Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(18), 4478-4479, DOI:10.1021/ic971583p

Table 1. Crystal Data for $C_{30}H_{25}N_4P_3$ (4).

Identification code	bc143s
Empirical formula	$C_{33.50}H_{28.50}N_4P_3$
Formula mass	580.01
Crystal size, mm	0.49 × 0.38 × 0.18
Crystal color, habit	colorless needle
Crystal system	Triclinic
Space group	$P\bar{1}$
a, Å	8.6689(8)
b, Å	12.7115(2)
c, Å	14.882(2)
α, °	110.033(6)
β, °	101.039(9)
γ, °	96.837(5)
Volume, Å^3	1481.6(2)
Z, formula units/cell	2
Density (calculated), Mg·m^{-3}	1.300
Absorption coefficient, mm^{-1}	0.231
F(000)	605
Absorption correction	None
Range Transmission Coefficients	0.97 and 0.82

Table 2. Data Collection Parameters for $C_{30}H_{25}N_4P_3$ (4).

Diffractometer	Siemens SMART
Temperature, K	151(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	6362
θ range	$1.50 < \theta < 28.27$
θ range, data collection	$1.50 < \theta < 28.27$
Scan type	ω scans
Index ranges	$-11 \le h \le 11$,
	$-16 \le k \le 16$,
	$-19 \le l \le 19$
Reflections collected	16217
Independent reflections	7153 (R(int) = 0.0176)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 3. Structure Solution and Refinement for $C_{30}H_{25}N_4P_3$ (4).

System used[1,2]	Siemens SHELXTL
Structure solution	direct
Data/ restraints/ parameters	7145 / 2/ 376
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0411P)^2+0.8470P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0358, wR2 = 0.0906
Reflections observed	6246
R indices (all data)	R1 = 0.0431, wR2 = 0.0994
Goodness-of-fit[4] on F^2	1.031
Largest diff. peak and hole	0.344 and -0.244

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\sum\|F_o|-|F_c\|}{\sum|F_o|}$; $wR2 = \sqrt{\frac{\sum[w(F_o^2-F_c^2)^2]}{\sum[w(F_o^2)^2]}}$;

4) $GooF = S = \sqrt{\frac{\sum[w(F_o^2-F_c^2)^2]}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined

Table 4. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $C_{30}H_{25}N_4P_3$ (4).

U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	Ueq
P(1)	0.06324(4)	0.67475(3)	0.34914(3)	0.01918(8)
P(2)	-0.11764(4)	0.43295(3)	0.22041(3)	0.02135(9)
P(3)	-0.04814(4)	0.80534(3)	0.22196(3)	0.02186(9)
N(1)	-0.06247(14)	0.76134(10)	0.31913(9)	0.0206(2)
N(2)	-0.09777(13)	0.56130(10)	0.31880(9)	0.0204(2)
N(3)	-0.04732(15)	0.46309(11)	0.13085(9)	0.0235(2)
N(4)	-0.00675(15)	0.69418(11)	0.13270(9)	0.0235(2)
C(11)	0.1061(2)	0.73570(12)	0.48469(10)	0.0202(3)
C(12)	0.0376(2)	0.82278(13)	0.53876(11)	0.0258(3)
C(13)	0.0810(2)	0.86587(13)	0.64164(11)	0.0292(3)
C(14)	0.1923(2)	0.82267(13)	0.69154(11)	0.0280(3)
C(15)	0.2627(2)	0.73726(13)	0.63905(11)	0.0256(3)
C(16)	0.2212(2)	0.69454(12)	0.53625(11)	0.0229(3)
C(21)	0.0563(2)	0.38322(12)	0.26961(11)	0.0230(3)
C(22)	0.1092(2)	0.40793(13)	0.37049(11)	0.0261(3)
C(23)	0.2327(2)	0.3610(2)	0.40629(14)	0.0349(4)
C(24)	0.3029(2)	0.2876(2)	0.3418(2)	0.0424(4)
C(25)	0.2501(3)	0.2605(2)	0.2415(2)	0.0464(5)
C(26)	0.1272(2)	0.3076(2)	0.20492(13)	0.0357(4)
C(31)	0.1560(2)	0.89040(12)	0.27301(11)	0.0232(3)
C(32)	0.2556(2)	0.89937(14)	0.21129(13)	0.0310(3)
C(33)	0.4082(2)	0.96839(15)	0.25066(14)	0.0370(4)
C(34)	0.4622(2)	1.02979(14)	0.35118(14)	0.0347(4)
C(35)	0.3626(2)	1.02454(13)	0.41289(13)	0.0316(3)
C(36)	0.2103(2)	0.95524(13)	0.37409(12)	0.0264(3)
C(41)	-0.2204(2)	0.71906(12)	0.32401(10)	0.0204(3)
C(42)	-0.3453(2)	0.77832(13)	0.32984(11)	0.0243(3)
C(43)	-0.4917(2)	0.72424(14)	0.33494(11)	0.0270(3)
C(44)	-0.5118(2)	0.61420(14)	0.33408(11)	0.0264(3)
C(45)	-0.3858(2)	0.55467(13)	0.32869(11)	0.0244(3)
C(46)	-0.2403(2)	0.60817(12)	0.32391(10)	0.0201(3)
C(51)	-0.1516(2)	0.49332(13)	0.06059(10)	0.0237(3)
C(52)	-0.2763(2)	0.40912(14)	-0.01146(11)	0.0309(3)
C(53)	-0.3841(2)	0.4360(2)	-0.07811(12)	0.0363(4)
C(54)	-0.3679(2)	0.5471(2)	-0.07449(12)	0.0359(4)
C(55)	-0.2430(2)	0.63095(15)	-0.00486(11)	0.0302(3)
C(56)	-0.1338(2)	0.60526(13)	0.06312(10)	0.0238(3)
C(1S)	0.3385(5)	0.0126(4)	-0.0196(2)	0.0932(11)

C(2S)	0.4670(6)	0.1048(4)	0.0132(2)	0.1026(13)
C(3S)	0.6271(5)	0.0926(3)	0.0319(2)	0.0907(11)
C(4S)	0.1588(9)	0.0204(5)	-0.0386(5)	0.086(2)

Table 5. Bond lengths (Å) for $C_{30}H_{25}N_4P_3$ (4).

P(1)-N(1)	1.7420(12)	P(1)-N(2)	1.7507(12)
P(1)-C(11)	1.8388(14)	P(2)-N(3)	1.7030(13)
P(2)-N(2)	1.7423(12)	P(2)-C(21)	1.8251(15)
P(3)-N(4)	1.7051(13)	P(3)-N(1)	1.7395(12)
P(3)-C(31)	1.829(2)	N(1)-C(41)	1.435(2)
N(2)-C(46)	1.438(2)	N(3)-H(3)	0.890(8)
N(3)-C(51)	1.433(2)	N(4)-H(4)	0.893(8)
N(4)-C(56)	1.424(2)	C(11)-C(12)	1.398(2)
C(11)-C(16)	1.402(2)	C(12)-C(13)	1.393(2)
C(13)-C(14)	1.384(2)	C(14)-C(15)	1.386(2)
C(15)-C(16)	1.392(2)	C(21)-C(22)	1.394(2)
C(21)-C(26)	1.400(2)	C(22)-C(23)	1.392(2)
C(23)-C(24)	1.380(3)	C(24)-C(25)	1.380(3)
C(25)-C(26)	1.394(2)	C(31)-C(36)	1.397(2)
C(31)-C(32)	1.398(2)	C(32)-C(33)	1.392(2)
C(33)-C(34)	1.382(3)	C(34)-C(35)	1.388(2)
C(35)-C(36)	1.391(2)	C(41)-C(42)	1.390(2)
C(41)-C(46)	1.399(2)	C(42)-C(43)	1.398(2)
C(43)-C(44)	1.384(2)	C(44)-C(45)	1.400(2)
C(45)-C(46)	1.387(2)	C(51)-C(52)	1.399(2)
C(51)-C(56)	1.400(2)	C(52)-C(53)	1.388(2)
C(53)-C(54)	1.384(3)	C(54)-C(55)	1.386(2)
C(55)-C(56)	1.400(2)	C(1S)-C(3S)#1	1.363(5)
C(1S)-C(2S)	1.393(6)	C(1S)-C(4S)	1.551(7)
C(2S)-C(3S)	1.400(5)	C(3S)-C(1S)#1	1.363(5)

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

Table 6. Bond angles (°) for $C_{30}H_{25}N_4P_3$ (4).

N(1)-P(1)-N(2)	92.49(6)	N(1)-P(1)-C(11)	100.62(6)
N(2)-P(1)-C(11)	101.95(6)	N(3)-P(2)-N(2)	108.10(6)
N(3)-P(2)-C(21)	97.53(6)	N(2)-P(2)-C(21)	99.39(6)
N(4)-P(3)-N(1)	106.80(6)	N(4)-P(3)-C(31)	97.24(6)
N(1)-P(3)-C(31)	98.21(6)	C(41)-N(1)-P(3)	117.12(9)
C(41)-N(1)-P(1)	107.85(9)	P(3)-N(1)-P(1)	120.16(7)
C(46)-N(2)-P(2)	116.07(9)	C(46)-N(2)-P(1)	107.60(9)
P(2)-N(2)-P(1)	121.02(7)	H(3)-N(3)-C(51)	115.3(12)
H(3)-N(3)-P(2)	118.5(12)	C(51)-N(3)-P(2)	119.63(10)
H(4)-N(4)-C(56)	114.1(12)	H(4)-N(4)-P(3)	116.8(12)
C(56)-N(4)-P(3)	120.04(10)	C(12)-C(11)-C(16)	118.53(13)
C(12)-C(11)-P(1)	124.61(11)	C(16)-C(11)-P(1)	116.79(10)
C(13)-C(12)-C(11)	120.50(14)	C(14)-C(13)-C(12)	120.32(14)
C(13)-C(14)-C(15)	119.90(14)	C(14)-C(15)-C(16)	120.14(14)
C(15)-C(16)-C(11)	120.57(13)	C(22)-C(21)-C(26)	118.48(14)
C(22)-C(21)-P(2)	121.23(11)	C(26)-C(21)-P(2)	119.85(12)
C(23)-C(22)-C(21)	120.71(15)	C(24)-C(23)-C(22)	120.2(2)
C(25)-C(24)-C(23)	119.8(2)	C(24)-C(25)-C(26)	120.4(2)
C(25)-C(26)-C(21)	120.3(2)	C(36)-C(31)-C(32)	118.71(14)
C(36)-C(31)-P(3)	120.14(11)	C(32)-C(31)-P(3)	120.94(12)
C(33)-C(32)-C(31)	120.4(2)	C(34)-C(33)-C(32)	120.3(2)
C(33)-C(34)-C(35)	119.9(2)	C(34)-C(35)-C(36)	120.1(2)
C(35)-C(36)-C(31)	120.54(15)	C(42)-C(41)-C(46)	120.83(13)
C(42)-C(41)-N(1)	126.00(13)	C(46)-C(41)-N(1)	113.16(12)
C(41)-C(42)-C(43)	118.45(14)	C(44)-C(43)-C(42)	120.74(13)
C(43)-C(44)-C(45)	120.82(14)	C(46)-C(45)-C(44)	118.59(14)
C(45)-C(46)-C(41)	120.56(13)	C(45)-C(46)-N(2)	126.54(13)
C(41)-C(46)-N(2)	112.90(12)	C(52)-C(51)-C(56)	119.06(14)
C(52)-C(51)-N(3)	119.16(14)	C(56)-C(51)-N(3)	121.77(13)
C(53)-C(52)-C(51)	120.9(2)	C(54)-C(53)-C(52)	120.0(2)
C(53)-C(54)-C(55)	119.8(2)	C(54)-C(55)-C(56)	120.9(2)
C(55)-C(56)-C(51)	119.37(14)	C(55)-C(56)-N(4)	118.78(14)
C(51)-C(56)-N(4)	121.85(13)	C(3S)#1-C(1S)-C(2S)	117.6(4)
C(3S)#1-C(1S)-C(4S)	117.0(4)	C(2S)-C(1S)-C(4S)	125.3(4)
C(1S)-C(2S)-C(3S)	122.6(3)	C(1S)#1-C(3S)-C(2S)	119.8(4)

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

Table 7. Anisotropic displacement parameters ($Å^2$) for $C_{30}H_{25}N_4P_3$ (4).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P(1)	0.0150(2)	0.0232(2)	0.0183(2)	0.00562(13)	0.00488(13)	0.00528(13)
P(2)	0.0203(2)	0.0215(2)	0.0198(2)	0.00394(13)	0.00622(13)	0.00448(13)
P(3)	0.0203(2)	0.0256(2)	0.0209(2)	0.00912(14)	0.00562(14)	0.00717(14)
N(1)	0.0166(5)	0.0254(6)	0.0211(6)	0.0090(5)	0.0056(4)	0.0062(4)
N(2)	0.0157(5)	0.0217(5)	0.0207(6)	0.0036(4)	0.0052(4)	0.0043(4)
N(3)	0.0218(6)	0.0280(6)	0.0205(6)	0.0071(5)	0.0069(5)	0.0070(5)
N(4)	0.0209(6)	0.0280(6)	0.0206(6)	0.0075(5)	0.0053(5)	0.0064(5)
C(11)	0.0172(6)	0.0220(6)	0.0194(6)	0.0061(5)	0.0045(5)	0.0016(5)
C(12)	0.0252(7)	0.0276(7)	0.0231(7)	0.0073(6)	0.0048(6)	0.0087(6)
C(13)	0.0326(8)	0.0286(7)	0.0228(7)	0.0038(6)	0.0085(6)	0.0082(6)
C(14)	0.0299(8)	0.0299(7)	0.0196(7)	0.0074(6)	0.0033(6)	-0.0002(6)
C(15)	0.0229(7)	0.0279(7)	0.0249(7)	0.0124(6)	0.0009(6)	0.0010(6)
C(16)	0.0195(7)	0.0218(6)	0.0251(7)	0.0072(5)	0.0041(5)	0.0033(5)
C(21)	0.0225(7)	0.0223(6)	0.0268(7)	0.0103(6)	0.0092(6)	0.0060(5)
C(22)	0.0240(7)	0.0264(7)	0.0283(7)	0.0108(6)	0.0072(6)	0.0036(6)
C(23)	0.0300(8)	0.0410(9)	0.0374(9)	0.0224(8)	0.0036(7)	0.0051(7)
C(24)	0.0333(9)	0.0514(11)	0.0600(12)	0.0355(10)	0.0169(9)	0.0210(8)
C(25)	0.0521(12)	0.0521(11)	0.0572(12)	0.0296(10)	0.0324(10)	0.0351(10)
C(26)	0.0459(10)	0.0381(9)	0.0342(9)	0.0169(7)	0.0206(8)	0.0221(8)
C(31)	0.0233(7)	0.0218(6)	0.0266(7)	0.0105(6)	0.0071(6)	0.0067(5)
C(32)	0.0318(8)	0.0310(8)	0.0318(8)	0.0119(7)	0.0122(7)	0.0042(6)
C(33)	0.0346(9)	0.0334(8)	0.0474(10)	0.0172(8)	0.0193(8)	0.0027(7)
C(34)	0.0262(8)	0.0266(8)	0.0492(10)	0.0144(7)	0.0072(7)	0.0004(6)
C(35)	0.0319(8)	0.0237(7)	0.0345(8)	0.0081(6)	0.0039(7)	0.0036(6)
C(36)	0.0263(7)	0.0246(7)	0.0284(7)	0.0092(6)	0.0078(6)	0.0067(6)
C(41)	0.0158(6)	0.0266(7)	0.0166(6)	0.0050(5)	0.0046(5)	0.0052(5)
C(42)	0.0207(7)	0.0282(7)	0.0230(7)	0.0065(6)	0.0060(5)	0.0092(6)
C(43)	0.0173(7)	0.0367(8)	0.0245(7)	0.0061(6)	0.0060(5)	0.0103(6)
C(44)	0.0156(6)	0.0369(8)	0.0231(7)	0.0065(6)	0.0066(5)	0.0037(6)
C(45)	0.0209(7)	0.0280(7)	0.0215(7)	0.0058(6)	0.0064(5)	0.0036(5)
C(46)	0.0160(6)	0.0251(6)	0.0165(6)	0.0039(5)	0.0044(5)	0.0056(5)
C(51)	0.0216(7)	0.0318(7)	0.0161(6)	0.0053(5)	0.0068(5)	0.0075(6)
C(52)	0.0308(8)	0.0321(8)	0.0225(7)	0.0022(6)	0.0070(6)	0.0029(6)
C(53)	0.0280(8)	0.0491(10)	0.0193(7)	0.0027(7)	0.0005(6)	0.0009(7)
C(54)	0.0286(8)	0.0556(11)	0.0215(7)	0.0135(7)	0.0025(6)	0.0093(7)
C(55)	0.0303(8)	0.0401(9)	0.0225(7)	0.0133(6)	0.0068(6)	0.0108(7)
C(56)	0.0216(7)	0.0321(7)	0.0164(6)	0.0061(5)	0.0066(5)	0.0070(6)
C(1S)	0.119(3)	0.108(3)	0.0411(14)	0.013(2)	0.009(2)	0.042(2)

C(2S)	0.149(4)	0.108(3)	0.054(2)	0.022(2)	0.017(2)	0.077(3)
C(3S)	0.134(3)	0.098(2)	0.0432(14)	0.0229(15)	0.016(2)	0.055(2)
C(4S)	0.120(5)	0.058(3)	0.070(4)	0.018(3)	-0.003(4)	0.038(3)

Table 8. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $C_{30}H_{25}N_4P_3$ (4).

	x	y	z	Ueq
H(3)	0.0564(10)	0.4930(15)	0.1438(13)	0.028
H(4)	0.0838(14)	0.6707(15)	0.1492(13)	0.028
H(12A)	-0.0391(2)	0.85281(13)	0.50511(11)	0.031
H(13A)	0.0340(2)	0.92519(13)	0.67769(11)	0.035
H(14A)	0.2204(2)	0.85152(13)	0.76168(11)	0.034
H(15A)	0.3394(2)	0.70781(13)	0.67329(11)	0.031
H(16A)	0.2714(2)	0.63700(12)	0.50074(11)	0.027
H(22A)	0.0604(2)	0.45733(13)	0.41532(11)	0.031
H(23A)	0.2689(2)	0.3796(2)	0.47533(14)	0.042
H(24A)	0.3873(2)	0.2558(2)	0.3665(2)	0.051
H(25A)	0.2978(3)	0.2095(2)	0.1972(2)	0.056
H(26A)	0.0913(2)	0.2883(2)	0.13576(13)	0.043
H(32A)	0.2189(2)	0.85811(14)	0.14205(13)	0.037
H(33A)	0.4756(2)	0.97332(15)	0.20826(14)	0.044
H(34A)	0.5672(2)	1.07549(14)	0.37795(14)	0.042
H(35A)	0.3985(2)	1.06834(13)	0.48174(13)	0.038
H(36A)	0.1426(2)	0.95199(13)	0.41670(12)	0.032
H(42A)	-0.3314(2)	0.85380(13)	0.33035(11)	0.029
H(43A)	-0.5784(2)	0.76347(14)	0.33905(11)	0.032
H(44A)	-0.6124(2)	0.57861(14)	0.33718(11)	0.032
H(45A)	-0.3998(2)	0.47924(13)	0.32833(11)	0.029
H(52A)	-0.2873(2)	0.33253(14)	-0.01479(11)	0.037
H(53A)	-0.4688(2)	0.3781(2)	-0.12619(12)	0.044
H(54A)	-0.4422(2)	0.5658(2)	-0.11958(12)	0.043
H(55A)	-0.2313(2)	0.70688(15)	-0.00327(11)	0.036
H(2SA)	0.4452(6)	0.1789(4)	0.0233(2)	0.123
H(3SA)	0.7114(5)	0.1573(3)	0.0531(2)	0.109
H(4SA)	0.1493(9)	0.0997(5)	-0.0275(5)	0.130
H(4SB)	0.1100(9)	-0.0049(5)	0.0066(5)	0.130
H(4SC)	0.1036(9)	-0.0286(5)	-0.1069(5)	0.130

Table 9. Least Squares Planes and Dihedral Angles for $C_{30}H_{25}N_4P_3$ (4).

A. Least Squares Planes

Plane	atom	deviation (Å)	atom	deviation (Å)
1	0.493 x + -0.139 y + 13.380 z = 4.1335			
	N(1)	0.0001	C(43)	0.0051
	N(2)	0.0060	C(44)	-0.0011
	C(41)	-0.0066	C(45)	-0.0027
	C(42)	0.0016	C(46)	-0.0024
2	-6.716 x + 0.863 y + 10.897z = 2.1115			
	N(3)	0.0319	C(53)	-0.0068
	N(4)	-0.0209	C(54)	0.0202
	C(51)	-0.0069	C(55)	0.0122
	C(52)	-0.0274	C(56)	-0.0023
3	5.084 x + 9.295 y + -5.108 z = 2.4621			
	C(21)	0.0090	C(24)	0.0044
	C(22)	-0.0079	C(25)	-0.0032
	C(23)	0.0012	C(26)	-0.0035
4	-4.026 x + 11.797 y + -5.182 z = 8.4487			
	C(31)	-0.0145	C(34)	-0.0121
	C(32)	0.0098	C(35)	0.0072
	C(33)	0.0035	C(36)	0.0061
5	-2.933 x + 0.495 y + 13.714 z = 4.9367			
	P(1)	0.0000	N(2)	0.0000
	N(1)	0.0000		
6	8.428 x + -1.555 y + 0.432 z = 1.5659			
	N(1)	-0.0067	P(2)	-0.0036
	N(2)	0.0067	P(3)	0.0036
7	7.231 x + -1.354 y + 5.131 z = 0.3028			

N(3)	0.0050	P(2)	-0.0031
N(4)	-0.0051	P(3)	0.0032

B. Dihedral Angles

plane	angle (°)	plane	angle (°)
1-2	54.1	3-4	64.8
1-5	23.0	1-6	73.2
5-6	96.3	6-7	19.9
2-7	107.3		

Table 10. Crystal data for $C_{31}H_{27}N_4P_3Si$ (6).

Identification code	bc190
Empirical formula	$C_{31}H_{27}N_4P_3Si$
Formula mass	576.57
Crystal size, mm	0.40 × 0.26 × 0.17
Crystal color, habit	Colorless Prism
Crystal system	Triclinic
Space group	$P\bar{1}$
a, Å	10.291(3)
b, Å	17.108(8)
c, Å	17.824(5)
α, °	106.029(10)
β, °	106.254(6)
γ, °	96.298(18)
Volume, Å^3	2835.4(18)
Z, formula units/cell	4
Density (calculated), Mg·m^{-3}	1.351
Absorption coefficient, mm^{-1}	0.281
F(000)	1200
Absorption correction	Semi-empirical from equivalents
Range Transmission Coefficients	0.9538 and 0.8959

Table 11. Data collection parameters for $C_{31}H_{27}N_4P_3Si$ (6).

Diffractometer	Siemens SMART CCD
Temperature, K	171(2)
Radiation source	sealed tube
Wavelength, Å	0.71073 MoKα
Monochromator	graphite
Cell measurement	
Reflections used	7480
θ range	$1.47 < \theta < 31.31$
θ range, data collection	$1.47 < \theta < 31.28$
Scan type	0.3° ω scan
Index ranges	$-14 \le h \le 14$,
	$-24 \le k \le 23$,
	$0 \le l \le 25$
Reflections collected	37489
Independent reflections	16836 (R(int) = 0.0362)
Standard reflections	50 frames re-measured
Stability of standards	no decay observed

Table 12. Structure Solution and Refinement for $C_{31}H_{27}N_4P_3Si$ (6).

System used[1,2]	SHELXS-97 (Sheldrick, 1990)
Structure solution	direct
Data/ restraints/ parameters	16836 / 0/ 711
Hydrogen atoms	riding, with riding isotropic U
weighting scheme	calc $w^{-1}=[\sigma^2(F_o^2)+(0.0411P)^2+0.8470P]$ where $P=(F_o^2+2F_c^2)\div 3$
Final R indices[3] [I>2σ(I)]	R1 = 0.0447, wR2 = 0.0980
Reflections observed	13886
R indices (all data)	R1 = 0.0597, wR2 = 0.1080
Goodness-of-fit[4] on F^2	1.106
Largest diff. peak and hole	0.789 and -0.388

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1) G. M. Sheldrick, SHELXTL, *A Program for Crystal Structure Determination.* Version 5.03, 1995, Siemens Analytical X-ray Instruments, Madison, Wisconsin.

2) Scattering factors (neutral atoms) are from "International Tables for Crystallography" Vol. C, D. Reidel Publishing Co. Boston, 1991.

3) $R1 = \frac{\sum\|F_o|-|F_c\|}{\sum|F_o|}$; $wR2 = \sqrt{\frac{\sum[w(F_o^2-F_c^2)^2]}{\sum[w(F_o^2)^2]}}$;

4) $GooF = S = \sqrt{\frac{\sum[w(F_o^2-F_c^2)^2]}{(M-N)}}$ where M is the number of reflections and N is the number of parameters refined.

Table 13. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for $C_{31}H_{27}N_4P_3Si$. (6)

U_{eq} is defined as one-third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	Ueq
Si11	0.87493(5)	-0.03709(3)	0.16065(3)	0.02131(9)
P11	0.73938(4)	0.07083(3)	0.30309(3)	0.01872(8)
P21	0.84655(4)	-0.09066(3)	0.30925(3)	0.01827(8)
P31	0.58364(4)	0.01171(3)	0.11622(3)	0.02047(9)
N11	0.73020(13)	-0.02540(8)	0.31883(9)	0.0185(3)
N21	0.58603(14)	0.03750(9)	0.21913(9)	0.0207(3)
N31	0.85566(14)	-0.11170(9)	0.21032(8)	0.0194(3)
N41	0.69735(14)	-0.05392(9)	0.10603(9)	0.0208(3)
C11	0.9710(2)	-0.06968(14)	0.08779(13)	0.0338(4)
C111	0.67376(17)	0.12413(10)	0.38538(11)	0.0217(3)
C121	0.67810(18)	0.09696(11)	0.45267(11)	0.0251(3)
C131	0.6434(2)	0.14433(13)	0.51882(12)	0.0300(4)
C141	0.6034(2)	0.21897(13)	0.51828(13)	0.0319(4)
C151	0.5973(2)	0.24614(13)	0.45154(14)	0.0352(4)
C161	0.6330(2)	0.19969(12)	0.38563(13)	0.0313(4)
C211	1.00800(16)	-0.01486(11)	0.36592(10)	0.0207(3)
C221	1.12675(18)	-0.02638(13)	0.34410(12)	0.0298(4)
C231	1.25290(19)	0.02760(15)	0.39036(14)	0.0368(5)
C241	1.2628(2)	0.09293(14)	0.45945(13)	0.0363(5)
C251	1.1468(2)	0.10436(12)	0.48268(12)	0.0300(4)
C261	1.02030(17)	0.05078(11)	0.43651(11)	0.0231(3)
C311	0.69366(17)	0.10546(11)	0.12104(11)	0.0224(3)
C321	0.6952(2)	0.18329(12)	0.17288(12)	0.0288(4)
C331	0.7734(2)	0.25467(13)	0.17217(14)	0.0377(5)
C341	0.8489(2)	0.24910(14)	0.11840(15)	0.0385(5)
C351	0.8447(2)	0.17226(14)	0.06453(15)	0.0375(5)
C361	0.7677(2)	0.10097(12)	0.06573(12)	0.0294(4)
C411	0.58580(16)	-0.06454(10)	0.28667(10)	0.0191(3)
C421	0.52544(18)	-0.13039(11)	0.30484(11)	0.0246(3)
C431	0.38404(19)	-0.16227(11)	0.26578(12)	0.0289(4)
C441	0.30590(18)	-0.12820(12)	0.21099(12)	0.0288(4)
C451	0.36581(17)	-0.06098(12)	0.19390(11)	0.0262(4)
C461	0.50664(16)	-0.02929(10)	0.23225(10)	0.0203(3)
C511	0.73529(17)	-0.17212(10)	0.15004(10)	0.0198(3)
C521	0.70262(19)	-0.25481(11)	0.14472(11)	0.0246(3)
C531	0.5820(2)	-0.30516(11)	0.08469(12)	0.0284(4)
C541	0.4956(2)	-0.27350(12)	0.03054(12)	0.0292(4)
C551	0.52854(18)	-0.19092(12)	0.03493(11)	0.0260(3)

C561	0.64821(17)	-0.14008(10)	0.09480(10)	0.0203(3)
Si12	0.30381(5)	0.32216(3)	0.18448(3)	0.02481(10)
P12	0.18975(4)	0.49960(3)	0.26728(3)	0.02063(9)
P22	0.30912(5)	0.47616(3)	0.12283(3)	0.02258(9)
P32	0.40319(5)	0.42650(3)	0.37325(3)	0.02182(9)
N12	0.33576(14)	0.51006(9)	0.35073(9)	0.0212(3)
N22	0.28533(14)	0.53572(9)	0.21218(9)	0.0211(3)
N32	0.37518(15)	0.39375(10)	0.14468(10)	0.0253(3)
N42	0.42547(15)	0.36534(9)	0.28503(9)	0.0249(3)
C12	0.3217(2)	0.21547(13)	0.13468(14)	0.0391(5)
C112	0.13573(16)	0.59735(11)	0.30739(11)	0.0220(3)
C122	0.10800(19)	0.65080(12)	0.26059(12)	0.0283(4)
C132	0.0524(2)	0.71960(13)	0.28696(14)	0.0339(4)
C142	0.0232(2)	0.73637(14)	0.36018(15)	0.0366(5)
C152	0.0497(2)	0.68417(15)	0.40718(15)	0.0392(5)
C162	0.1053(2)	0.61531(13)	0.38102(13)	0.0313(4)
C212	0.13228(18)	0.42074(12)	0.06167(11)	0.0249(3)
C222	0.1154(2)	0.34740(13)	-0.00233(12)	0.0328(4)
C232	-0.0154(2)	0.30568(15)	-0.05597(13)	0.0389(5)
C242	-0.1311(2)	0.33560(14)	-0.04683(13)	0.0379(5)
C252	-0.1162(2)	0.40865(13)	0.01573(13)	0.0326(4)
C262	0.01494(19)	0.45142(12)	0.06934(12)	0.0272(4)
C312	0.24663(19)	0.36364(12)	0.37151(11)	0.0267(4)
C322	0.1593(2)	0.40190(14)	0.41028(15)	0.0378(5)
C332	0.0439(2)	0.35491(18)	0.41476(18)	0.0500(6)
C342	0.0167(3)	0.26972(18)	0.38211(16)	0.0530(7)
C352	0.1044(3)	0.23063(16)	0.34657(15)	0.0537(7)
C362	0.2201(3)	0.27699(13)	0.34156(14)	0.0395(5)
C412	0.41157(17)	0.58800(10)	0.27370(10)	0.0201(3)
C422	0.50427(18)	0.64527(11)	0.26221(11)	0.0248(3)
C432	0.62670(19)	0.68566(11)	0.32658(12)	0.0280(4)
C442	0.65506(18)	0.67022(11)	0.40145(12)	0.0274(4)
C452	0.56067(18)	0.61434(11)	0.41379(11)	0.0239(3)
C462	0.43948(17)	0.57314(10)	0.34947(10)	0.0201(3)
C512	0.51936(18)	0.41613(11)	0.19468(12)	0.0252(3)
C522	0.6258(2)	0.45314(12)	0.17431(14)	0.0315(4)
C532	0.7590(2)	0.47649(13)	0.23097(15)	0.0376(5)
C542	0.7860(2)	0.46077(13)	0.30545(15)	0.0377(5)
C552	0.68090(19)	0.42197(13)	0.32541(13)	0.0323(4)
C562	0.54668(18)	0.40054(11)	0.27012(11)	0.0252(3)

Table 14. Bond lengths (Å) for $C_{31}H_{27}N_4P_3Si$ (6).

Si11-N41	1.7619(15)	Si11-N31	1.7661(16)
Si11-C11	1.848(2)	P11-N11	1.7416(16)
P11-N21	1.7506(15)	P11-C111	1.8411(18)
P21-N31	1.7313(15)	P21-N11	1.7354(15)
P21-C211	1.8240(18)	P31-N41	1.7197(16)
P31-N21	1.7564(16)	P31-C311	1.8256(19)
N11-C411	1.442(2)	N21-C461	1.441(2)
N31-C511	1.455(2)	N41-C561	1.444(2)
C111-C121	1.393(3)	C111-C161	1.401(3)
C121-C131	1.395(3)	C131-C141	1.386(3)
C141-C151	1.380(3)	C151-C161	1.392(3)
C211-C261	1.400(2)	C211-C221	1.400(2)
C221-C231	1.391(3)	C231-C241	1.386(3)
C241-C251	1.386(3)	C251-C261	1.390(2)
C311-C321	1.391(3)	C311-C361	1.396(3)
C321-C331	1.392(3)	C331-C341	1.384(3)
C341-C351	1.385(3)	C351-C361	1.388(3)
C411-C421	1.386(2)	C411-C461	1.399(2)
C421-C431	1.396(3)	C431-C441	1.385(3)
C441-C451	1.392(3)	C451-C461	1.389(2)
C511-C521	1.388(2)	C511-C561	1.409(2)
C521-C531	1.393(3)	C531-C541	1.389(3)
C541-C551	1.391(3)	C551-C561	1.389(2)
Si12-N32	1.7654(17)	Si12-N42	1.7705(16)
Si12-C12	1.850(2)	P12-N12	1.7450(15)
P12-N22	1.7483(15)	P12-C112	1.8394(19)
P22-N32	1.7224(18)	P22-N22	1.7352(16)
P22-C212	1.8273(19)	P32-N42	1.7222(17)
P32-N12	1.7507(16)	P32-C312	1.8238(19)
N12-C462	1.442(2)	N22-C412	1.448(2)
N32-C512	1.445(2)	N42-C562	1.448(2)
C112-C162	1.394(3)	C112-C122	1.399(2)
C122-C132	1.388(3)	C132-C142	1.381(3)
C142-C152	1.383(3)	C152-C162	1.388(3)
C212-C262	1.394(3)	C212-C222	1.399(3)
C222-C232	1.388(3)	C232-C242	1.380(3)
C242-C252	1.386(3)	C252-C262	1.395(3)
C312-C322	1.393(3)	C312-C362	1.396(3)
C322-C332	1.393(3)	C332-C342	1.376(4)
C342-C352	1.371(4)	C352-C362	1.396(3)
C412-C422	1.388(2)	C412-C462	1.400(2)

C422-C432	1.394(3)	C432-C442	1.389(3)
C442-C452	1.392(3)	C452-C462	1.388(2)
C512-C522	1.389(3)	C512-C562	1.400(3)
C522-C532	1.393(3)	C532-C542	1.385(3)
C542-C552	1.388(3)	C552-C562	1.393(3)

Table 15. Bond angles (°) for $C_{31}H_{27}N_4P_3Si$ (6).

N41-Si11-N31	94.94(7)	N41-Si11-C11	109.95(9)
N31-Si11-C11	110.56(9)	N11-P11-N21	93.28(7)
N11-P11-C111	98.08(8)	N21-P11-C111	100.02(8)
N31-P21-N11	107.60(7)	N31-P21-C211	99.37(7)
N11-P21-C211	99.38(8)	N41-P31-N21	106.58(7)
N41-P31-C311	97.71(8)	N21-P31-C311	100.25(8)
C411-N11-P21	116.47(11)	C411-N11-P11	106.18(11)
P21-N11-P11	126.36(8)	C461-N21-P11	105.35(11)
C461-N21-P31	111.19(11)	P11-N21-P31	122.81(8)
C511-N31-P21	111.39(11)	C511-N31-Si11	102.11(11)
P21-N31-Si11	125.36(9)	C561-N41-P31	117.08(11)
C561-N41-Si11	103.17(11)	P31-N41-Si11	129.24(9)
C121-C111-C161	118.42(17)	C121-C111-P11	122.06(13)
C161-C111-P11	119.10(14)	C111-C121-C131	120.55(17)
C141-C131-C121	120.42(19)	C151-C141-C131	119.56(18)
C141-C151-C161	120.43(19)	C151-C161-C111	120.62(19)
C261-C211-C221	118.37(16)	C261-C211-P21	121.39(13)
C221-C211-P21	119.92(14)	C231-C221-C211	120.60(18)
C241-C231-C221	120.25(18)	C251-C241-C231	119.86(18)
C241-C251-C261	120.14(18)	C251-C261-C211	120.75(16)
C321-C311-C361	118.37(17)	C321-C311-P31	121.61(14)
C361-C311-P31	119.70(14)	C311-C321-C331	120.84(19)
C341-C331-C321	120.1(2)	C331-C341-C351	119.62(19)
C341-C351-C361	120.2(2)	C351-C361-C311	120.74(19)
C421-C411-C461	120.97(15)	C421-C411-N11	126.18(15)
C461-C411-N11	112.85(14)	C411-C421-C431	118.36(17)
C441-C431-C421	120.73(17)	C431-C441-C451	121.00(16)
C461-C451-C441	118.52(17)	C451-C461-C411	120.40(16)
C451-C461-N21	125.80(16)	C411-C461-N21	113.74(14)
C521-C511-C561	120.29(16)	C521-C511-N31	125.37(15)
C561-C511-N31	114.33(14)	C511-C521-C531	119.04(17)
C541-C531-C521	120.71(17)	C531-C541-C551	120.54(17)
C561-C551-C541	119.21(17)	C551-C561-C511	120.20(16)
C551-C561-N41	125.64(16)	C511-C561-N41	114.15(14)
N32-Si12-N42	94.70(8)	N32-Si12-C12	111.30(10)
N42-Si12-C12	110.92(9)	N12-P12-N22	93.67(7)
N12-P12-C112	99.48(8)	N22-P12-C112	96.72(8)
N32-P22-N22	106.78(8)	N32-P22-C212	98.27(8)
N22-P22-C212	101.25(8)	N42-P32-N12	107.65(8)
N42-P32-C312	99.83(9)	N12-P32-C312	99.56(8)
C462-N12-P12	105.86(11)	C462-N12-P32	112.60(11)

P12-N12-P32	124.16(9)	C412-N22-P22	113.77(11)
C412-N22-P12	105.57(11)	P22-N22-P12	125.69(9)
C512-N32-P22	113.47(12)	C512-N32-Si12	103.17(12)
P22-N32-Si12	127.10(9)	C562-N42-P32	112.45(12)
C562-N42-Si12	102.85(12)	P32-N42-Si12	128.64(9)
C162-C112-C122	117.88(17)	C162-C112-P12	120.53(14)
C122-C112-P12	121.15(14)	C132-C122-C112	120.92(18)
C142-C132-C122	120.30(19)	C132-C142-C152	119.60(19)
C142-C152-C162	120.3(2)	C152-C162-C112	121.03(19)
C262-C212-C222	118.37(17)	C262-C212-P22	124.01(15)
C222-C212-P22	117.27(15)	C232-C222-C212	120.6(2)
C242-C232-C222	120.6(2)	C232-C242-C252	119.57(19)
C242-C252-C262	120.2(2)	C212-C262-C252	120.62(19)
C322-C312-C362	118.32(19)	C322-C312-P32	119.40(15)
C362-C312-P32	121.79(17)	C332-C322-C312	120.7(2)
C342-C332-C322	120.0(3)	C352-C342-C332	120.2(2)
C342-C352-C362	120.3(2)	C352-C362-C312	120.3(2)
C422-C412-C462	120.28(15)	C422-C412-N22	126.43(15)
C462-C412-N22	113.22(14)	C412-C422-C432	118.75(17)
C442-C432-C422	120.94(17)	C432-C442-C452	120.39(17)
C462-C452-C442	118.85(17)	C452-C462-C412	120.77(15)
C452-C462-N12	125.56(15)	C412-C462-N12	113.60(14)
C522-C512-C562	120.32(17)	C522-C512-N32	125.12(18)
C562-C512-N32	114.51(16)	C512-C522-C532	119.0(2)
C542-C532-C522	120.63(19)	C532-C542-C552	120.74(19)
C542-C552-C562	119.0(2)	C552-C562-C512	120.28(18)
C552-C562-N42	125.16(18)	C512-C562-N42	114.49(15)

Table 16. Anisotropic displacement parameters ($Å^2$) for $C_{31}H_{27}N_4P_3Si$ (6).

The anisotropic displacement factor exponent takes the form:

$-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si11	0.0172(2)	0.0243(2)	0.0222(2)	0.00832(18)	0.00605(17)	0.00246(17)
P11	0.01617(18)	0.01846(19)	0.02058(19)	0.00594(15)	0.00537(15)	0.00204(14)
P21	0.01693(18)	0.01925(19)	0.01794(19)	0.00620(15)	0.00414(15)	0.00426(14)
P31	0.01751(18)	0.0234(2)	0.0203(2)	0.00896(16)	0.00380(15)	0.00443(15)
N11	0.0148(6)	0.0178(6)	0.0220(7)	0.0061(5)	0.0054(5)	0.0022(5)
N21	0.0164(6)	0.0241(7)	0.0211(7)	0.0085(5)	0.0045(5)	0.0028(5)
N31	0.0184(6)	0.0210(6)	0.0169(6)	0.0050(5)	0.0041(5)	0.0037(5)
N41	0.0188(6)	0.0211(7)	0.0222(7)	0.0080(5)	0.0055(5)	0.0031(5)
C11	0.0274(9)	0.0475(12)	0.0333(10)	0.0169(9)	0.0152(8)	0.0108(8)
C111	0.0177(7)	0.0207(8)	0.0234(8)	0.0041(6)	0.0053(6)	0.0015(6)
C121	0.0249(8)	0.0234(8)	0.0264(8)	0.0060(7)	0.0093(7)	0.0050(6)
C131	0.0289(9)	0.0345(10)	0.0265(9)	0.0064(8)	0.0122(7)	0.0059(7)
C141	0.0263(9)	0.0321(10)	0.0318(10)	-0.0004(8)	0.0116(8)	0.0059(7)
C151	0.0385(11)	0.0253(9)	0.0402(11)	0.0048(8)	0.0136(9)	0.0126(8)
C161	0.0366(10)	0.0274(9)	0.0318(10)	0.0103(8)	0.0114(8)	0.0112(8)
C211	0.0174(7)	0.0244(8)	0.0196(7)	0.0091(6)	0.0032(6)	0.0037(6)
C221	0.0197(8)	0.0384(10)	0.0279(9)	0.0060(8)	0.0063(7)	0.0080(7)
C231	0.0178(8)	0.0520(13)	0.0389(11)	0.0138(10)	0.0085(8)	0.0049(8)
C241	0.0223(9)	0.0433(12)	0.0337(10)	0.0101(9)	0.0019(8)	-0.0069(8)
C251	0.0284(9)	0.0311(9)	0.0222(8)	0.0049(7)	0.0028(7)	-0.0037(7)
C261	0.0202(7)	0.0271(8)	0.0209(8)	0.0080(7)	0.0056(6)	0.0028(6)
C311	0.0210(7)	0.0251(8)	0.0232(8)	0.0128(7)	0.0046(6)	0.0067(6)
C321	0.0389(10)	0.0265(9)	0.0257(9)	0.0129(7)	0.0113(8)	0.0119(8)
C331	0.0537(13)	0.0224(9)	0.0334(10)	0.0099(8)	0.0086(9)	0.0058(9)
C341	0.0371(11)	0.0320(10)	0.0474(13)	0.0220(9)	0.0087(9)	0.0002(8)
C351	0.0360(10)	0.0406(11)	0.0501(13)	0.0267(10)	0.0223(10)	0.0109(9)
C361	0.0327(9)	0.0285(9)	0.0326(10)	0.0140(8)	0.0140(8)	0.0092(7)
C411	0.0162(7)	0.0187(7)	0.0204(7)	0.0028(6)	0.0067(6)	0.0022(5)
C421	0.0247(8)	0.0219(8)	0.0279(9)	0.0068(7)	0.0111(7)	0.0033(6)
C431	0.0264(9)	0.0226(8)	0.0356(10)	0.0043(7)	0.0148(8)	-0.0023(7)
C441	0.0176(7)	0.0306(9)	0.0301(9)	0.0007(7)	0.0076(7)	-0.0034(7)
C451	0.0171(7)	0.0333(9)	0.0252(8)	0.0068(7)	0.0055(6)	0.0038(7)
C461	0.0174(7)	0.0216(8)	0.0211(7)	0.0047(6)	0.0077(6)	0.0025(6)
C511	0.0203(7)	0.0201(7)	0.0173(7)	0.0030(6)	0.0065(6)	0.0043(6)
C521	0.0307(9)	0.0217(8)	0.0215(8)	0.0062(6)	0.0090(7)	0.0059(7)
C531	0.0359(10)	0.0191(8)	0.0271(9)	0.0023(7)	0.0123(8)	0.0006(7)
C541	0.0277(9)	0.0266(9)	0.0256(9)	0.0028(7)	0.0056(7)	-0.0028(7)
C551	0.0229(8)	0.0283(9)	0.0232(8)	0.0070(7)	0.0038(7)	0.0030(7)

C561	0.0213(7)	0.0197(7)	0.0198(7)	0.0053(6)	0.0080(6)	0.0039(6)
Si12	0.0214(2)	0.0236(2)	0.0244(2)	0.00472(19)	0.00418(18)	0.00072(18)
P12	0.01774(18)	0.0223(2)	0.0210(2)	0.00849(16)	0.00450(15)	0.00139(15)
P22	0.0208(2)	0.0272(2)	0.01806(19)	0.00784(17)	0.00464(16)	0.00132(16)
P32	0.0214(2)	0.0224(2)	0.0205(2)	0.00948(16)	0.00300(16)	0.00284(16)
N12	0.0193(6)	0.0223(7)	0.0214(7)	0.0099(5)	0.0040(5)	0.0017(5)
N22	0.0194(6)	0.0243(7)	0.0179(6)	0.0070(5)	0.0049(5)	0.0001(5)
N32	0.0208(7)	0.0262(7)	0.0260(7)	0.0069(6)	0.0057(6)	0.0021(6)
N42	0.0212(7)	0.0244(7)	0.0245(7)	0.0054(6)	0.0039(6)	0.0018(5)
C12	0.0448(12)	0.0262(10)	0.0375(11)	0.0015(8)	0.0099(9)	0.0037(8)
C112	0.0159(7)	0.0242(8)	0.0256(8)	0.0101(7)	0.0046(6)	0.0020(6)
C122	0.0281(9)	0.0316(9)	0.0294(9)	0.0146(8)	0.0096(7)	0.0094(7)
C132	0.0317(10)	0.0350(10)	0.0400(11)	0.0188(9)	0.0100(8)	0.0135(8)
C142	0.0316(10)	0.0343(11)	0.0485(12)	0.0140(9)	0.0164(9)	0.0143(8)
C152	0.0448(12)	0.0432(12)	0.0410(12)	0.0164(10)	0.0253(10)	0.0177(10)
C162	0.0343(10)	0.0346(10)	0.0325(10)	0.0166(8)	0.0160(8)	0.0092(8)
C212	0.0231(8)	0.0307(9)	0.0189(8)	0.0110(7)	0.0028(6)	-0.0007(7)
C222	0.0302(9)	0.0386(11)	0.0231(9)	0.0054(8)	0.0050(7)	0.0016(8)
C232	0.0384(11)	0.0405(12)	0.0240(9)	0.0025(8)	0.0018(8)	-0.0050(9)
C242	0.0282(9)	0.0452(12)	0.0308(10)	0.0154(9)	-0.0017(8)	-0.0097(8)
C252	0.0235(8)	0.0413(11)	0.0339(10)	0.0212(9)	0.0037(7)	0.0006(8)
C262	0.0255(8)	0.0308(9)	0.0250(8)	0.0143(7)	0.0036(7)	0.0027(7)
C312	0.0262(8)	0.0286(9)	0.0251(8)	0.0153(7)	0.0032(7)	0.0011(7)
C322	0.0373(11)	0.0392(11)	0.0518(13)	0.0300(10)	0.0205(10)	0.0119(9)
C332	0.0356(11)	0.0704(18)	0.0662(17)	0.0479(15)	0.0230(12)	0.0146(11)
C342	0.0412(13)	0.0667(17)	0.0457(14)	0.0303(13)	0.0047(11)	-0.0178(12)
C352	0.0708(18)	0.0393(13)	0.0368(12)	0.0102(10)	0.0107(12)	-0.0225(12)
C362	0.0529(13)	0.0301(10)	0.0325(11)	0.0108(8)	0.0128(10)	-0.0028(9)
C412	0.0185(7)	0.0200(7)	0.0193(7)	0.0052(6)	0.0041(6)	0.0024(6)
C422	0.0249(8)	0.0234(8)	0.0269(9)	0.0096(7)	0.0096(7)	0.0019(6)
C432	0.0226(8)	0.0220(8)	0.0375(10)	0.0079(7)	0.0102(7)	-0.0004(6)
C442	0.0203(8)	0.0213(8)	0.0318(9)	0.0038(7)	0.0016(7)	-0.0003(6)
C452	0.0224(8)	0.0223(8)	0.0224(8)	0.0055(6)	0.0023(6)	0.0035(6)
C462	0.0190(7)	0.0190(7)	0.0219(8)	0.0068(6)	0.0059(6)	0.0032(6)
C512	0.0197(7)	0.0214(8)	0.0301(9)	0.0040(7)	0.0055(7)	0.0046(6)
C522	0.0266(9)	0.0291(9)	0.0398(11)	0.0102(8)	0.0131(8)	0.0060(7)
C532	0.0230(9)	0.0314(10)	0.0566(14)	0.0111(9)	0.0139(9)	0.0030(7)
C542	0.0200(8)	0.0336(10)	0.0477(12)	0.0036(9)	0.0034(8)	0.0032(7)
C552	0.0239(8)	0.0316(10)	0.0335(10)	0.0049(8)	0.0018(7)	0.0079(7)
C562	0.0200(8)	0.0225(8)	0.0281(9)	0.0030(7)	0.0053(7)	0.0041(6)

Table 17. Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for $C_{31}H_{27}N_4P_3Si$ (6).

	x	y	z	Ueq
H11	0.935(2)	0.0423(13)	0.2131(13)	0.025(5)
H1A1	1.0686	-0.0638	0.1188	0.041
H1B1	0.9631	-0.0347	0.0521	0.041
H1C1	0.9323	-0.1278	0.0538	0.041
H121	0.7049	0.0457	0.4535	0.030
H131	0.6472	0.1253	0.5645	0.036
H141	0.5802	0.2512	0.5635	0.038
H151	0.5686	0.2969	0.4506	0.042
H161	0.6297	0.2194	0.3404	0.038
H221	1.1211	-0.0715	0.2973	0.036
H231	1.3325	0.0196	0.3745	0.044
H241	1.3491	0.1298	0.4908	0.044
H251	1.1536	0.1489	0.5303	0.036
H261	0.9413	0.0588	0.4531	0.028
H321	0.6422	0.1878	0.2092	0.035
H331	0.7749	0.3073	0.2087	0.045
H341	0.9034	0.2977	0.1184	0.046
H351	0.8946	0.1683	0.0266	0.045
H361	0.7653	0.0486	0.0285	0.035
H421	0.5790	-0.1533	0.3429	0.030
H431	0.3410	-0.2078	0.2769	0.035
H441	0.2100	-0.1510	0.1847	0.035
H451	0.3116	-0.0373	0.1568	0.031
H521	0.7617	-0.2767	0.1815	0.030
H531	0.5586	-0.3618	0.0807	0.034
H541	0.4134	-0.3085	-0.0098	0.035
H551	0.4698	-0.1696	-0.0026	0.031
H12	0.177(2)	0.3289(14)	0.1845(14)	0.032(6)
H1A2	0.2653	0.1965	0.0763	0.047
H1B2	0.2905	0.1782	0.1620	0.047
H1C2	0.4188	0.2152	0.1394	0.047
H122	0.1275	0.6398	0.2101	0.034
H132	0.0343	0.7553	0.2545	0.041
H142	-0.0149	0.7835	0.3781	0.044
H152	0.0297	0.6955	0.4576	0.047
H162	0.1229	0.5799	0.4138	0.038
H222	0.1941	0.3259	-0.0092	0.039
H232	-0.0253	0.2561	-0.0993	0.047
H242	-0.2205	0.3063	-0.0832	0.045

H252	-0.1955	0.4297	0.0221	0.039
H262	0.0244	0.5019	0.1115	0.033
H322	0.1786	0.4606	0.4339	0.045
H332	-0.0159	0.3817	0.4404	0.060
H342	-0.0631	0.2379	0.3842	0.064
H352	0.0862	0.1717	0.3253	0.064
H362	0.2812	0.2495	0.3177	0.047
H422	0.4847	0.6567	0.2114	0.030
H432	0.6917	0.7243	0.3191	0.034
H442	0.7394	0.6980	0.4445	0.033
H452	0.5789	0.6046	0.4653	0.029
H522	0.6080	0.4624	0.1225	0.038
H532	0.8320	0.5034	0.2184	0.045
H542	0.8775	0.4767	0.3433	0.045
H552	0.7002	0.4102	0.3760	0.039

Table 18. Least Squares Planes and Dihedral Angles for $C_{31}H_{27}N_4P_3Si$ (6).

A. Least Squares Planes

Plane	atom	deviation (Å)	atom	deviation (Å)
1	-5.126 x + 8.082 y + 12.479 z = 0.0445			
	N(1)	-0.0140	C(43)	-0.0079
	N(2)	-0.0107	C(44)	-0.0157
	C(41)	0.0084	C(45)	0.0076
	C(42)	0.0123	C(46)	0.0199
2	-7.956 x + 2.424 y + 13.803 z = -4.1945			
	N(3)	0.0196	C(53)	-0.0069
	N(4)	-0.0206	C(54)	0.0098
	C(51)	-0.0017	C(55)	0.0090
	C(52)	-0.0158	C(56)	0.0065
3	1.174 x + -14.123 y + 13.122 z = 6.2040			
	C(21)	-0.0090	C(24)	-0.0047
	C(22)	-0.0068	C(25)	0.0023
	C(23)	0.0000	C(26)	0.0045
4	6.620 x + -7.005 y + 9.8032 z = 5.0247			
	C(31)	0.0150	C(34)	0.0106
	C(32)	-0.0119	C(35)	-0.0072
	C(33)	-0.0009	C(36)	-0.0055
5	-8.023 x + 2.968 y + 13.474 z = -1.6375			
	P(1)	0.0000	N(2)	0.0000
	N(2)	0.0000		
6	6.430 x + -11.274 y + -2.648 z = 3.5883			
	N(1)	-0.0241	P(2)	0.0136
	N(2)	0.0221	P(3)	-0.0116
7	6.116 x + 11.643 y + -2.313 z = 3.4203			

N(3)	0.0259	P(2)	-0.0139
N(4)	-0.0284	P(3)	0.0165

8 -4.495 x + 9.039 y + 11.830 z = 2.3675

N(1)	0.0000	Si(1)	0.0000
N(2)	0.0000		

B. Dihedral Angles

plane	angle (°)	plane	angle (°)
Table 19. 1-2	27.3	3-4	42.3
1-5	26.3	1-6	78.1
5-6	104.4	2-7	103.2
6-7	2.3	2-8	32.3
7-8	70.9		