C(24)-C(25)-C(26)-C(27)	-55.1(9)
C(25)-C(26)-C(27)-C(28)	55.5(9)
C(26)-C(27)-C(28)-C(23)	-57.1(8)
C(22)-C(23)-C(28)-C(27)	-179.3(5)
C(24)-C(23)-C(28)-C(27)	56.5(7)
C(23)-C(22)-N(1)-N(2)	-178.9(4)
P(2)-C(22)-N(1)-N(2)	-0.9(5)
C(23)-C(22)-N(1)-Sb(1)	6.2(7)

P(2)-C(22)-N(1)-Sb(1)	-175.8(3)
C(20)-C(21)-N(2)-N(1)	-177.6(4)
P(2)-C(21)-N(2)-N(1)	0.2(5)
C(20)-C(21)-N(2)-Sb(1)#1	-1.2(8)
P(2)-C(21)-N(2)-Sb(1)#1	176.7(3)
C(22)-N(1)-N(2)-C(21)	0.4(5)
Sb(1)-N(1)-N(2)-C(21)	177.1(3)
C(22)-N(1)-N(2)-Sb(1)#1	-177.2(3)
Sb(1)-N(1)-N(2)-Sb(1)#1	-0.5(3)
C(6)-C(7)-N(3)-N(4)	-178.7(4)
P(1)-C(7)-N(3)-N(4)	0.0(5)
C(6)-C(7)-N(3)-Sb(1)	-4.1(7)
P(1)-C(7)-N(3)-Sb(1)	174.6(3)
C(9)-C(8)-N(4)-N(3)	-177.8(4)
P(1)-C(8)-N(4)-N(3)	0.3(5)
C(9)-C(8)-N(4)-Sb(1)#1	5.7(7)
P(1)-C(8)-N(4)-Sb(1)#1	-176.1(3)
C(7)-N(3)-N(4)-C(8)	-0.2(5)
Sb(1)-N(3)-N(4)-C(8)	-176.6(3)
C(7)-N(3)-N(4)-Sb(1)#1	177.4(3)
Sb(1)-N(3)-N(4)-Sb(1)#1	1.0(3)
N(3)-C(7)-P(1)-C(8)	0.1(4)
C(6)-C(7)-P(1)-C(8)	178.7(4)
N(4)-C(8)-P(1)-C(7)	-0.2(4)
C(9)-C(8)-P(1)-C(7)	177.7(4)
N(2)-C(21)-P(2)-C(22)	-0.6(4)
C(20)-C(21)-P(2)-C(22)	177.1(5)
N(1)-C(22)-P(2)-C(21)	0.8(4)
C(23)-C(22)-P(2)-C(21)	178.7(4)
C(7)-N(3)-Sb(1)-N(2)#1	109.8(5)

N(4)-N(3)-Sb(1)-N(2)#1	-75.3(3)
C(7)-N(3)-Sb(1)-N(4)#1	-176.6(4)
N(4)-N(3)-Sb(1)-N(4)#1	-1.8(4)
C(7)-N(3)-Sb(1)-N(1)	-102.8(5)
N(4)-N(3)-Sb(1)-N(1)	72.1(2)
C(7)-N(3)-Sb(1)-Sb(1)#1	-175.7(5)
N(4)-N(3)-Sb(1)-Sb(1)#1	-0.9(2)
C(22)-N(1)-Sb(1)-N(2)#1	176.0(4)
N(2)-N(1)-Sb(1)-N(2)#1	0.9(4)
C(22)-N(1)-Sb(1)-N(3)	101.1(5)
N(2)-N(1)-Sb(1)-N(3)	-74.0(2)
C(22)-N(1)-Sb(1)-N(4)#1	-111.2(5)
N(2)-N(1)-Sb(1)-N(4)#1	73.7(2)
C(22)-N(1)-Sb(1)-Sb(1)#1	175.6(5)
N(2)-N(1)-Sb(1)-Sb(1)#1	0.4(2)

Symmetry transformations used to generate equivalent atoms:

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

3.4 Crystal structural analysis data for **9**

Table 1. Crystal data and structure refinement for 121201-1a.

Identification code	121201-1a
Empirical formula	C14 H26 Li N2 O P
Formula weight	276.28
Temperature	153(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/m
Unit cell dimensions	a = 9.9007(11) A alpha = 90 deg.
	b = 18.4778(10) A beta = 114.866(12) deg.
	c = 10.4804(10) A gamma = 90 deg.
Volume	1739.6(3) A^3
Z, Calculated density	4, 1.055 Mg/m^3
Absorption coefficient	0.152 mm^-1
F(000)	600
Crystal size	0.22 x0.15 x 0.10 mm
Theta range for data collection	3.07 to 25.50 deg.
Limiting indices	-11<=h<=9, -22<=k<=13, -10<=l<=12
Reflections collected / unique	3558 / 1670 [R(int) = 0.0265]
Completeness to theta = 25.50	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.70177
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1670 / 0 / 94
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0633, wR2 = 0.1727
R indices (all data)	R1 = 0.0892, wR2 = 0.1914
Extinction coefficient	0.020(4)
Largest diff. peak and hole	0.329 and -0.271 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 121201-1a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	0	2274(1)	0	59(1)
N(1)	610(2)	922(1)	644(2)	55(1)
C(5)	1051(3)	1587(1)	1116(2)	49(1)
O(1)	2643(4)	0	-573(3)	78(1)
C(4)	2369(3)	1670(2)	2548(3)	62(1)
C(6)	2662(6)	628(2)	-1364(4)	103(1)
C(2)	2789(5)	2477(2)	2833(5)	112(2)
C(3)	1941(5)	1392(3)	3680(4)	115(2)
C(1)	3722(4)	1285(2)	2549(4)	105(1)
Li(1A)	1552(8)	0	545(7)	63(2)
C(7)	2365(10)	389(3)	-2733(6)	168(3)

Table 3. Bond lengths [A] and angles [deg] for 121201-1a.

P(1)-C(5)#1	1.743(2)
P(1)-C(5)	1.743(2)
N(1)-C(5)	1.329(3)
N(1)-N(1)#1	1.383(4)
N(1)-Li(1A)	1.965(4)
N(1)-Li(1A)#2	2.606(6)
C(5)-C(4)	1.527(4)
O(1)-C(6)#3	1.430(4)
O(1)-C(6)	1.430(4)
O(1)-Li(1A)	1.899(8)
C(4)-C(3)	1.508(5)
C(4)-C(1)	1.517(5)
C(4)-C(2)	1.542(5)
C(6)-C(7)	1.408(6)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
Li(1A)-N(1)#3	1.965(4)
Li(1A)-N(1)#2	2.606(6)
Li(1A)-N(1)#1	2.606(6)

Li(1A)-Li(1A)#2	2.792(14)
C(7)-C(7)#3	1.438(10)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700

C(5)#1-P(1)-C(5)	86.58(16)
C(5)-N(1)-N(1)#1	112.28(14)
C(5)-N(1)-Li(1A)	137.1(3)
N(1)#1-N(1)-Li(1A)	100.8(2)
C(5)-N(1)-Li(1A)#2	149.1(2)
N(1)#1-N(1)-Li(1A)#2	47.78(15)
Li(1A)-N(1)-Li(1A)#2	73.8(3)
N(1)-C(5)-C(4)	118.1(2)
N(1)-C(5)-P(1)	114.43(18)
C(4)-C(5)-P(1)	127.51(18)
C(6)#3-O(1)-C(6)	108.4(4)
C(6)#3-O(1)-Li(1A)	120.5(2)
C(6)-O(1)-Li(1A)	120.5(2)
C(3)-C(4)-C(1)	112.3(3)
C(3)-C(4)-C(5)	109.4(3)
C(1)-C(4)-C(5)	110.0(2)
C(3)-C(4)-C(2)	108.7(3)
C(1)-C(4)-C(2)	106.7(3)
C(5)-C(4)-C(2)	109.7(2)
C(7)-C(6)-O(1)	106.8(3)
C(7)-C(6)-H(6A)	110.4
O(1)-C(6)-H(6A)	110.4
C(7)-C(6)-H(6B)	110.4
O(1)-C(6)-H(6B)	110.4
H(6A)-C(6)-H(6B)	108.6

C(4)-C(2)-H(2A)	109.5
C(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(4)-C(1)-H(1A)	109.5
C(4)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(4)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-Li(1A)-N(1)#3	116.0(2)
O(1)-Li(1A)-N(1)	116.0(2)
N(1)#3-Li(1A)-N(1)	120.2(4)
O(1)-Li(1A)-N(1)#2	105.7(3)
N(1)#3-Li(1A)-N(1)#2	31.40(13)
N(1)-Li(1A)-N(1)#2	106.2(3)
O(1)-Li(1A)-N(1)#1	105.7(3)
N(1)#3-Li(1A)-N(1)#1	106.2(3)
N(1)-Li(1A)-N(1)#1	31.40(13)
N(1)#2-Li(1A)-N(1)#1	81.6(2)
O(1)-Li(1A)-Li(1A)#2	124.2(5)
N(1)#3-Li(1A)-Li(1A)#2	63.7(2)

N(1)-Li(1A)-Li(1A)#2	63.7(2)
N(1)#2-Li(1A)-Li(1A)#2	42.52(12)
N(1)#1-Li(1A)-Li(1A)#2	42.52(12)
C(6)-C(7)-C(7)#3	108.2(2)
C(6)-C(7)-H(7A)	110.1
C(7)#3-C(7)-H(7A)	110.1
C(6)-C(7)-H(7B)	110.1
C(7)#3-C(7)-H(7B)	110.1
H(7A)-C(7)-H(7B)	108.4

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z #2 -x,-y,-z #3 x,-y,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 121201-1a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
P(1)	77(1)	40(1)	54(1)	0	21(1)	0
N(1)	60(1)	45(1)	54(1)	4(1)	20(1)	3(1)
C(5)	57(2)	50(1)	43(1)	-2(1)	25(1)	-1(1)
O(1)	96(2)	71(2)	80(2)	0	49(2)	0
C(4)	61(2)	76(2)	45(2)	-7(1)	18(1)	-1(1)
C(6)	143(4)	83(2)	107(3)	8(2)	76(3)	-21(2)
C(2)	107(3)	108(3)	82(3)	-27(2)	2(2)	-24(2)
C(3)	106(3)	186(4)	48(2)	13(2)	27(2)	-21(3)
C(1)	72(2)	137(3)	81(3)	-20(2)	8(2)	17(2)
Li(1A)	64(4)	53(3)	69(4)	0	27(3)	0
C(7)	284(9)	142(4)	111(4)	21(3)	118(5)	1(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 121201-1a.

	x	y	z	U(eq)
H(6A)	1910	970	-1389	124
H(6B)	3628	862	-942	124
H(2A)	1969	2740	2866	168
H(2B)	3016	2667	2093	168
H(2C)	3643	2525	3716	168
H(3A)	1094	1656	3653	173
H(3B)	2761	1455	4583	173
H(3C)	1697	887	3526	173
H(1A)	4567	1376	3423	158
H(1B)	3923	1461	1785	158
H(1C)	3533	774	2441	158
H(7A)	3121	569	-3012	201
H(7B)	1405	569	-3394	201

Table 6. Torsion angles [deg] for 121201-1a.

N(1)#1-N(1)-C(5)-C(4)	178.6(3)
Li(1A)-N(1)-C(5)-C(4)	-43.7(5)
Li(1A)#2-N(1)-C(5)-C(4)	135.4(4)
N(1)#1-N(1)-C(5)-P(1)	-0.4(4)
Li(1A)-N(1)-C(5)-P(1)	137.2(4)
Li(1A)#2-N(1)-C(5)-P(1)	-43.6(5)
C(5)#1-P(1)-C(5)-N(1)	0.17(13)
C(5)#1-P(1)-C(5)-C(4)	-178.7(3)
N(1)-C(5)-C(4)-C(3)	-66.2(3)
P(1)-C(5)-C(4)-C(3)	112.7(3)
N(1)-C(5)-C(4)-C(1)	57.6(4)
P(1)-C(5)-C(4)-C(1)	-123.5(3)
N(1)-C(5)-C(4)-C(2)	174.7(3)
P(1)-C(5)-C(4)-C(2)	-6.4(4)
C(6)#3-O(1)-C(6)-C(7)	12.6(8)
Li(1A)-O(1)-C(6)-C(7)	-132.1(5)
C(6)#3-O(1)-Li(1A)-N(1)#3	4.4(6)
C(6)-O(1)-Li(1A)-N(1)#3	144.8(3)
C(6)#3-O(1)-Li(1A)-N(1)	-144.8(3)
C(6)-O(1)-Li(1A)-N(1)	-4.4(6)
C(6)#3-O(1)-Li(1A)-N(1)#2	-27.4(4)
C(6)-O(1)-Li(1A)-N(1)#2	113.0(3)
C(6)#3-O(1)-Li(1A)-N(1)#1	-113.0(3)
C(6)-O(1)-Li(1A)-N(1)#1	27.4(4)
C(6)#3-O(1)-Li(1A)-Li(1A)#2	-70.2(3)
C(6)-O(1)-Li(1A)-Li(1A)#2	70.2(3)
C(5)-N(1)-Li(1A)-O(1)	-63.3(6)
N(1)#1-N(1)-Li(1A)-O(1)	77.3(4)

Li(1A)#2-N(1)-Li(1A)-O(1)	117.1(5)
C(5)-N(1)-Li(1A)-N(1)#3	148.7(3)
N(1)#1-N(1)-Li(1A)-N(1)#3	-70.6(5)
Li(1A)#2-N(1)-Li(1A)-N(1)#3	-30.8(2)
C(5)-N(1)-Li(1A)-N(1)#2	179.5(3)
N(1)#1-N(1)-Li(1A)-N(1)#2	-39.8(3)
Li(1A)#2-N(1)-Li(1A)-N(1)#2	0.0
C(5)-N(1)-Li(1A)-N(1)#1	-140.6(5)
Li(1A)#2-N(1)-Li(1A)-N(1)#1	39.8(3)
C(5)-N(1)-Li(1A)-Li(1A)#2	179.5(3)
N(1)#1-N(1)-Li(1A)-Li(1A)#2	-39.8(3)
O(1)-C(6)-C(7)-C(7)#3	-7.7(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z #2 -x,-y,-z #3 x,-y,z

3.5 Crystal structural analysis data for**10**

Table 1. Crystal data and structure refinement for 121222-4a.

Identification code	121222-4a
Empirical formula	C30 H54 N6 P3 Sb
Formula weight	713.45
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.0959(5) A alpha = 81.355(3) deg.
	b = 11.0582(4) A beta = 76.325(3) deg.
	c = 17.7867(6) A gamma = 79.091(4) deg.
Volume	1882.96(13) A^3
Z, Calculated density	2, 1.258 Mg/m^3
Absorption coefficient	0.887 mm^-1
F(000)	744
Crystal size	0.31 x 0.26 x 0.12 mm
Theta range for data collection	2.63 to 25.50 deg.
Limiting indices	-12<=h<=11, -13<=k<=13, -21<=l<=20
Reflections collected / unique	13437 / 7003 [R(int) = 0.0400]
Completeness to theta = 25.50	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.88318
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7003 / 0 / 410
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.0712
R indices (all data)	R1 = 0.0544, wR2 = 0.0782
Largest diff. peak and hole	0.849 and -0.726 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 121222-4a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6574(4)	4814(4)	5922(2)	80(1)
C(2)	7572(4)	4033(4)	6402(2)	56(1)
C(3)	8420(5)	2996(4)	5923(3)	94(2)
C(4)	6754(5)	3438(4)	7161(2)	83(1)
C(5)	8545(3)	4798(3)	6575(2)	44(1)
C(6)	10357(3)	5727(3)	6832(2)	42(1)
C(7)	11647(4)	6113(4)	6965(2)	50(1)
C(8)	11314(9)	7280(11)	7395(9)	98(6)
C(9)	12420(11)	5066(10)	7413(8)	95(6)
C(10)	12607(10)	6428(13)	6163(5)	85(5)
C(11)	7919(4)	9307(4)	7958(2)	72(1)
C(12)	7565(4)	8764(3)	8810(2)	49(1)
C(13)	8645(5)	8995(4)	9227(3)	91(2)
C(14)	6159(5)	9418(4)	9196(3)	97(2)
C(15)	7498(3)	7396(3)	8906(2)	41(1)
C(16)	7425(4)	5194(3)	9286(2)	49(1)
C(17)	7530(5)	3827(4)	9583(2)	67(1)
C(18)	7600(6)	3674(5)	10450(3)	130(2)
C(19)	8863(5)	3142(5)	9119(3)	115(2)
C(20)	6287(5)	3296(4)	9507(3)	87(2)
C(21)	3313(5)	11694(4)	8129(3)	90(2)
C(22)	2974(4)	10583(4)	7828(2)	55(1)
C(23)	2465(4)	9675(4)	8528(2)	71(1)

C(24)	1825(4)	11010(5)	7371(3)	96(2)
C(25)	4255(3)	9993(3)	7291(2)	45(1)
C(26)	6261(3)	9337(3)	6277(2)	39(1)
C(27)	7451(3)	9094(3)	5586(2)	46(1)
C(28)	8826(3)	9039(4)	5829(2)	60(1)
C(29)	7410(4)	7885(4)	5282(2)	67(1)
C(30)	7326(4)	10160(4)	4931(2)	61(1)
C(8')	12897(11)	5197(18)	6596(12)	116(10)
C(9')	11773(17)	7358(16)	6611(14)	128(12)
C(10')	11568(15)	5910(20)	7826(7)	117(11)
N(1)	6857(3)	6872(3)	8482(1)	40(1)
N(2)	6824(3)	5619(3)	8697(2)	44(1)
N(3)	8108(3)	5833(2)	6946(1)	37(1)
N(4)	9136(3)	6362(2)	7098(1)	39(1)
N(5)	5955(3)	8462(2)	6889(2)	42(1)
N(6)	4812(3)	8827(3)	7450(2)	44(1)
P(1)	10332(1)	4435(1)	6367(1)	62(1)
P(2)	8075(1)	6317(1)	9627(1)	61(1)
P(3)	5117(1)	10714(1)	6404(1)	52(1)
Sb(1)	6118(1)	6649(1)	7512(1)	36(1)

Table 3. Bond lengths [A] and angles [deg] for 121222-4a.

C(1)-C(2)	1.532(5)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(2)-C(5)	1.520(5)
C(2)-C(4)	1.532(5)
C(2)-C(3)	1.534(5)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-N(3)	1.357(4)
C(5)-P(1)	1.734(3)
C(6)-N(4)	1.317(4)
C(6)-C(7)	1.523(4)
C(6)-P(1)	1.761(4)
C(7)-C(9')	1.441(14)
C(7)-C(10')	1.500(12)
C(7)-C(9)	1.503(8)
C(7)-C(8')	1.540(13)
C(7)-C(8)	1.541(9)
C(7)-C(10)	1.555(9)
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(12)	1.528(5)
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-C(15)	1.509(5)
C(12)-C(14)	1.520(5)
C(12)-C(13)	1.532(5)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-N(1)	1.353(4)
C(15)-P(2)	1.743(3)
C(16)-N(2)	1.315(4)
C(16)-C(17)	1.517(5)
C(16)-P(2)	1.751(4)
C(17)-C(20)	1.523(5)
C(17)-C(19)	1.531(6)
C(17)-C(18)	1.544(6)
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(22)	1.536(6)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-C(25)	1.515(5)
C(22)-C(23)	1.529(5)
C(22)-C(24)	1.533(5)
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)-N(6)	1.323(4)
C(25)-P(3)	1.766(3)
C(26)-N(5)	1.361(4)
C(26)-C(27)	1.519(4)
C(26)-P(3)	1.737(4)
C(27)-C(29)	1.526(5)
C(27)-C(28)	1.536(4)
C(27)-C(30)	1.537(4)
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(8')-H(8'1)	0.9600
C(8')-H(8'2)	0.9600
C(8')-H(8'3)	0.9600
C(9')-H(9'1)	0.9600
C(9')-H(9'2)	0.9600
C(9')-H(9'3)	0.9600
C(10')-H(10D)	0.9600
C(10')-H(10E)	0.9600
C(10')-H(10F)	0.9600
N(1)-N(2)	1.385(4)
N(1)-Sb(1)	2.098(3)
N(2)-Sb(1)	2.436(3)
N(3)-N(4)	1.379(3)
N(3)-Sb(1)	2.120(3)
N(5)-N(6)	1.375(3)
N(5)-Sb(1)	2.137(3)
N(6)-Sb(1)	2.517(3)

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(5)-C(2)-C(4)	110.5(3)

C(5)-C(2)-C(1)	111.8(3)
C(4)-C(2)-C(1)	109.7(3)
C(5)-C(2)-C(3)	109.1(3)
C(4)-C(2)-C(3)	108.3(4)
C(1)-C(2)-C(3)	107.3(3)
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
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
N(3)-C(5)-C(2)	123.5(3)
N(3)-C(5)-P(1)	111.4(2)
C(2)-C(5)-P(1)	125.1(3)
N(4)-C(6)-C(7)	119.5(3)
N(4)-C(6)-P(1)	115.1(2)
C(7)-C(6)-P(1)	125.3(3)
C(9')-C(7)-C(10')	115.0(11)
C(9')-C(7)-C(9)	139.1(6)
C(10')-C(7)-C(9)	52.3(7)
C(9')-C(7)-C(6)	110.8(5)
C(10')-C(7)-C(6)	106.7(5)
C(9)-C(7)-C(6)	110.1(4)
C(9')-C(7)-C(8')	110.1(11)

C(10')-C(7)-C(8')	106.5(10)
C(9)-C(7)-C(8')	55.3(7)
C(6)-C(7)-C(8')	107.3(5)
C(9')-C(7)-C(8)	54.0(9)
C(10')-C(7)-C(8)	63.4(8)
C(9)-C(7)-C(8)	109.8(7)
C(6)-C(7)-C(8)	112.4(4)
C(8')-C(7)-C(8)	140.2(6)
C(9')-C(7)-C(10)	56.2(9)
C(10')-C(7)-C(10)	143.7(6)
C(9)-C(7)-C(10)	108.3(7)
C(6)-C(7)-C(10)	109.1(4)
C(8')-C(7)-C(10)	56.9(7)
C(8)-C(7)-C(10)	107.0(7)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
C(12)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(15)-C(12)-C(14)	107.5(3)

C(15)-C(12)-C(11)	113.1(3)
C(14)-C(12)-C(11)	109.1(3)
C(15)-C(12)-C(13)	109.6(3)
C(14)-C(12)-C(13)	108.5(3)
C(11)-C(12)-C(13)	108.9(3)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(1)-C(15)-C(12)	123.5(3)
N(1)-C(15)-P(2)	111.0(3)
C(12)-C(15)-P(2)	125.2(3)
N(2)-C(16)-C(17)	119.1(3)
N(2)-C(16)-P(2)	114.0(3)
C(17)-C(16)-P(2)	126.9(3)
C(16)-C(17)-C(20)	111.7(3)
C(16)-C(17)-C(19)	108.2(3)
C(20)-C(17)-C(19)	110.4(4)
C(16)-C(17)-C(18)	108.3(4)
C(20)-C(17)-C(18)	108.8(4)
C(19)-C(17)-C(18)	109.3(4)
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
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(25)-C(22)-C(23)	111.9(3)
C(25)-C(22)-C(24)	108.8(3)
C(23)-C(22)-C(24)	108.6(3)
C(25)-C(22)-C(21)	108.9(3)
C(23)-C(22)-C(21)	108.4(3)
C(24)-C(22)-C(21)	110.3(4)
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
N(6)-C(25)-C(22)	120.9(3)
N(6)-C(25)-P(3)	113.3(3)
C(22)-C(25)-P(3)	125.7(3)
N(5)-C(26)-C(27)	122.8(3)
N(5)-C(26)-P(3)	111.0(2)
C(27)-C(26)-P(3)	126.2(2)
C(26)-C(27)-C(29)	110.2(3)
C(26)-C(27)-C(28)	109.5(3)
C(29)-C(27)-C(28)	110.6(3)
C(26)-C(27)-C(30)	109.3(3)
C(29)-C(27)-C(30)	108.7(3)
C(28)-C(27)-C(30)	108.4(3)
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
C(7)-C(8')-H(8'1)	109.5
C(7)-C(8')-H(8'2)	109.5
H(8'1)-C(8')-H(8'2)	109.5
C(7)-C(8')-H(8'3)	109.5
H(8'1)-C(8')-H(8'3)	109.5
H(8'2)-C(8')-H(8'3)	109.5
C(7)-C(9')-H(9'1)	109.5
C(7)-C(9')-H(9'2)	109.5
H(9'1)-C(9')-H(9'2)	109.5
C(7)-C(9')-H(9'3)	109.5
H(9'1)-C(9')-H(9'3)	109.5
H(9'2)-C(9')-H(9'3)	109.5
C(7)-C(10')-H(10D)	109.5
C(7)-C(10')-H(10E)	109.5
H(10D)-C(10')-H(10E)	109.5
C(7)-C(10')-H(10F)	109.5
H(10D)-C(10')-H(10F)	109.5
H(10E)-C(10')-H(10F)	109.5
C(15)-N(1)-N(2)	114.6(3)

C(15)-N(1)-Sb(1)	157.2(2)
N(2)-N(1)-Sb(1)	86.17(17)
C(16)-N(2)-N(1)	111.8(3)
C(16)-N(2)-Sb(1)	167.9(2)
N(1)-N(2)-Sb(1)	59.26(14)
C(5)-N(3)-N(4)	115.5(3)
C(5)-N(3)-Sb(1)	131.8(2)
N(4)-N(3)-Sb(1)	111.86(19)
C(6)-N(4)-N(3)	110.4(3)
C(26)-N(5)-N(6)	115.0(3)
C(26)-N(5)-Sb(1)	155.8(2)
N(6)-N(5)-Sb(1)	88.82(17)
C(25)-N(6)-N(5)	112.1(3)
C(25)-N(6)-Sb(1)	169.9(2)
N(5)-N(6)-Sb(1)	58.08(15)
C(5)-P(1)-C(6)	87.64(16)
C(15)-P(2)-C(16)	88.53(16)
C(26)-P(3)-C(25)	88.61(16)
N(1)-Sb(1)-N(3)	91.54(10)
N(1)-Sb(1)-N(5)	103.52(10)
N(3)-Sb(1)-N(5)	101.11(10)
N(1)-Sb(1)-N(2)	34.57(9)
N(3)-Sb(1)-N(2)	84.39(9)
N(5)-Sb(1)-N(2)	138.08(10)
N(1)-Sb(1)-N(6)	92.57(10)
N(3)-Sb(1)-N(6)	133.25(9)
N(5)-Sb(1)-N(6)	33.10(8)
N(2)-Sb(1)-N(6)	121.45(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for 121222-4a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	69(3)	87(4)	101(3)	-33(3)	-29(3)	-27(3)
C(2)	57(3)	42(2)	76(3)	-29(2)	-7(2)	-12(2)
C(3)	89(4)	72(4)	134(4)	-66(3)	-13(3)	-15(3)
C(4)	95(4)	57(3)	103(3)	-20(3)	-6(3)	-36(3)
C(5)	43(2)	37(2)	52(2)	-17(2)	-5(2)	-3(2)
C(6)	34(2)	43(2)	45(2)	-7(2)	-4(2)	0(2)
C(7)	33(2)	59(3)	59(2)	-10(2)	-12(2)	-5(2)
C(8)	51(5)	104(11)	160(14)	-76(11)	-31(7)	-6(5)
C(9)	78(8)	87(8)	134(14)	18(8)	-64(10)	-15(6)
C(10)	53(6)	118(13)	87(6)	-4(6)	-5(5)	-36(8)
C(11)	92(3)	53(3)	73(3)	-3(2)	-11(2)	-29(3)
C(12)	48(2)	43(2)	57(2)	-15(2)	-6(2)	-10(2)
C(13)	118(4)	72(4)	108(4)	-11(3)	-55(3)	-41(3)
C(14)	86(4)	57(3)	131(4)	-43(3)	27(3)	-4(3)
C(15)	34(2)	44(2)	42(2)	-11(2)	3(2)	-7(2)
C(16)	47(2)	50(2)	46(2)	1(2)	-6(2)	-8(2)
C(17)	77(3)	48(3)	75(3)	11(2)	-23(2)	-12(2)
C(18)	229(7)	86(4)	94(4)	43(3)	-80(4)	-54(5)
C(19)	93(4)	54(4)	180(6)	-5(4)	-21(4)	10(3)
C(20)	93(4)	51(3)	114(4)	16(3)	-23(3)	-25(3)
C(21)	91(4)	52(3)	110(4)	-29(3)	24(3)	-7(3)
C(22)	43(2)	40(2)	68(3)	-7(2)	4(2)	4(2)
C(23)	53(3)	67(3)	76(3)	-10(2)	17(2)	-3(2)
C(24)	58(3)	106(4)	102(4)	-2(3)	-10(3)	27(3)

C(25)	37(2)	34(2)	59(2)	-4(2)	-9(2)	-2(2)
C(26)	41(2)	38(2)	40(2)	-3(2)	-9(2)	-12(2)
C(27)	46(2)	48(2)	41(2)	-5(2)	-2(2)	-10(2)
C(28)	46(2)	74(3)	52(2)	3(2)	1(2)	-11(2)
C(29)	83(3)	55(3)	56(2)	-18(2)	3(2)	-9(2)
C(30)	68(3)	66(3)	45(2)	3(2)	-6(2)	-17(2)
C(8')	39(7)	148(19)	180(20)	-85(18)	-28(9)	6(8)
C(9')	82(14)	118(16)	210(30)	40(19)	-82(18)	-70(13)
C(10')	65(10)	240(30)	73(9)	-23(12)	-30(7)	-59(15)
N(1)	44(2)	36(2)	41(2)	-8(1)	-5(1)	-8(1)
N(2)	47(2)	37(2)	48(2)	0(1)	-8(1)	-11(1)
N(3)	35(2)	31(2)	47(2)	-14(1)	-7(1)	-3(1)
N(4)	35(2)	35(2)	46(2)	-9(1)	-7(1)	-6(1)
N(5)	37(2)	32(2)	49(2)	-4(1)	-4(1)	3(1)
N(6)	37(2)	36(2)	49(2)	-7(1)	4(1)	1(1)
P(1)	45(1)	53(1)	86(1)	-36(1)	-7(1)	7(1)
P(2)	71(1)	61(1)	58(1)	-3(1)	-26(1)	-15(1)
P(3)	53(1)	37(1)	57(1)	2(1)	-7(1)	-2(1)
Sb(1)	31(1)	30(1)	47(1)	-7(1)	-6(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 121222-4a.

	x	y	z	U(eq)
H(1A)	6014	5466	6210	120
H(1B)	5991	4298	5814	120
H(1C)	7090	5167	5441	120
H(3A)	8946	3353	5446	141
H(3B)	7808	2518	5806	141
H(3C)	9035	2469	6216	141
H(4A)	7382	2910	7445	125
H(4B)	6147	2957	7042	125
H(4C)	6220	4075	7470	125
H(8A)	12156	7493	7460	147
H(8B)	10726	7119	7896	147
H(8C)	10852	7955	7096	147
H(9A)	12749	4383	7106	143
H(9B)	11815	4806	7889	143
H(9C)	13189	5338	7529	143
H(10A)	12101	7039	5849	128
H(10B)	12936	5692	5905	128
H(10C)	13379	6749	6242	128
H(11A)	8746	8827	7694	108
H(11B)	8061	10148	7932	108
H(11C)	7172	9288	7714	108
H(13A)	8412	8682	9767	136
H(13B)	8660	9868	9181	136
H(13C)	9538	8578	8993	136
H(14A)	5470	9281	8942	146

H(14B)	6176	10291	9155	146
H(14C)	5943	9096	9735	146
H(18A)	8342	4057	10508	196
H(18B)	7757	2809	10635	196
H(18C)	6744	4062	10747	196
H(19A)	8793	3180	8586	172
H(19B)	9004	2292	9338	172
H(19C)	9629	3526	9140	172
H(20A)	5458	3746	9791	130
H(20B)	6373	2438	9715	130
H(20C)	6247	3368	8968	130
H(21A)	4058	11421	8395	136
H(21B)	2514	12060	8481	136
H(21C)	3580	12297	7698	136
H(23A)	2264	8967	8349	107
H(23B)	1643	10076	8848	107
H(23C)	3167	9414	8826	107
H(24A)	2130	11584	6931	144
H(24B)	1016	11407	7702	144
H(24C)	1611	10305	7194	144
H(28A)	8844	9813	6006	90
H(28B)	9577	8888	5391	90
H(28C)	8915	8381	6242	90
H(29A)	7608	7200	5661	100
H(29B)	8087	7796	4805	100
H(29C)	6509	7899	5188	100
H(30A)	6460	10221	4782	91
H(30B)	8070	10002	4490	91
H(30C)	7371	10924	5112	91
H(8'1)	13054	5359	6039	174

H(8'2)	12716	4365	6754	174
H(8'3)	13701	5297	6766	174
H(9'1)	12615	7569	6679	191
H(9'2)	11002	7923	6854	191
H(9'3)	11788	7412	6066	191
H(10D)	12432	6003	7929	175
H(10E)	11379	5087	8022	175
H(10F)	10842	6503	8078	175

Table 6. Torsion angles [deg] for 121222-4a.

C(4)-C(2)-C(5)-N(3)	-65.3(5)
C(1)-C(2)-C(5)-N(3)	57.2(5)
C(3)-C(2)-C(5)-N(3)	175.6(3)
C(4)-C(2)-C(5)-P(1)	111.6(4)
C(1)-C(2)-C(5)-P(1)	-125.9(3)
C(3)-C(2)-C(5)-P(1)	-7.4(5)
N(4)-C(6)-C(7)-C(9')	-60.1(12)
P(1)-C(6)-C(7)-C(9')	122.1(12)
N(4)-C(6)-C(7)-C(10')	65.8(11)
P(1)-C(6)-C(7)-C(10')	-112.1(10)
N(4)-C(6)-C(7)-C(9)	121.0(7)
P(1)-C(6)-C(7)-C(9)	-56.8(7)
N(4)-C(6)-C(7)-C(8')	179.6(9)
P(1)-C(6)-C(7)-C(8')	1.8(10)
N(4)-C(6)-C(7)-C(8)	-1.7(8)
P(1)-C(6)-C(7)-C(8)	-179.6(7)
N(4)-C(6)-C(7)-C(10)	-120.3(6)
P(1)-C(6)-C(7)-C(10)	61.9(7)
C(14)-C(12)-C(15)-N(1)	76.0(4)
C(11)-C(12)-C(15)-N(1)	-44.5(5)
C(13)-C(12)-C(15)-N(1)	-166.3(3)
C(14)-C(12)-C(15)-P(2)	-97.5(4)
C(11)-C(12)-C(15)-P(2)	142.0(3)
C(13)-C(12)-C(15)-P(2)	20.2(4)
N(2)-C(16)-C(17)-C(20)	-33.5(5)
P(2)-C(16)-C(17)-C(20)	148.5(3)
N(2)-C(16)-C(17)-C(19)	88.2(4)
P(2)-C(16)-C(17)-C(19)	-89.7(4)

N(2)-C(16)-C(17)-C(18)	-153.4(4)
P(2)-C(16)-C(17)-C(18)	28.6(5)
C(23)-C(22)-C(25)-N(6)	-0.3(5)
C(24)-C(22)-C(25)-N(6)	-120.3(4)
C(21)-C(22)-C(25)-N(6)	119.5(4)
C(23)-C(22)-C(25)-P(3)	177.4(3)
C(24)-C(22)-C(25)-P(3)	57.5(4)
C(21)-C(22)-C(25)-P(3)	-62.7(4)
N(5)-C(26)-C(27)-C(29)	48.8(4)
P(3)-C(26)-C(27)-C(29)	-130.8(3)
N(5)-C(26)-C(27)-C(28)	-73.1(4)
P(3)-C(26)-C(27)-C(28)	107.3(3)
N(5)-C(26)-C(27)-C(30)	168.2(3)
P(3)-C(26)-C(27)-C(30)	-11.4(4)
C(12)-C(15)-N(1)-N(2)	-175.5(3)
P(2)-C(15)-N(1)-N(2)	-1.2(4)
C(12)-C(15)-N(1)-Sb(1)	30.2(8)
P(2)-C(15)-N(1)-Sb(1)	-155.5(5)
C(17)-C(16)-N(2)-N(1)	-177.9(3)
P(2)-C(16)-N(2)-N(1)	0.3(4)
C(17)-C(16)-N(2)-Sb(1)	-137.3(11)
P(2)-C(16)-N(2)-Sb(1)	40.9(13)
C(15)-N(1)-N(2)-C(16)	0.6(4)
Sb(1)-N(1)-N(2)-C(16)	170.9(2)
C(15)-N(1)-N(2)-Sb(1)	-170.3(3)
C(2)-C(5)-N(3)-N(4)	175.9(3)
P(1)-C(5)-N(3)-N(4)	-1.4(3)
C(2)-C(5)-N(3)-Sb(1)	7.6(5)
P(1)-C(5)-N(3)-Sb(1)	-169.68(15)
C(7)-C(6)-N(4)-N(3)	-177.5(3)

P(1)-C(6)-N(4)-N(3)	0.5(3)
C(5)-N(3)-N(4)-C(6)	0.6(4)
Sb(1)-N(3)-N(4)-C(6)	171.20(19)
C(27)-C(26)-N(5)-N(6)	-177.7(3)
P(3)-C(26)-N(5)-N(6)	1.9(3)
C(27)-C(26)-N(5)-Sb(1)	-8.5(7)
P(3)-C(26)-N(5)-Sb(1)	171.2(4)
C(22)-C(25)-N(6)-N(5)	179.2(3)
P(3)-C(25)-N(6)-N(5)	1.2(4)
C(22)-C(25)-N(6)-Sb(1)	167.9(12)
P(3)-C(25)-N(6)-Sb(1)	-10.1(15)
C(26)-N(5)-N(6)-C(25)	-2.1(4)
Sb(1)-N(5)-N(6)-C(25)	-177.7(2)
C(26)-N(5)-N(6)-Sb(1)	175.6(3)
N(3)-C(5)-P(1)-C(6)	1.3(2)
C(2)-C(5)-P(1)-C(6)	-175.9(3)
N(4)-C(6)-P(1)-C(5)	-1.1(3)
C(7)-C(6)-P(1)-C(5)	176.8(3)
N(1)-C(15)-P(2)-C(16)	1.1(2)
C(12)-C(15)-P(2)-C(16)	175.3(3)
N(2)-C(16)-P(2)-C(15)	-0.8(3)
C(17)-C(16)-P(2)-C(15)	177.2(4)
N(5)-C(26)-P(3)-C(25)	-1.0(2)
C(27)-C(26)-P(3)-C(25)	178.6(3)
N(6)-C(25)-P(3)-C(26)	-0.1(3)
C(22)-C(25)-P(3)-C(26)	-178.0(3)
C(15)-N(1)-Sb(1)-N(3)	78.9(6)
N(2)-N(1)-Sb(1)-N(3)	-77.81(17)
C(15)-N(1)-Sb(1)-N(5)	-22.9(6)
N(2)-N(1)-Sb(1)-N(5)	-179.62(16)

C(15)-N(1)-Sb(1)-N(2)	156.7(7)
C(15)-N(1)-Sb(1)-N(6)	-54.5(6)
N(2)-N(1)-Sb(1)-N(6)	148.77(17)
C(5)-N(3)-Sb(1)-N(1)	132.8(3)
N(4)-N(3)-Sb(1)-N(1)	-35.8(2)
C(5)-N(3)-Sb(1)-N(5)	-123.1(3)
N(4)-N(3)-Sb(1)-N(5)	68.3(2)
C(5)-N(3)-Sb(1)-N(2)	98.9(3)
N(4)-N(3)-Sb(1)-N(2)	-69.63(19)
C(5)-N(3)-Sb(1)-N(6)	-132.2(3)
N(4)-N(3)-Sb(1)-N(6)	59.2(2)
C(26)-N(5)-Sb(1)-N(1)	116.3(5)
N(6)-N(5)-Sb(1)-N(1)	-73.49(18)
C(26)-N(5)-Sb(1)-N(3)	21.9(6)
N(6)-N(5)-Sb(1)-N(3)	-167.81(17)
C(26)-N(5)-Sb(1)-N(2)	115.9(5)
N(6)-N(5)-Sb(1)-N(2)	-73.8(2)
C(26)-N(5)-Sb(1)-N(6)	-170.2(6)
C(16)-N(2)-Sb(1)-N(1)	-44.7(12)
C(16)-N(2)-Sb(1)-N(3)	56.3(12)
N(1)-N(2)-Sb(1)-N(3)	100.95(18)
C(16)-N(2)-Sb(1)-N(5)	-44.1(13)
N(1)-N(2)-Sb(1)-N(5)	0.6(2)
C(16)-N(2)-Sb(1)-N(6)	-82.0(12)
N(1)-N(2)-Sb(1)-N(6)	-37.4(2)
C(25)-N(6)-Sb(1)-N(1)	123.5(14)
N(5)-N(6)-Sb(1)-N(1)	111.07(18)
C(25)-N(6)-Sb(1)-N(3)	28.9(14)
N(5)-N(6)-Sb(1)-N(3)	16.5(2)
C(25)-N(6)-Sb(1)-N(5)	12.4(13)

C(25)-N(6)-Sb(1)-N(2)	143.7(13)
N(5)-N(6)-Sb(1)-N(2)	131.24(17)

Symmetry transformations used to generate equivalent atoms:

4. X-ray crystal structure of **9**

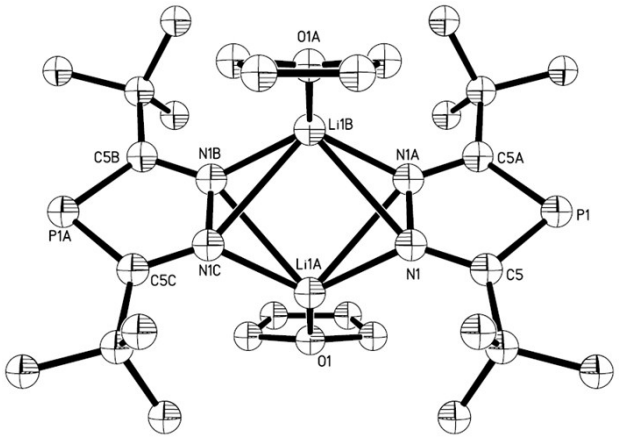


Figure 26. X-ray crystal structure of **9**. Drawn with ellipsoids at 30% probability, tBu groups and hydrogen atoms omitted for clarity. Selected bond distances [Å] and angles (deg). **9**: N(1)-Li(1A) 1.965(4), N(1)-Li(1B) 2.606(6), O(1)-Li(1A) 1.899(8), Li(1A)-N(1C) 1.965(4), Li(1A)-N(1B) 2.606(6), Li(1A)-N(1A) 2.606(6); N(1A)-N(1)-Li(1A) 100.8(2),N(1A)-N(1)-Li(1B) 47.78(15), Li(1A)-N(1)-Li(1B) 73.8(3), O(1)-Li(1A)-N(1C) 116.0(2), N(1C)-Li(1A)-N(1) 120.2(4), O(1)-Li(1A)-N(1B) 105.7(3), N(1C)-Li(1A)-N(1B) 31.40(13), N(1)-Li(1A)-N(1B) 106.2(3), O(1)-Li(1A)-N(1A) 105.7(3), N(1C)-Li(1A)-N(1A) 106.2(3), N(1)-Li(1A)-N(1A) 31.40(13), N(1B)-Li(1A)-N(1A) 81.6(2), O(1)-Li(1A)-Li(1B) 124.2(5), N(1C)-Li(1A)-Li(1B) 63.7(2), N(1)-Li(1A)-Li(1B) 63.7(2), N(1B)-Li(1A)-Li(1B) 42.52(12), N(1A)-Li(1A)-Li(1B) 42.52(12).

5. Theoretically computed data of **4**, **5**, **6** and **10**

Cartesian Coordinates of the Optimized Geometries of Compound **4**, **5**, **6**, and **10** by M11 method[3] with the combination of 6-31G(d) basis set for C, N, P and H atoms anddefz-TZVP basis set and psuedopotential for Sb atoms. All calculations were performed using Gaussian 09 package.[4]

Compound **4**:

Sb	0.000212000	-0.000661000	1.337599000
Sb	0.000071000	0.000687000	-1.337755000
P	-0.038574000	4.742831000	-0.000642000
P	4.734687000	0.037652000	0.000862000
P	-4.734367000	-0.037503000	0.001672000
P	0.038173000	-4.742819000	-0.001667000
N	-0.347993000	2.243441000	0.590764000
N	0.310599000	2.248558000	-0.591093000
N	2.239847000	-0.288769000	-0.601466000
N	2.234802000	0.325847000	0.601518000
N	-2.234367000	-0.326006000	0.601788000
N	-2.239632000	0.289083000	-0.600969000
N	-0.311021000	-2.248412000	-0.591714000
N	0.347843000	-2.243567000	0.589966000
C	-0.646552000	3.461629000	1.038616000
C	0.589983000	3.471176000	-1.039384000
C	1.463730000	3.658280000	-2.272718000
C	0.811755000	3.054931000	-3.527539000
C	1.706281000	5.153335000	-2.523279000
C	2.811988000	2.967054000	-2.000228000
C	-1.523074000	3.635224000	2.271919000
C	-1.791137000	5.126248000	2.520681000
C	-0.860137000	3.044638000	3.527078000
C	-2.859192000	2.920380000	2.001164000
C	3.461029000	-0.549505000	-1.060535000
C	3.451567000	0.605206000	1.061375000
C	3.611947000	1.345696000	2.380528000
C	5.045323000	1.882702000	2.500993000
C	3.333395000	0.391728000	3.556653000
C	2.624248000	2.522825000	2.422130000
C	3.633799000	-1.287736000	-2.379378000
C	5.074819000	-1.804325000	-2.497641000
C	2.663088000	-2.478858000	-2.422309000
C	3.343319000	-0.337920000	-3.555976000
C	-3.451077000	-0.605504000	1.061751000
C	-3.460872000	0.549832000	-1.059807000
C	-3.633804000	1.288090000	-2.378647000

C	-2.663860000	2.479876000	-2.421254000
C	-3.342395000	0.338563000	-3.555260000
C	-5.075141000	1.803707000	-2.497272000
C	-3.611262000	-1.346524000	2.380642000
C	-5.044516000	-1.883867000	2.501017000
C	-3.332812000	-0.393050000	3.557194000
C	-2.623267000	-2.523424000	2.421618000
C	-0.590622000	-3.470898000	-1.040041000
C	0.646545000	-3.461847000	1.037582000
C	1.523439000	-3.635595000	2.270633000
C	1.791677000	-5.126654000	2.519032000
C	2.859473000	-2.920624000	1.999609000
C	0.860901000	-3.045394000	3.526179000
C	-1.465157000	-3.657532000	-2.272879000
C	-1.708474000	-5.152459000	-2.523509000
C	-0.813664000	-3.054188000	-3.527951000
C	-2.812945000	-2.965761000	-1.999532000
H	0.614484000	1.978232000	-3.414342000
H	1.484776000	3.178224000	-4.389894000
H	-0.139192000	3.557369000	-3.757154000
H	2.351150000	5.281527000	-3.405567000
H	2.205073000	5.624993000	-1.663809000
H	0.761916000	5.687123000	-2.707489000
H	2.675508000	1.893181000	-1.813921000
H	3.301036000	3.399627000	-1.113731000
H	3.485695000	3.089321000	-2.863050000
H	-0.855932000	5.676409000	2.703478000
H	-2.437497000	5.244607000	3.403255000
H	-2.298547000	5.588088000	1.660909000
H	-0.645210000	1.971189000	3.414891000
H	-1.534461000	3.157797000	4.389801000
H	0.082514000	3.563066000	3.755288000
H	-3.356157000	3.342907000	1.114201000
H	-3.534458000	3.032228000	2.864166000
H	-2.703980000	1.848789000	1.816518000
H	5.782671000	1.066195000	2.480244000
H	5.161995000	2.423740000	3.451807000
H	5.277013000	2.575291000	1.678094000
H	2.313126000	-0.021376000	3.505336000
H	3.431708000	0.932270000	4.510487000
H	4.043217000	-0.448677000	3.556811000
H	2.708647000	3.150126000	1.521030000
H	2.816986000	3.148045000	3.307725000
H	1.586306000	2.170181000	2.483407000

H	5.800530000	-0.977508000	-2.475199000
H	5.200811000	-2.343184000	-3.448502000
H	5.314853000	-2.493979000	-1.674668000
H	2.754350000	-3.104310000	-1.520567000
H	2.866613000	-3.101788000	-3.307094000
H	1.620411000	-2.140964000	-2.486209000
H	2.317295000	0.060801000	-3.505827000
H	3.450374000	-0.877118000	-4.509632000
H	4.041250000	0.512383000	-3.555388000
H	-2.755943000	3.105311000	-1.519582000
H	-2.867495000	3.102635000	-3.306131000
H	-1.620879000	2.142778000	-2.484728000
H	-3.449624000	0.877750000	-4.508904000
H	-4.039713000	-0.512233000	-3.554877000
H	-2.316103000	-0.059458000	-3.504926000
H	-5.315834000	2.493268000	-1.674411000
H	-5.800303000	0.976407000	-2.474922000
H	-5.201286000	2.342405000	-3.448204000
H	-5.782028000	-1.067501000	2.480638000
H	-5.160979000	-2.425270000	3.451649000
H	-5.276146000	-2.576212000	1.677898000
H	-2.312590000	0.020170000	3.506099000
H	-3.431087000	-0.934037000	4.510779000
H	-4.042704000	0.447290000	3.557715000
H	-2.707329000	-3.150124000	1.520070000
H	-2.815954000	-3.149290000	3.306767000
H	-1.585443000	-2.170500000	2.483333000
H	0.856569000	-5.676938000	2.701931000
H	2.438251000	-5.245117000	3.401435000
H	2.298939000	-5.588267000	1.659057000
H	3.534924000	-3.032481000	2.862465000
H	2.704233000	-1.848997000	1.815017000
H	3.356281000	-3.343114000	1.112545000
H	-0.081629000	-3.563957000	3.754559000
H	0.645874000	-1.971927000	3.414437000
H	1.535535000	-3.158764000	4.388629000
H	-0.764420000	-5.686645000	-2.708165000
H	-2.353763000	-5.280288000	-3.405542000
H	-2.207113000	-5.623997000	-1.663881000
H	0.137050000	-3.556812000	-3.758127000
H	-0.616103000	-1.977533000	-3.414646000
H	-1.487157000	-3.177197000	-4.389978000
H	-3.487187000	-3.087602000	-2.861997000
H	-2.675867000	-1.891993000	-1.813112000

H	-3.301684000	-3.398256000	-1.112823000

Compound **5**:

Sb	0.000066000	-0.000034000	1.375280000
Sb	-0.000037000	-0.000036000	-1.375577000
P	-3.317847000	-3.353270000	0.000123000
P	-3.353274000	3.317768000	0.000117000
P	3.353349000	-3.317798000	0.000034000
P	3.317721000	3.353351000	0.000026000
N	-1.651144000	-1.491255000	0.658819000
N	-1.475511000	-1.664969000	-0.658784000
N	-1.664961000	1.475442000	-0.658781000
N	-1.491182000	1.651147000	0.658803000
N	1.491261000	-1.651187000	0.658748000
N	1.664960000	-1.475532000	-0.658853000
N	1.475463000	1.664951000	-0.658851000
N	1.651191000	1.491189000	0.658732000
C	-2.575855000	-2.278012000	1.184236000
C	-2.251411000	-2.598864000	-1.184092000
C	-2.072391000	-2.935165000	-2.644656000
C	-0.791419000	-3.765117000	-2.820412000
C	-3.288572000	-3.664644000	-3.212254000
C	-2.914018000	-2.102827000	2.644846000
C	-3.756970000	-0.830445000	2.820938000
C	-3.631019000	-3.326578000	3.212071000
C	-2.598901000	2.251291000	-1.184082000
C	-2.277929000	2.575872000	1.184211000
C	-2.102672000	2.914118000	2.644794000
C	-0.830306000	3.757118000	2.820771000
C	-3.326414000	3.631109000	3.212050000
C	-2.935279000	2.072181000	-2.644618000
C	-3.765231000	0.791192000	-2.820255000
C	-3.664797000	3.288323000	-3.212250000
C	2.278069000	-2.575861000	1.184158000
C	2.598901000	-2.251371000	-1.184167000
C	2.935212000	-2.072307000	-2.644724000
C	3.664868000	-3.288389000	-3.212306000
C	3.765005000	-0.791230000	-2.820463000
C	2.102913000	-2.914032000	2.644769000
C	0.830586000	-3.757066000	2.820867000
C	3.326715000	-3.630948000	3.211991000
C	2.251254000	2.598936000	-1.184158000
C	2.575880000	2.277985000	1.184132000

C	2.914136000	2.102756000	2.644715000
C	3.757216000	0.830443000	2.820698000
C	3.631046000	3.326547000	3.211967000
C	2.072099000	2.935322000	-2.644688000
C	0.791007000	3.765119000	-2.820309000
C	3.288144000	3.665014000	-3.212305000
H	-0.596173000	-3.957894000	-3.881432000
H	-0.895743000	-4.727584000	-2.305901000
H	0.075538000	-3.250504000	-2.387758000
H	-4.200002000	-3.068263000	-3.095452000
H	-3.438466000	-4.618352000	-2.690927000
H	-3.145572000	-3.880446000	-4.276266000
H	-3.251009000	0.041870000	2.388850000
H	-3.952018000	-0.637649000	3.881989000
H	-4.718175000	-0.944256000	2.306084000
H	-4.583171000	-3.486051000	2.690739000
H	-3.848222000	-3.186152000	4.276140000
H	-3.025376000	-4.231841000	3.094948000
H	0.042000000	3.251164000	2.388660000
H	-0.637457000	3.952225000	3.881802000
H	-0.944176000	4.718295000	2.305877000
H	-3.485951000	4.583227000	2.690675000
H	-3.185934000	3.848376000	4.276099000
H	-4.231663000	3.025429000	3.095013000
H	-3.250590000	-0.075736000	-2.387577000
H	-3.958061000	0.595883000	-3.881255000
H	-4.727673000	0.895539000	-2.305701000
H	-4.618477000	3.438243000	-2.690880000
H	-3.880655000	3.145257000	-4.276241000
H	-3.068415000	4.199764000	-3.095537000
H	4.618591000	-3.438144000	-2.690966000
H	3.880664000	-3.145363000	-4.276316000
H	3.068619000	-4.199906000	-3.095509000
H	4.727474000	-0.895432000	-2.305930000
H	3.250277000	0.075665000	-2.387823000
H	3.957782000	-0.595962000	-3.881480000
H	-0.041763000	-3.251161000	2.388782000
H	0.637807000	-3.952126000	3.881919000
H	0.944457000	-4.718265000	2.306014000
H	3.486259000	-4.583085000	2.690655000
H	3.186307000	-3.848165000	4.276059000
H	4.231932000	-3.025236000	3.094869000
H	3.251314000	-0.041896000	2.388589000
H	3.952334000	0.637609000	3.881730000

H	4.718385000	0.944370000	2.305804000
H	3.848327000	3.186084000	4.276015000
H	3.025298000	4.231752000	3.094931000
H	4.583149000	3.486151000	2.690586000
H	-0.075860000	3.250364000	-2.387644000
H	0.595677000	3.957948000	-3.881305000
H	0.895235000	4.727562000	-2.305734000
H	3.145053000	3.880865000	-4.276294000
H	4.199670000	3.068761000	-3.095596000
H	3.437928000	4.618709000	-2.690923000
H	-1.985247000	1.943905000	-3.185000000
H	-1.944141000	-1.985104000	-3.184995000
H	1.985148000	-1.944181000	-3.185086000
H	1.943945000	1.985286000	-3.185091000
H	-1.964794000	1.965454000	3.185218000
H	1.965481000	1.964820000	3.185140000
H	1.965034000	-1.965344000	3.185151000
H	-1.965321000	-1.965009000	3.185228000

Compound **6**:

Sb	1.374500000	-0.001385000	0.004495000
P	0.009642000	1.152216000	-4.567544000
P	-0.014100000	-4.564449000	-1.169205000
N	-0.668652000	-2.169031000	-0.447071000
C	-4.826613000	-4.750829000	-0.826989000
N	0.657396000	-2.125349000	-0.633494000
N	0.665950000	0.633622000	-2.120802000
N	-0.660158000	0.449524000	-2.170246000
C	4.825347000	1.541029000	-4.561936000
C	-2.661318000	0.389911000	-3.526191000
C	-3.302178000	1.119770000	-4.710665000
C	-4.803559000	0.813512000	-4.775856000
C	-1.187508000	0.668142000	-3.368867000
C	2.657209000	-3.286292000	-1.339480000
C	-3.325726000	-4.687777000	-1.136320000
C	-5.062229000	-0.696960000	-4.860022000
C	1.199597000	1.010120000	-3.276748000
C	3.324369000	1.241323000	-4.659002000
C	2.674218000	1.327406000	-3.274741000
C	-2.677868000	-3.514194000	-0.394861000
C	-1.203440000	-3.362949000	-0.673723000
C	5.080893000	2.912092000	-3.921779000
C	2.910809000	2.719770000	-2.654886000

C	-5.081182000	-4.851128000	0.683039000
C	1.183221000	-3.281184000	-1.019946000
C	5.062495000	-3.940449000	-2.923162000
C	-4.398311000	-1.438944000	-3.692453000
C	4.800950000	-4.584764000	-1.555083000
C	-2.899757000	-1.129389000	-3.639133000
C	-4.412503000	-3.693165000	1.435581000
C	-2.914380000	-3.641133000	1.123645000
C	3.298855000	-4.674727000	-1.259017000
C	2.897899000	-2.663118000	-2.729436000
C	4.397189000	-2.561306000	-3.023071000
C	4.408900000	3.015695000	-2.546178000
H	-5.310498000	-3.837351000	-1.216210000
H	-5.287125000	-5.601648000	-1.350233000
H	5.306755000	0.759041000	-3.948115000
H	5.288150000	1.491683000	-5.558469000
H	-3.167092000	0.735032000	-2.602617000
H	-2.811886000	0.788735000	-5.643406000
H	-3.125088000	2.203489000	-4.623560000
H	-5.289329000	1.213975000	-3.868366000
H	-5.259865000	1.328684000	-5.633819000
H	3.161371000	-2.637295000	-0.596102000
H	-2.838240000	-5.626122000	-0.817129000
H	-3.151151000	-4.589058000	-2.219556000
H	-4.648089000	-1.080503000	-5.808255000
H	-6.143438000	-0.898804000	-4.879445000
H	2.839043000	1.972641000	-5.329628000
H	3.150268000	0.244190000	-5.093563000
H	3.174381000	0.586183000	-2.620161000
H	-3.179359000	-2.584703000	-0.730059000
H	4.670838000	3.698036000	-4.578996000
H	6.161735000	3.098817000	-3.837739000
H	2.417105000	2.776953000	-1.670681000
H	2.422264000	3.474107000	-3.295547000
H	-6.161834000	-4.870306000	0.887842000
H	-4.668075000	-5.804402000	1.055015000
H	4.651168000	-4.592745000	-3.712547000
H	6.144102000	-3.860624000	-3.107296000
H	-4.561158000	-2.524060000	-3.782587000
H	-4.866105000	-1.122662000	-2.742353000
H	5.283975000	-3.976557000	-0.769718000
H	5.258115000	-5.584019000	-1.508464000
H	-2.412405000	-1.645546000	-2.795449000
H	-2.405737000	-1.491594000	-4.557171000

H	-4.878392000	-2.738730000	1.129925000
H	-4.573398000	-3.794079000	2.519996000
H	-2.422220000	-4.564029000	1.475958000
H	-2.423713000	-2.803925000	1.647368000
H	3.119726000	-5.113523000	-0.264675000
H	2.811305000	-5.338717000	-1.994904000
H	2.409694000	-1.676024000	-2.784019000
H	2.406847000	-3.298863000	-3.486299000
H	4.562093000	-2.124408000	-4.020124000
H	4.862062000	-1.874969000	-2.292037000
H	4.570408000	4.014450000	-2.111824000
H	4.871470000	2.287312000	-1.855451000
Sb	-1.374654000	0.004534000	0.004384000
P	0.013388000	4.575099000	1.151428000
P	-0.010444000	-1.165617000	4.572739000
N	0.659202000	-0.637808000	2.131351000
C	4.798883000	-1.588896000	4.591299000
N	-0.666170000	-0.446107000	2.176933000
N	-0.657369000	2.177698000	0.449985000
N	0.668223000	2.126448000	0.638474000
C	-4.796724000	4.794234000	0.803817000
C	2.677010000	3.281747000	1.330622000
C	3.323891000	4.667716000	1.246594000
C	4.824730000	4.575100000	1.548305000
C	1.202297000	3.282680000	1.013551000
C	-2.673534000	-0.385249000	3.524882000
C	3.299230000	-1.280518000	4.680453000
C	5.079880000	3.935185000	2.919430000
C	-1.183990000	3.377141000	0.666289000
C	-3.296505000	4.722509000	1.114436000
C	-2.657194000	3.536255000	0.385635000
C	2.658344000	-1.348447000	3.290807000
C	1.185673000	-1.022412000	3.287457000
C	-5.050143000	4.881021000	-0.707229000
C	-2.892434000	3.649368000	-1.134204000
C	5.049593000	-2.955920000	3.940727000
C	-1.199947000	-0.667905000	3.372300000
C	-5.072587000	0.708592000	4.856711000
C	4.412752000	2.557109000	3.020306000
C	-4.820269000	-0.802705000	4.770011000
C	2.914604000	2.660561000	2.722273000
C	4.386946000	-3.042215000	2.559424000
C	2.890141000	-2.736498000	2.659711000
C	-3.320050000	-1.114757000	4.706719000

C	-2.907647000	1.134765000	3.638519000
C	-4.405124000	1.449148000	3.690347000
C	-4.389967000	3.710324000	-1.447358000
H	5.289567000	-0.805010000	3.987405000
H	5.254903000	-1.551033000	5.591443000
H	-5.287875000	3.888563000	1.201867000
H	-5.250760000	5.653777000	1.318343000
H	3.178314000	2.629454000	0.588089000
H	2.835797000	5.336340000	1.977929000
H	3.149709000	5.102681000	0.249658000
H	5.309249000	3.962734000	0.767198000
H	5.284695000	5.572979000	1.499894000
H	-3.177705000	-0.728063000	2.599561000
H	2.804710000	-2.015775000	5.339963000
H	3.127740000	-0.286964000	5.124019000
H	4.665689000	4.590403000	3.704887000
H	6.160625000	3.854926000	3.108396000
H	-2.801601000	5.653616000	0.785720000
H	-3.123203000	4.633808000	2.198672000
H	-3.165309000	2.613959000	0.730486000
H	3.167162000	-0.603808000	2.646858000
H	-4.629629000	5.827220000	-1.088829000
H	-6.130583000	4.906265000	-0.912540000
H	-2.408207000	2.803085000	-1.649298000
H	-2.393056000	4.564821000	-1.495598000
H	6.129676000	-3.149570000	3.862676000
H	4.629141000	-3.744805000	4.587778000
H	-4.656892000	1.088782000	5.805610000
H	-6.152905000	0.915175000	4.876155000
H	4.574180000	2.122254000	4.018803000
H	4.879142000	1.868812000	2.292114000
H	-5.306466000	-1.199352000	3.861034000
H	-5.279949000	-1.317549000	5.626374000
H	2.424493000	1.674424000	2.777590000
H	2.422768000	3.298410000	3.476876000
H	4.859824000	-2.311347000	1.878447000
H	4.544250000	-4.038214000	2.117318000
H	2.391460000	-3.493323000	3.289606000
H	2.403709000	-2.781055000	1.671269000
H	-3.147057000	-2.199010000	4.617880000
H	-2.830305000	-0.787273000	5.641021000
H	-2.417983000	1.650088000	2.795638000
H	-2.413339000	1.494980000	4.557213000
H	-4.564484000	2.534695000	3.781132000

H	-4.873005000	1.134769000	2.739735000
H	-4.549521000	3.801742000	-2.532795000
H	-4.863484000	2.762666000	-1.132447000

Compound **10**:

Sb	0.393872000	-0.070588000	-1.342695000
P	4.355558000	-1.201841000	0.822472000
P	-3.245201000	-2.418517000	0.362043000
P	-1.749324000	3.312759000	0.803761000
N	-1.178371000	-1.097561000	-0.377109000
N	2.827672000	0.118455000	-0.797035000
N	-1.428630000	-0.612036000	0.857450000
N	2.032026000	-0.805597000	-0.192353000
N	-1.256836000	1.686726000	-1.142808000
N	-0.144446000	1.694104000	-0.364117000
C	4.069778000	0.062558000	-0.390210000
C	-2.474835000	-1.186079000	1.393433000
C	2.991167000	-3.597586000	2.159589000
C	-2.966185000	-3.750862000	-2.395868000
C	2.661748000	-1.601415000	0.694731000
C	-2.210125000	2.449700000	-0.674926000
C	-2.230813000	-1.553498000	-3.281644000
C	-2.033580000	-2.044237000	-0.826900000
C	1.423080000	1.395003000	2.285180000
C	4.542065000	1.858011000	-2.085055000
C	-0.208487000	2.491777000	0.715887000
C	0.971137000	2.710470000	1.642897000
C	-2.975840000	-0.759315000	2.764556000
C	5.127829000	0.981275000	-0.974849000
C	-4.171368000	1.060695000	-1.211317000
C	0.583681000	3.693167000	2.754158000
C	1.105547000	-2.012581000	2.588269000
C	-1.924430000	-2.634680000	-2.226693000
C	1.956281000	-2.679212000	1.497049000
C	-4.472958000	3.516508000	-0.786319000
C	-3.332954000	2.731542000	-2.883097000
C	5.697975000	1.866043000	0.145489000
C	2.126780000	3.301107000	0.820050000
C	-0.542689000	-3.266607000	-2.470852000
C	1.053583000	-3.518728000	0.587187000
C	-3.548945000	2.455258000	-1.388761000
C	6.262932000	0.120159000	-1.554871000

C	-1.914458000	0.050209000	3.513576000
C	-4.221854000	0.124045000	2.577499000
C	-3.350976000	-2.005041000	3.579452000
H	3.623330000	-4.091085000	1.412248000
H	2.469986000	-4.368623000	2.738559000
H	3.638732000	-3.038720000	2.845027000
H	-3.982058000	-3.365377000	-2.255742000
H	-2.800571000	-4.558161000	-1.673774000
H	-2.892725000	-4.167876000	-3.407128000
H	-2.070664000	-1.961849000	-4.286657000
H	-1.611998000	-0.653477000	-3.180752000
H	-3.276288000	-1.237164000	-3.202350000
H	0.615782000	0.944006000	2.869892000
H	2.276361000	1.585622000	2.948316000
H	1.743855000	0.674581000	1.531349000
H	4.133449000	1.243027000	-2.894109000
H	5.330519000	2.498908000	-2.496895000
H	3.738033000	2.498468000	-1.708851000
H	-3.486244000	0.291916000	-1.583334000
H	-5.119172000	0.992835000	-1.759949000
H	-4.361547000	0.844465000	-0.154687000
H	-0.246063000	3.300223000	3.354904000
H	0.285521000	4.665625000	2.345279000
H	1.443121000	3.846984000	3.416671000
H	0.568177000	-2.781786000	3.159022000
H	0.370501000	-1.337928000	2.140635000
H	1.738546000	-1.439485000	3.277181000
H	-4.652588000	3.322938000	0.278853000
H	-5.440360000	3.503458000	-1.301731000
H	-4.042540000	4.520286000	-0.885129000
H	-2.859968000	3.708257000	-3.036981000
H	-4.296440000	2.724107000	-3.406959000
H	-2.688555000	1.962690000	-3.323779000
H	4.913298000	2.490470000	0.585421000
H	6.480236000	2.521092000	-0.256827000
H	6.136582000	1.253069000	0.941792000
H	2.970672000	3.525394000	1.484024000
H	1.819423000	4.226412000	0.319255000
H	2.458919000	2.580064000	0.064825000
H	-0.377171000	-4.096839000	-1.777144000
H	0.298972000	-2.571380000	-2.354538000
H	-0.496109000	-3.654466000	-3.495056000
H	1.619788000	-3.927717000	-0.258699000
H	0.220017000	-2.922715000	0.207895000

H	0.627364000	-4.352313000	1.158150000
H	6.726614000	-0.496692000	-0.776164000
H	7.036273000	0.766983000	-1.986766000
H	5.886252000	-0.545075000	-2.340044000
H	-1.018143000	-0.551076000	3.702657000
H	-2.320378000	0.379015000	4.478037000
H	-1.627110000	0.932583000	2.930927000
H	-3.953023000	1.050673000	2.054287000
H	-4.640175000	0.390632000	3.556038000
H	-4.994643000	-0.397730000	1.999521000
H	-4.155923000	-2.570144000	3.093912000
H	-3.695899000	-1.708734000	4.577307000
H	-2.485336000	-2.669133000	3.691360000

Comparison of selected bond distances (Å), bond angles (°) and torsion angles (°) for complex **4**, **5**, **6** and **10**

Item	Sb-Sb(Å)		Sb-N $_{avg}$ (Å)		N-Sb-N $_{avg}$ (°)		N-Sb-Sb $_{avg}$ (°)		Sb-Sb-N-N $_{avg}$ (°)	
Complex	Exp.*	Calc.*	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
4	2.6691(8)	2.6753	2.393(6)	2.3825	85.03(7)	84.440	72.89(15)	71.87	-23.6(4)	-28.50
5α, 5β	2.7429 $_{avg}$	2.7508	2.385(5)	2.3373	85.27(19)	84.606	73.30(13)	72.14	0.3(4)	11.09
6	2.7399(5)	2.7492	2.348(8)	2.3304	85.16(12)	84.648	73.11(18)	72.21	-0.25(2)	-8.69
10	–	–	2.118(3)	2.1108	33.83(9)	33.511	–	–	–	–

*Exp.: experimental value; *Calc.: calculated value.

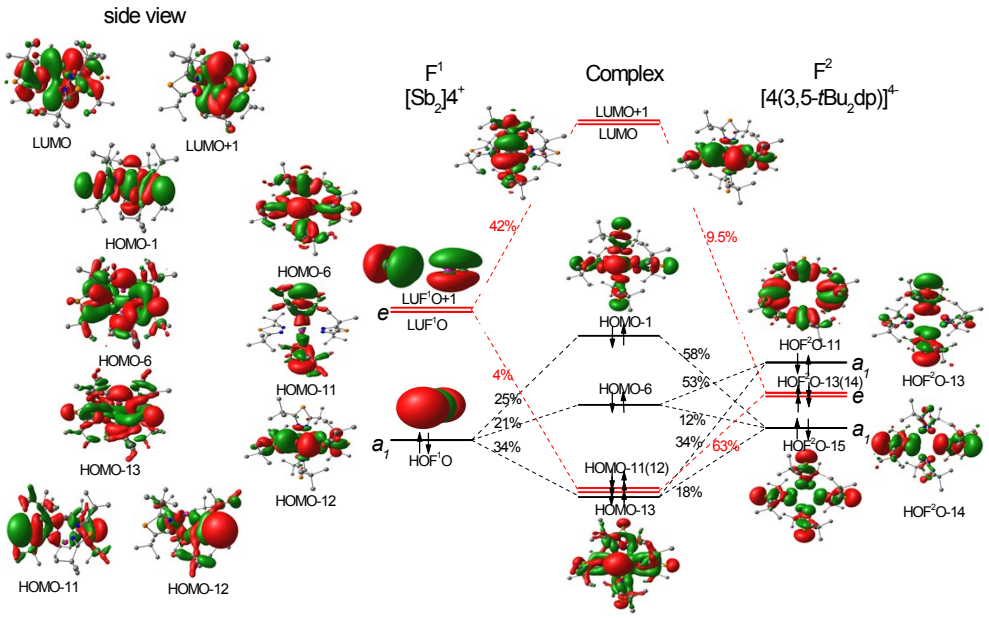


Figure 27. MO-FO interaction diagram for the main interaction between $[Sb–Sb]^{4+}$unit (F^1) and the four coordinating 1,2,4-diazaphospholides $\{4[3,5\text{-}t\text{Bu}_2\text{dp}]\}^{4-}$ (F^2). The orbital energy levels of F^1 were shifted with a vshift of22 eV, while the orbital energy levels of F^2were shifted with a vshift of –10 eV.

Cartesian Coordinates of the Optimized Geometries of Compound $Bi_2[3,5\text{-}t\text{Bu}_2\text{dp}]_4$ by M11 method with the combination of 6-31G(d) basis set for C, N, P and H atoms anddefz-TZVP basis set and psuedopotential for Bi atoms. All calculations were performed using Gaussian 09 package.

Bi	-0.000436000	0.000103000	-1.398255105
Bi	-0.000257000	-0.000143000	1.395519105
P	-3.319741252	-3.566501271	0.001221000
P	3.566567270	-3.319004251	0.002669000
P	-3.566249271	3.319970254	0.000786000
P	3.320162255	3.565373271	0.002914000
N	-1.787218137	-1.564611117	-0.643242051
N	-1.429545107	-1.896460144	0.640878047
N	1.895858146	-1.429203110	0.641679052
N	1.564631120	-1.786864138	-0.642603048
N	-1.564372119	1.787311134	-0.643307049
N	-1.896696146	1.429410108	0.640622046
N	1.429170111	1.895845145	0.641337050
N	1.787419134	1.563966119	-0.642629052
C	-2.777540210	-2.323066178	-1.133662088
C	-2.115789159	-2.936917227	1.133692087
C	-1.780244136	-3.558449273	2.493278189
C	-1.753834133	-2.512389192	3.627565277
C	-2.832229219	-4.624311351	2.866252220
C	-0.399456030	-4.248673325	2.383727184
C	-3.422593259	-2.034495156	-2.493063189
C	-4.416526338	-3.156580243	-2.860344221
C	-2.382375184	-1.942461146	-3.629238277
C	-4.203322322	-0.702556052	-2.387037183
C	2.936453223	-2.115056164	1.134837089
C	2.323457177	-2.777015214	-1.132691085
C	2.035516156	-3.422075263	-2.492219189
C	3.157424244	-4.416501340	-2.858701221
C	1.944730147	-2.381821183	-3.628459275
C	0.703171051	-4.202221321	-2.387062181
C	3.558111271	-1.779015138	2.494247192
C	4.621990354	-2.832473217	2.868777221
C	4.250881323	-0.399618031	2.383029184
C	2.511973190	-1.749163133	3.628342279
C	-2.322400177	2.777971215	-1.133738088
C	-2.937347226	2.115537159	1.133150088
C	-3.559855270	1.779229137	2.492113189
C	-4.250215327	0.398619030	2.381119182
C	-2.514661194	1.751804135	3.627160277

C	-4.625811352	2.831142214	2.865021216
C	-2.033200153	3.423351263	-2.492859191
C	-3.154805240	4.417844339	-2.860089221
C	-1.941299147	2.383480180	-3.629368280
C	-0.700993053	4.203551323	-2.386282184
C	2.115190162	2.936301222	1.134529087
C	2.778398213	2.321986175	-1.132316089
C	3.425051261	2.032993155	-2.490877190
C	4.415230335	3.157875240	-2.859823219
C	4.210399321	0.703975051	-2.381549181
C	2.386100184	1.934664148	-3.627613279
C	1.778296134	3.558628272	2.493439191
C	2.830099217	4.624485355	2.866964217
C	1.750346135	2.513330191	3.628381279
C	0.397797030	4.249114326	2.381913181
H	-0.965590076	-1.765578137	3.490320269
H	-1.559389117	-3.008374232	4.585859348
H	-2.711176208	-1.986865150	3.706945283
H	-2.571185198	-5.080061389	3.828551295
H	-2.879773217	-5.424717426	2.120422164
H	-3.832802292	-4.187658321	2.958620225
H	0.381339029	-3.540520271	2.092018162
H	-0.422991032	-5.043917387	1.630786124
H	-0.120306009	-4.698100356	3.345192254
H	-3.914348300	-4.126188314	-2.950123226
H	-4.890322373	-2.929881223	-3.822652291
H	-5.210753400	-3.254837250	-2.112856162
H	-1.688585128	-1.106798082	-3.494655267
H	-2.891431220	-1.783288138	-4.587167353
H	-1.795460136	-2.863531217	-3.707023284
H	-4.993239383	-0.775787061	-1.631683127
H	-4.673014359	-0.458202035	-3.348299255
H	-3.548186272	0.125017010	-2.100642159
H	4.127284314	-3.914724301	-2.948007226
H	2.931089223	-4.890361373	-3.821063294
H	3.254942249	-5.210647400	-2.111028162
H	1.109133082	-1.687821128	-3.494563265
H	1.786256135	-2.890790222	-4.586550348
H	2.866032220	-1.795151139	-3.705412283
H	0.775604061	-4.992240381	-1.631736124
H	0.459172035	-4.671717357	-3.348511254
H	-0.124274009	-3.546741269	-2.101080159
H	4.183484319	-3.832130295	2.962266225
H	5.077988390	-2.571059196	3.830859291

H	5.422501390	-2.882408218	2.123221162
H	5.046325387	-0.425632032	1.630383124
H	4.700482358	-0.119938009	3.344260257
H	3.544199270	0.382021029	2.090003161
H	1.766897138	-0.959454075	3.490155266
H	3.008269228	-1.554663119	4.586458350
H	1.984429151	-2.705300208	3.708787286
H	-5.044820385	0.422762032	1.627521127
H	-4.700495359	0.118936009	3.342029256
H	-3.541923268	-0.382104029	2.089529161
H	-3.011413228	1.556755121	4.584932351
H	-1.989009154	2.708980207	3.707640283
H	-1.767926133	0.963496074	3.489898266
H	-5.425653434	2.879334222	2.118628163
H	-4.189048321	3.831575294	2.958393224
H	-5.082326389	2.569525195	3.826802290
H	-4.124584314	3.916075301	-2.950289224
H	-2.927670225	4.891883371	-3.822175291
H	-3.252941250	5.211848400	-2.112348163
H	-1.105938084	1.689318128	-3.494831266
H	-1.781703136	2.892801223	-4.587088352
H	-2.862579217	1.796954135	-3.707576285
H	-0.774128058	4.993329381	-1.630773122
H	-0.456198035	4.673372358	-3.347370258
H	0.126265010	3.548057269	-2.099786162
H	3.909587297	4.125453313	-2.952010225
H	4.890587374	2.930826222	-3.821280293
H	5.208562400	3.260633249	-2.111992159
H	4.681610357	0.459297035	-3.341993256
H	3.557842270	-0.125256010	-2.093971160
H	4.999546382	0.781484061	-1.625817123
H	1.794958137	2.852878218	-3.707161283
H	1.696290129	1.095825084	-3.492497267
H	2.896638223	1.776570138	-4.584927351
H	3.830469292	4.187664322	2.960725224
H	2.568070196	5.080861388	3.828698295
H	2.878667221	5.424437438	2.120715164
H	2.707493208	1.987698149	3.709277283
H	0.962116074	1.766583134	3.490718268
H	1.554839118	3.010000230	4.586101351
H	0.117618009	4.699107359	3.342813253
H	-0.382813029	3.540979269	2.089664160
H	0.422406032	5.043952387	1.628579127

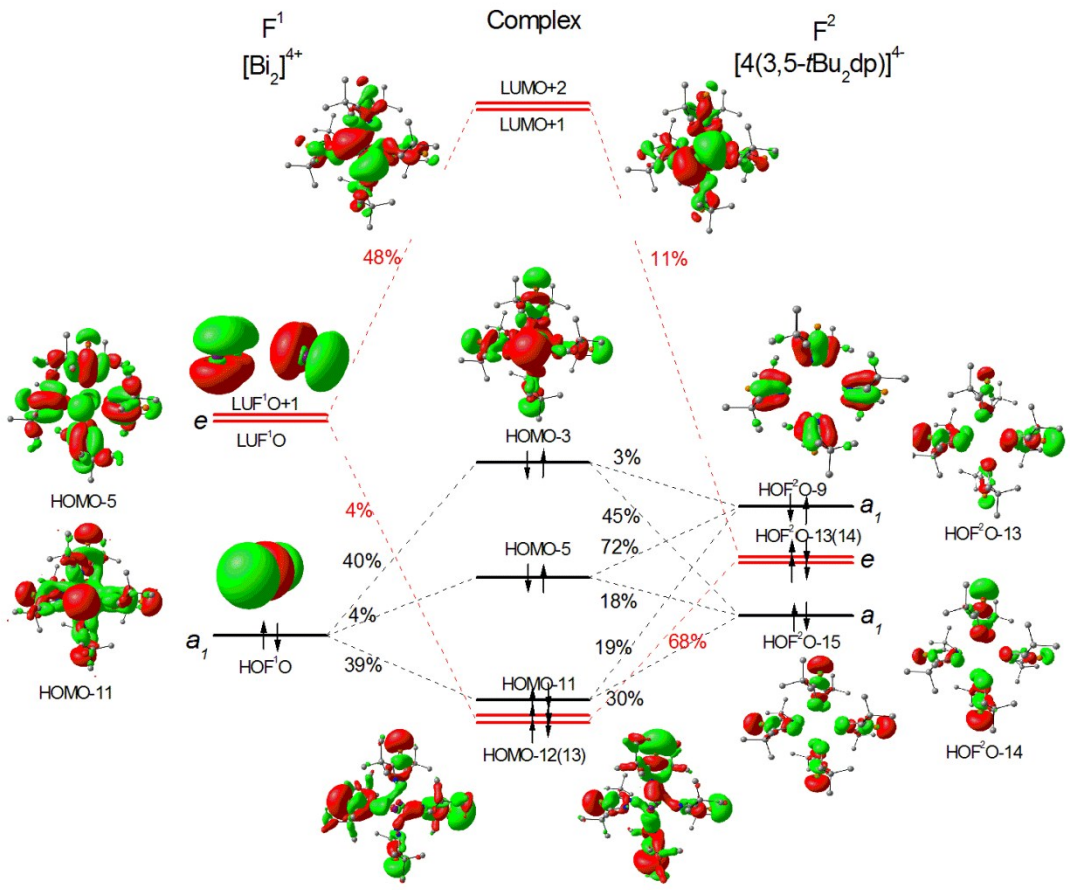


Figure 28. MO-FO interaction diagram for the main interaction between $[Bi–Bi]^{4+}$unit (F^1) and the four coordinating 1,2,4-diazaphospholides $\{4[3,5\text{-}t\text{Bu}_2\text{dp}]\}^{4-}$ (F^2). The orbital energy levels of F^1 were shifted with a vshift of24eV, while the orbital energy levels of F^2were shifted with a vshift of –11.5eV.

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