

Table 1. Experimental details

## A. Crystal Data

Empirical Formula	$C_{42}H_{24}N_3O_6P_3 \cdot 2C_6H_4Cl_2$
Formula Weight	4097.02
Crystal Color, Habit	colourless, prismatic
Crystal Dimensions	0.55 X 0.22 X 0.17 mm
Crystal System	orthorhombic
No. of Reflections Used for Unit	
Cell Determination ( $2\theta$ range)	23 ( 18.6 - 24.4° )
Omega Scan Peak Width at Half-height	0.32°
Lattice Parameters	a = 14.880(3) Å b = 23.277(4) Å c = 13.429(4) Å
	V = 4651(1) Å <sup>3</sup>
Space Group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (#19)
Z value	4
D <sub>calc</sub>	5.850 g/cm <sup>3</sup>
F <sub>000</sub>	8144.00
$\mu(MoK\alpha)$	4.16 cm <sup>-1</sup>

## B. Intensity Measurements

Diffractometer	Rigaku AFC6S
Radiation	MoK $\alpha$ ( $\lambda = 0.71069$ Å) graphite monochromated

2

Temperature	-73.0°C
Scan Type	$\omega$ -2 $\theta$
Scan Rate	8.0°/min (in $\omega$ ) (up to 4 scans)
Scan Width	(1.15 + 0.34 tan $\theta$ )°
$2\theta_{max}$	50.1°
No. of Reflections Measured	Total: 4595
Corrections	Lorentz-polarization Absorption (trans. factors: 0.540 - 1.0000) Decay (0.51%)

## C. Structure Solution and Refinement

Structure Solution	Direct Methods (SAPI91)
Refinement	Full-matrix least-squares (SHELX76)
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ( $I > 3.00\sigma(I)$ )	1405
No. Variables	314
Reflection/Parameter Ratio	4.24
Residuals: R; Rw	0.0614 ; 0.0625
Goodness of Fit Indicator	2.58
Max Shift/Error in Final Cycle	0.10
Maximum peak in Final Diff. Map	0.45 e <sup>-</sup> /Å <sup>3</sup>
Minimum peak in Final Diff. Map	-0.38 e <sup>-</sup> /Å <sup>3</sup>

Table 2. Atomic coordinates and  $B_{iso}/B_{eq}$ 

atom	x	y	z	$B_{eq}$
Cl(1)	0.6181(5)	0.0311(3)	0.6243(6)	7.5(2)
Cl(2)	0.6217(5)	0.1312(4)	0.7767(6)	7.4(2)
Cl(3A)	0.1171(8)	0.0563(3)	0.8410(9)	9.8(4)
Cl(3B)	-0.0277(15)	0.0401(10)	0.9274(16)	3.2(7)
Cl(4)	0.1205(7)	0.1087(4)	0.6338(8)	10.7(3)
P(1)	1.0022(5)	0.2112(2)	0.3383(3)	2.4(1)
P(2)	1.0023(6)	0.0920(2)	0.3254(3)	2.3(1)
P(3)	1.0047(6)	0.1582(2)	0.1551(3)	2.3(1)
O(1)	1.0836(10)	0.2498(8)	0.3849(13)	3.3(4)
O(2)	0.9193(8)	0.2489(7)	0.3816(11)	1.9(4)
O(3)	1.0840(8)	0.0513(7)	0.3639(11)	1.9(4)
O(4)	0.9216(10)	0.0517(8)	0.3625(13)	3.3(4)
O(5)	0.9273(10)	0.1600(7)	0.0733(11)	2.4(4)
O(6)	1.0881(10)	0.1644(7)	0.0778(11)	2.7(4)
N(1)	0.9995(15)	0.1499(6)	0.3863(9)	2.8(3)
N(2)	1.0034(15)	0.0983(6)	0.2088(9)	2.8(4)
N(3)	1.0021(14)	0.2134(6)	0.2226(9)	2.6(3)
C(1)	1.049(2)	0.291(1)	0.448(2)	1.8(5)
C(2)	0.959(2)	0.291(1)	0.446(2)	2.5(6)
C(3)	0.902(2)	0.326(1)	0.501(2)	2.8(6)
C(4)	0.810(2)	0.330(1)	0.501(2)	3.0(6)
C(5)	0.761(2)	0.364(1)	0.563(2)	4.1(7)

4

Table 2. Atomic coordinates and  $B_{iso}/B_{eq}$  (continued)

atom	x	y	z	$B_{eq}$
C(6)	0.809(2)	0.399(1)	0.631(2)	4.2(7)
C(7)	0.903(2)	0.402(1)	0.631(2)	2.9(6)
C(8)	0.941(1)	0.366(1)	0.573(1)	1.1(4)
C(9)	1.038(2)	0.364(1)	0.571(2)	3.8(6)
C(10)	1.104(2)	0.400(1)	0.638(2)	5.5(8)
C(11)	1.195(2)	0.398(1)	0.634(2)	4.4(7)
C(12)	1.240(2)	0.364(1)	0.572(2)	3.5(7)
C(13)	1.196(2)	0.325(1)	0.507(2)	3.4(7)
C(14)	1.099(1)	0.329(1)	0.514(2)	1.7(5)
C(15)	1.051(1)	0.010(1)	0.430(1)	0.8(4)
C(16)	0.964(2)	0.007(1)	0.420(2)	3.2(6)
C(17)	0.906(1)	-0.031(1)	0.482(2)	1.6(5)
C(18)	0.811(2)	-0.031(1)	0.477(2)	3.8(7)
C(19)	0.762(2)	-0.071(1)	0.531(2)	2.6(5)
C(20)	0.810(2)	-0.111(1)	0.587(2)	5.1(8)
C(21)	0.902(2)	-0.114(1)	0.590(2)	2.8(6)
C(22)	0.949(2)	-0.071(1)	0.538(2)	2.7(6)
C(23)	1.047(2)	-0.071(1)	0.540(2)	3.0(6)
C(24)	1.105(2)	-0.107(1)	0.600(2)	4.4(7)
C(25)	1.193(2)	-0.106(1)	0.601(2)	3.6(6)
C(26)	1.236(2)	-0.065(1)	0.551(2)	5.8(8)
C(27)	1.196(2)	-0.028(1)	0.489(2)	2.5(6)

Table 2. Atomic coordinates and  $B_{iso}/B_{eq}$  (continued)

atom	x	y	z	$B_{eq}$
C(28)	1.103(2)	-0.030(1)	0.484(2)	3.8(7)
C(29)	0.967(2)	0.183(1)	-0.014(2)	2.7(5)
C(30)	1.057(2)	0.186(1)	-0.011(2)	2.3(5)
C(31)	1.113(2)	0.206(1)	-0.091(2)	2.6(5)
C(32)	1.204(2)	0.209(1)	-0.080(2)	3.5(6)
C(33)	1.260(2)	0.231(1)	-0.155(2)	4.8(6)
C(34)	1.211(1)	0.250(1)	-0.243(2)	2.6(4)
C(35)	1.122(2)	0.250(1)	-0.254(2)	5.0(6)
C(36)	1.068(1)	0.226(1)	-0.171(2)	2.2(4)
C(37)	0.975(1)	0.228(1)	-0.178(1)	3.0(5)
C(38)	0.928(2)	0.248(1)	-0.259(2)	4.4(6)
C(39)	0.843(2)	0.251(1)	-0.257(2)	3.5(5)
C(40)	0.777(2)	0.233(1)	-0.183(2)	3.3(5)
C(41)	0.824(2)	0.209(1)	-0.097(2)	3.9(6)
C(42)	0.918(1)	0.206(1)	-0.097(2)	2.4(5)
C(43)	0.521(1)	0.058(1)	0.672(1)	4.3(5)
C(44)	0.524(1)	0.103(1)	0.742(1)	4.4(5)
C(45)	0.444(1)	0.125(1)	0.781(1)	4.1(5)
C(46)	0.361(1)	0.103(1)	0.749(1)	6.5(8)
C(47)	0.359(1)	0.059(1)	0.679(1)	5.2(7)
C(48)	0.438(1)	0.037(1)	0.640(1)	4.8(6)
C(49)	0.018(1)	0.068(1)	0.783(1)	5.9(6)

Table 2. Atomic coordinates and  $B_{iso}/B_{eq}$  (continued)

atom	x	y	z	$B_{eq}$
C(50)	0.022(1)	0.090(1)	0.687(1)	5.1(6)
C(51)	-0.056(1)	0.102(1)	0.634(1)	5.0(6)
C(52)	-0.140(1)	0.090(1)	0.677(1)	8.1(9)
C(53)	-0.145(1)	0.068(1)	0.773(1)	3.9(5)
C(54)	-0.066(1)	0.057(1)	0.826(1)	6.3(8)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table 3. Calculated coordinates and  $B_{iso}$  for H-atoms

atom	x	y	z	$B_{eq}$
H(4)	0.7785	0.3062	0.4556	6.1800
H(5)	0.6976	0.3646	0.5605	6.1800
H(6)	0.7762	0.4221	0.6773	6.1800
H(7)	0.9357	0.4288	0.6709	6.1800
H(10)	1.0774	0.4262	0.6842	6.1800
H(11)	1.2280	0.4207	0.6793	6.1800
H(12)	1.3032	0.3661	0.5702	6.1800
H(13)	1.2265	0.2991	0.4640	6.1800
H(18)	0.7808	-0.0029	0.4376	6.1800
H(19)	0.6984	-0.0711	0.5309	6.1800
H(20)	0.7776	-0.1389	0.6253	6.1800
H(21)	0.9324	-0.1434	0.6245	6.1800
H(24)	1.0761	-0.1346	0.6413	6.1800
H(25)	1.2262	-0.1343	0.6370	6.1800
H(26)	1.2987	-0.0615	0.5599	6.1800
H(27)	1.2296	-0.0018	0.4490	6.1800
H(32)	1.2305	0.1937	-0.0214	6.1800
H(33)	1.3237	0.2347	-0.1479	6.1800
H(34)	1.2457	0.2635	-0.2977	6.1800
H(35)	1.0938	0.2640	-0.3129	6.1800
H(38)	0.9591	0.2601	-0.3172	6.1800
H(39)	0.8176	0.2682	-0.3149	6.1800
H(40)	0.7137	0.2358	-0.1894	6.1800

Table 3. Calculated coordinates and  $B_{iso}$  for H-atoms (continued)

atom	x	y	z	$B_{eq}$
H(41)	0.7913	0.1958	-0.0412	6.1800
H(45)	0.4456	0.1550	0.8284	15.5490
H(46)	0.3070	0.1181	0.7755	15.5490
H(47)	0.3023	0.0438	0.6577	15.5490
H(48)	0.4363	0.0064	0.5927	15.5490
H(51)	-0.0530	0.1170	0.5688	15.5490
H(52)	-0.1933	0.0981	0.6411	15.5490
H(53)	-0.2015	0.0602	0.8027	15.5490



9

Table 4. Anisotropic Displacement Parameters

atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Cl(1)	0.081(5)	0.063(5)	0.129(7)	0.018(5)	0.037(6)	0.025(5)
Cl(2)	0.092(6)	0.099(6)	0.091(5)	-0.018(5)	-0.021(6)	0.029(5)
Cl(3A)	0.112(9)	0.033(5)	0.18(1)	0.021(5)	-0.090(9)	-0.015(7)
Cl(4)	0.113(8)	0.154(9)	0.135(8)	-0.015(7)	0.041(8)	-0.040(7)
P(1)	0.027(3)	0.031(3)	0.033(3)	0.000(5)	0.015(5)	-0.003(2)
P(2)	0.028(3)	0.026(2)	0.033(3)	0.003(5)	0.003(5)	0.007(2)
P(3)	0.034(3)	0.029(3)	0.024(2)	-0.001(5)	0.009(5)	0.003(2)
N(1)	0.042(8)	0.023(7)	0.038(7)	-0.01(1)	0.00(2)	0.010(7)
N(2)	0.05(1)	0.026(8)	0.026(8)	-0.02(1)	0.01(1)	0.000(7)
N(3)	0.029(9)	0.043(9)	0.025(8)	-0.01(1)	0.00(1)	0.007(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 5. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Cl(1)	C(43)	1.71(2)	Cl(2)	C(44)	1.67(2)
Cl(3A)	C(49)	1.69(2)	Cl(3B)	C(54)	1.52(3)
Cl(4)	C(50)	1.68(2)	P(1)	O(1)	1.63(2)
P(1)	O(2)	1.62(2)	P(1)	N(1)	1.57(1)
P(1)	N(3)	1.55(1)	P(2)	O(3)	1.63(2)
P(2)	O(4)	1.60(2)	P(2)	N(1)	1.58(1)
P(2)	N(2)	1.57(1)	P(3)	O(5)	1.59(2)
P(3)	O(6)	1.62(2)	P(3)	N(2)	1.57(1)
P(3)	N(3)	1.57(1)	O(1)	C(1)	1.37(3)
O(2)	C(2)	1.43(3)	O(3)	C(15)	1.40(2)
O(4)	C(16)	1.44(3)	O(5)	C(29)	1.42(3)
O(6)	C(30)	1.38(3)	C(1)	C(2)	1.34(4)
C(1)	C(14)	1.45(3)	C(2)	C(3)	1.39(4)
C(3)	C(4)	1.38(3)	C(3)	C(8)	1.45(3)
C(4)	C(5)	1.36(4)	C(5)	C(6)	1.41(4)
C(6)	C(7)	1.40(3)	C(7)	C(8)	1.29(3)
C(8)	C(9)	1.44(3)	C(9)	C(10)	1.57(4)
C(9)	C(14)	1.45(3)	C(10)	C(11)	1.36(4)
C(11)	C(12)	1.33(4)	C(12)	C(13)	1.42(4)
C(13)	C(14)	1.45(3)	C(15)	C(16)	1.30(3)
C(15)	C(28)	1.40(3)	C(16)	C(17)	1.49(3)
C(17)	C(18)	1.41(3)	C(17)	C(22)	1.35(4)
C(18)	C(19)	1.39(4)	C(19)	C(20)	1.40(4)
C(20)	C(21)	1.37(4)	C(21)	C(22)	1.41(4)

11

Table 5. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(22)	C(23)	1.46(4)	C(23)	C(24)	1.44(4)
C(23)	C(28)	1.49(4)	C(24)	C(25)	1.31(4)
C(25)	C(26)	1.33(4)	C(26)	C(27)	1.34(4)
C(27)	C(28)	1.37(4)	C(29)	C(30)	1.35(3)
C(29)	C(42)	1.44(3)	C(30)	C(31)	1.44(3)
C(31)	C(32)	1.36(3)	C(31)	C(36)	1.35(3)
C(32)	C(33)	1.41(3)	C(33)	C(34)	1.46(3)
C(34)	C(35)	1.34(3)	C(35)	C(36)	1.47(3)
C(36)	C(37)	1.40(3)	C(37)	C(38)	1.38(3)
C(37)	C(42)	1.47(3)	C(38)	C(39)	1.26(3)
C(39)	C(40)	1.47(3)	C(40)	C(41)	1.46(3)
C(41)	C(42)	1.39(3)	C(43)	C(44)	1.39(2)
C(43)	C(48)	1.39(2)	C(44)	C(45)	1.39(2)
C(45)	C(46)	1.39(2)	C(46)	C(47)	1.39(2)
C(47)	C(48)	1.40(2)	C(49)	C(50)	1.39(3)
C(49)	C(54)	1.39(2)	C(50)	C(51)	1.40(2)
C(51)	C(52)	1.39(2)	C(52)	C(53)	1.40(3)
C(53)	C(54)	1.39(2)			

Table 6. Bond Lengths(Å) involving H-atoms

atom	atom	distance	atom	atom	distance
C(4)	H(4)	0.95	C(5)	H(5)	0.95
C(6)	H(6)	0.95	C(7)	H(7)	0.95
C(10)	H(10)	0.95	C(11)	H(11)	0.95
C(12)	H(12)	0.95	C(13)	H(13)	0.95
C(18)	H(18)	0.95	C(19)	H(19)	0.95
C(20)	H(20)	0.95	C(21)	H(21)	0.95
C(24)	H(24)	0.95	C(25)	H(25)	0.95
C(26)	H(26)	0.95	C(27)	H(27)	0.95
C(32)	H(32)	0.95	C(33)	H(33)	0.95
C(34)	H(34)	0.95	C(35)	H(35)	0.95
C(38)	H(38)	0.95	C(39)	H(39)	0.95
C(40)	H(40)	0.95	C(41)	H(41)	0.95
C(45)	H(45)	0.95	C(46)	H(46)	0.95
C(47)	H(47)	0.95	C(48)	H(48)	0.95
C(51)	H(51)	0.95	C(52)	H(52)	0.95
C(53)	H(53)	0.95			

Table 7. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	P(1)	O(2)	97.4(8)	O(1)	P(1)	N(1)	111(1)
O(1)	P(1)	N(3)	111.4(10)	O(2)	P(1)	N(1)	109.0(10)
O(2)	P(1)	N(3)	109.9(9)	N(1)	P(1)	N(3)	116.2(7)
O(3)	P(2)	O(4)	96.9(8)	O(3)	P(2)	N(1)	110.7(10)
O(3)	P(2)	N(2)	111.4(10)	O(4)	P(2)	N(1)	108(1)
O(4)	P(2)	N(2)	111(1)	N(1)	P(2)	N(2)	115.9(7)
O(5)	P(3)	O(6)	96.3(8)	O(5)	P(3)	N(2)	109.4(10)
O(5)	P(3)	N(3)	111.0(10)	O(6)	P(3)	N(2)	112.4(10)
O(6)	P(3)	N(3)	108.3(9)	N(2)	P(3)	N(3)	117.4(7)
P(1)	O(1)	C(1)	109(1)	P(1)	O(2)	C(2)	105(1)
P(2)	O(3)	C(15)	109(1)	P(2)	O(4)	C(16)	104(1)
P(3)	O(5)	C(29)	106(1)	P(3)	O(6)	C(30)	109(1)
P(1)	N(1)	P(2)	124.4(8)	P(2)	N(2)	P(3)	122.7(8)
P(1)	N(3)	P(3)	123.3(8)	O(1)	C(1)	C(2)	111(2)
O(1)	C(1)	C(14)	127(2)	C(2)	C(1)	C(14)	121(2)
O(2)	C(2)	C(1)	115(2)	O(2)	C(2)	C(3)	118(2)
C(1)	C(2)	C(3)	126(2)	C(2)	C(3)	C(4)	129(2)
C(2)	C(3)	C(8)	119(2)	C(4)	C(3)	C(8)	110(2)
C(3)	C(4)	C(5)	124(2)	C(4)	C(5)	C(6)	117(2)
C(5)	C(6)	C(7)	121(2)	C(6)	C(7)	C(8)	113(2)
C(3)	C(8)	C(7)	130(2)	C(3)	C(8)	C(9)	111(1)
C(7)	C(8)	C(9)	117(2)	C(8)	C(9)	C(10)	127(2)
C(8)	C(9)	C(14)	130(2)	C(10)	C(9)	C(14)	102(2)
C(9)	C(10)	C(11)	125(2)	C(10)	C(11)	C(12)	123(2)

A

Table 7. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(11)	C(12)	C(13)	122(2)	C(12)	C(13)	C(14)	112(2)
C(1)	C(14)	C(9)	110(1)	C(1)	C(14)	C(13)	115(2)
C(9)	C(14)	C(13)	133(2)	O(3)	C(15)	C(16)	108(1)
O(3)	C(15)	C(28)	125(2)	C(16)	C(15)	C(28)	124(2)
O(4)	C(16)	C(15)	117(2)	O(4)	C(16)	C(17)	117(2)
C(15)	C(16)	C(17)	123(2)	C(16)	C(17)	C(18)	123(2)
C(16)	C(17)	C(22)	116(2)	C(18)	C(17)	C(22)	119(2)
C(17)	C(18)	C(19)	119(2)	C(18)	C(19)	C(20)	117(2)
C(19)	C(20)	C(21)	123(2)	C(20)	C(21)	C(22)	117(2)
C(17)	C(22)	C(21)	121(2)	C(17)	C(22)	C(23)	119(2)
C(21)	C(22)	C(23)	118(2)	C(22)	C(23)	C(24)	128(2)
C(22)	C(23)	C(28)	123(2)	C(24)	C(23)	C(28)	108(2)
C(23)	C(24)	C(25)	126(2)	C(24)	C(25)	C(26)	118(2)
C(25)	C(26)	C(27)	124(2)	C(26)	C(27)	C(28)	116(2)
C(15)	C(28)	C(23)	111(2)	C(15)	C(28)	C(27)	124(2)
C(23)	C(28)	C(27)	124(2)	O(5)	C(29)	C(30)	114(1)
O(5)	C(29)	C(42)	124(1)	C(30)	C(29)	C(42)	120(2)
O(6)	C(30)	C(29)	109(1)	O(6)	C(30)	C(31)	125(1)
C(29)	C(30)	C(31)	125(2)	C(30)	C(31)	C(32)	120(2)
C(30)	C(31)	C(36)	114(2)	C(32)	C(31)	C(36)	124(2)
C(31)	C(32)	C(33)	122(2)	C(32)	C(33)	C(34)	112(2)
C(33)	C(34)	C(35)	126(2)	C(34)	C(35)	C(36)	116(2)
C(31)	C(36)	C(35)	117(1)	C(31)	C(36)	C(37)	123(1)
C(35)	C(36)	C(37)	118(1)	C(36)	C(37)	C(38)	124(1)

Table 7. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(36)	C(37)	C(42)	121(1)	C(38)	C(37)	C(42)	114(1)
C(37)	C(38)	C(39)	120(2)	C(38)	C(39)	C(40)	131(2)
C(39)	C(40)	C(41)	108(2)	C(40)	C(41)	C(42)	120(2)
C(29)	C(42)	C(37)	114(1)	C(29)	C(42)	C(41)	122(2)
C(37)	C(42)	C(41)	123(1)	Cl(1)	C(43)	C(44)	120(1)
Cl(1)	C(43)	C(48)	119(1)	C(44)	C(43)	C(48)	119(1)
Cl(2)	C(44)	C(43)	120(1)	Cl(2)	C(44)	C(45)	119(1)
C(43)	C(44)	C(45)	120(1)	C(44)	C(45)	C(46)	120(1)
C(45)	C(46)	C(47)	120(1)	C(46)	C(47)	C(48)	119(1)
C(43)	C(48)	C(47)	120(1)	Cl(3A)	C(49)	C(50)	115(1)
Cl(3A)	C(49)	C(54)	124(1)	C(50)	C(49)	C(54)	120(1)
Cl(4)	C(50)	C(49)	122(1)	Cl(4)	C(50)	C(51)	117(1)
C(49)	C(50)	C(51)	120(1)	C(50)	C(51)	C(52)	120(1)
C(51)	C(52)	C(53)	119(1)	C(52)	C(53)	C(54)	119(1)
Cl(3B)	C(54)	C(49)	94(1)	Cl(3B)	C(54)	C(53)	144(1)
C(49)	C(54)	C(53)	120(1)				

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Table 8. Least Squares Planes

## Plane number 1

Atoms defining plane	Distance
P(1)	0.004(8)
P(2)	0.002(8)
P(3)	0.002(9)
N(1)	-0.03(2)
N(2)	-0.01(2)
N(3)	-0.02(2)

## Plane number 2

Atoms defining plane	Distance
O(1)	-0.01(2)
O(2)	-0.03(2)
C(1)	0.02(3)
C(2)	0.02(3)
C(3)	0.05(2)
C(4)	0.07(3)
C(5)	0.02(3)
C(6)	-0.07(3)
C(7)	0.00(2)
C(8)	-0.01(2)
C(9)	0.01(3)
C(10)	-0.05(3)
C(11)	-0.04(3)
C(12)	0.03(3)
C(13)	0.03(3)
C(14)	0.01(2)



## Plane number 3

Atoms defining plane	Distance
O(3)	0.04(2)
O(4)	-0.03(2)
C(15)	-0.04(2)
C(16)	0.07(3)
C(17)	-0.04(2)
C(18)	-0.04(3)
C(19)	-0.03(2)
C(20)	0.02(3)
C(21)	0.08(2)
C(22)	-0.01(3)
C(23)	0.03(3)
C(24)	-0.02(3)
C(25)	0.00(3)
C(26)	-0.08(3)
C(27)	-0.02(3)
C(28)	0.02(3)

## Plane number 4

Atoms defining plane	Distance
O(5)	0.03(2)
O(6)	-0.04(2)
C(29)	0.05(2)
C(30)	0.00(2)
C(31)	0.04(2)
C(32)	-0.05(2)
C(33)	-0.09(2)
C(34)	0.00(2)
C(35)	0.05(3)
C(36)	0.05(2)
C(37)	0.04(2)
C(38)	0.05(2)
C(39)	-0.04(2)
C(40)	-0.10(2)
C(41)	-0.06(3)
C(42)	0.02(2)

## Plane number 5

Atoms defining plane	Distance
C(43)	0.00(2)
C(44)	0.00(2)
C(45)	0.00(2)
C(46)	0.00(2)
C(47)	0.00(2)
C(48)	0.00(2)

## Plane number 6

Atoms defining plane	Distance
C(49)	0.00(2)
C(50)	0.00(2)
C(51)	0.00(2)
C(52)	0.00(2)
C(53)	0.00(2)
C(54)	0.00(2)

## Summary

plane	mean deviation	$\chi^2$
1	0.0105	2.9
2	0.0301	31.5
3	0.0348	49.4
4	0.0440	82.5
5	0.0000	0.0
6	0.0000	0.0

## Dihedral angles between planes (°)

plane	1	2	3	4	5
2	89.69				
3	88.84	83.28			
4	89.37	108.66	25.38		
5	87.81	177.29	97.70	72.36	
6	89.18	111.52	28.24	2.87	69.49

## EXPERIMENTAL DETAILS

## A. Crystal Data

Empirical Formula	$C_{42}H_{24}N_3O_6P_3 \cdot C_8H_{10}$
Formula Weight	865.76
Crystal Color, Habit	colourless, needle
Crystal Dimensions	0.70 X 0.25 X 0.10 mm
Crystal System	triclinic
No. of Reflections Used for Unit	
Cell Determination ( $2\theta$ range)	22 ( 13.8 - 23.6° )
Omega Scan Peak Width	
at Half-height	0.40°
Lattice Parameters	$a = 12.724(3) \text{ \AA}$ $b = 19.347(5) \text{ \AA}$ $c = 9.124(5) \text{ \AA}$ $\alpha = 97.55(3)^\circ$ $\beta = 106.13(3)^\circ$ $\gamma = 72.46(2)^\circ$
	$V = 2054(1) \text{ \AA}^3$
Space Group	$P\bar{1} (\#2)$
Z value	2
$D_{calc}$	1.399 g/cm <sup>3</sup>
$F_{000}$	896
$\mu(\text{MoK}\alpha)$	2.02 cm <sup>-1</sup>

## B. Intensity Measurements

Diffractometer

Rigaku AFC6S

Radiation	MoK $\alpha$ ( $\lambda = 0.71069 \text{ \AA}$ ) graphite monochromated
Temperature	-103.0°C
Scan Type	$\omega$ - $2\theta$
Scan Rate	8.0°/min (in $\omega$ ) (up to 4 scans)
Scan Width	(1.68 + 0.34 tan $\theta$ )°
$2\theta_{max}$	50.1°
No. of Reflections Measured	Total: 7627 Unique: 7268 ( $R_{int} = 0.123$ )
Corrections	Lorentz-polarization Absorption (trans. factors: 0.7430 - 1.0000)

## C. Structure Solution and Refinement

Structure Solution	Direct Methods (SAPI91)
Refinement	Full-matrix least-squares
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ( $I > 3.00\sigma(I)$ )	2571
No. Variables	519
Reflection/Parameter Ratio	4.95
Residuals: R; $R_w$	0.081 ; 0.072
Goodness of Fit Indicator	3.11
Max Shift/Error in Final Cycle	0.003
Maximum peak in Final Diff. Map	0.44 $e^-/\text{\AA}^3$
Minimum peak in Final Diff. Map	-0.42 $e^-/\text{\AA}^3$

Table 1. Atomic coordinates and  $B_{eq}$ 

atom	x	y	z	$B_{eq}$
P(1)	0.2152(3)	0.2335(2)	0.1882(4)	2.61(9)
P(2)	-0.0082(3)	0.2949(2)	0.2022(4)	2.41(9)
P(3)	0.1050(3)	0.1566(2)	0.2998(4)	2.46(9)
O(1)	0.2551(7)	0.2101(5)	0.0302(10)	3.6(3)
O(2)	0.3235(7)	0.2606(5)	0.2832(9)	3.0(2)
O(3)	-0.1187(7)	0.3192(5)	0.0592(9)	3.2(2)
O(4)	-0.0457(7)	0.3620(5)	0.3196(9)	2.9(2)
O(5)	0.1313(7)	0.1372(4)	0.4756(9)	2.5(2)
O(6)	0.0831(7)	0.0807(4)	0.2256(9)	2.8(2)
N(1)	0.1018(9)	0.2977(6)	0.1633(13)	3.6(3)
N(2)	-0.0086(8)	0.2234(5)	0.2581(11)	2.2(3)
N(3)	0.2129(8)	0.1644(6)	0.2588(13)	3.4(3)
C(1)	0.3565(11)	0.2279(6)	0.0493(16)	2.6(4)
C(2)	0.4153(12)	0.2136(7)	-0.0691(17)	3.3(4)
C(3)	0.3743(12)	0.1884(8)	-0.2175(18)	4.1(4)
C(4)	0.4333(14)	0.1791(8)	-0.3253(17)	4.2(4)
C(5)	0.5378(16)	0.1926(9)	-0.284(2)	5.2(5)
C(6)	0.5817(13)	0.2203(9)	-0.140(2)	4.6(5)
C(7)	0.5213(11)	0.2315(7)	-0.0281(16)	3.2(4)
C(8)	0.5647(11)	0.2604(7)	0.1284(17)	3.0(4)
C(9)	0.6700(12)	0.2760(7)	0.1736(19)	3.7(4)
C(10)	0.7084(12)	0.3016(8)	0.320(2)	4.5(5)
C(11)	0.6448(12)	0.3141(8)	0.4289(17)	3.9(4)
C(12)	0.5404(11)	0.2987(8)	0.3835(17)	3.5(4)

Table 1. Atomic coordinates and  $B_{eq}$  (continued)

atom	x	y	z	$B_{eq}$
C(13)	0.5012(11)	0.2707(7)	0.2349(16)	2.6(4)
C(14)	0.3975(11)	0.2527(7)	0.1897(16)	2.5(4)
C(15)	-0.1799(11)	0.3903(7)	0.0941(16)	2.7(4)
C(16)	-0.2774(11)	0.4333(7)	-0.0135(15)	2.9(4)
C(17)	-0.3217(12)	0.4046(8)	-0.1605(16)	3.9(4)
C(18)	-0.4138(14)	0.4498(9)	-0.2554(18)	5.4(5)
C(19)	-0.4624(13)	0.5193(10)	-0.2026(18)	5.3(5)
C(20)	-0.4237(13)	0.5461(8)	-0.0625(17)	4.6(4)
C(21)	-0.3270(11)	0.5026(7)	0.0464(17)	3.4(4)
C(22)	-0.2827(13)	0.5288(8)	0.1993(17)	3.8(4)
C(23)	-0.3284(12)	0.5995(9)	0.2576(19)	4.6(5)
C(24)	-0.2885(15)	0.6211(8)	0.403(2)	5.2(5)
C(25)	-0.1968(13)	0.5756(9)	0.5040(17)	4.4(5)
C(26)	-0.1483(11)	0.5075(7)	0.4499(16)	3.4(4)
C(27)	-0.1880(10)	0.4825(7)	0.3007(15)	2.5(3)
C(28)	-0.1399(10)	0.4140(7)	0.2370(14)	2.2(3)
C(29)	0.1303(10)	0.0651(6)	0.4775(16)	2.2(3)
C(30)	0.1588(11)	0.0279(8)	0.6164(16)	3.0(4)
C(31)	0.1841(12)	0.0611(8)	0.7652(18)	4.0(4)
C(32)	0.2117(12)	0.0255(8)	0.8917(17)	3.8(4)
C(33)	0.2171(13)	-0.0468(10)	0.8779(17)	4.7(5)
C(34)	0.1929(12)	-0.0811(8)	0.7375(19)	4.2(4)
C(35)	0.1582(10)	-0.0469(7)	0.5957(16)	2.5(4)
C(36)	0.1339(11)	-0.0804(7)	0.4463(17)	3.1(4)

2

Table 1. Atomic coordinates and  $B_{iso}/B_{eq}$  (continued)

atom	x	y	z	$B_{eq}$
C(37)	0.1344(13)	-0.1542(7)	0.4191(18)	4.0(4)
C(38)	0.1159(13)	-0.1841(7)	0.278(2)	4.8(5)
C(39)	0.0910(12)	-0.1454(8)	0.1478(17)	4.0(4)
C(40)	0.0872(10)	-0.0733(7)	0.1699(15)	3.0(4)
C(41)	0.1077(10)	-0.0390(7)	0.3126(15)	2.6(4)
C(42)	0.1058(10)	0.0331(7)	0.3417(14)	2.2(3)
C(43)	0.4984(15)	0.0483(10)	0.210(2)	7.0(5)
C(44)	0.4990(12)	0.0220(8)	0.3600(17)	4.2(3)
C(45)	0.4159(12)	-0.0052(8)	0.3742(17)	4.2(3)
C(46)	0.5834(12)	0.0274(8)	0.4919(17)	3.7(3)
C(47)	0.0350(19)	0.3707(14)	0.789(3)	11.6(7)
C(48)	0.0150(19)	0.4354(12)	0.895(3)	8.1(6)
C(49)	0.1018(17)	0.4526(12)	1.025(3)	7.7(5)
C(50)	-0.0869(18)	0.4882(13)	0.875(2)	8.1(6)

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^* \cos \gamma + 2U_{13}aa^*cc^* \cos \beta + 2U_{23}bb^*cc^* \cos \alpha)$$

Table 2. Atomic coordinates and  $B_{eq}$  for H-atoms

atom	x	y	z	$B_{eq}$
H(1)	0.3038	0.1767	-0.2433	4.8204
H(2)	0.4022	0.1640	-0.4265	5.1150
H(3)	0.5821	0.1831	-0.3567	6.2149
H(4)	0.6526	0.2313	-0.1174	5.4955
H(5)	0.7147	0.2689	0.1028	4.4801
H(6)	0.7808	0.3113	0.3485	5.4168
H(7)	0.6724	0.3320	0.5304	4.7399
H(8)	0.4943	0.3071	0.4540	4.0769
H(9)	-0.2889	0.3561	-0.1929	4.7377
H(10)	-0.4436	0.4334	-0.3567	6.3149
H(11)	-0.5273	0.5496	-0.2680	6.3152
H(12)	-0.4591	0.5946	-0.0330	5.6119
H(13)	-0.3891	0.6326	0.1935	5.5283
H(14)	-0.3223	0.6690	0.4375	6.1950
H(15)	-0.1693	0.5921	0.6070	5.2908
H(16)	-0.0855	0.4764	0.5158	3.9769
H(17)	0.1819	0.1108	0.7752	4.7540
H(18)	0.2271	0.0500	0.9897	4.5815
H(19)	0.2377	-0.0734	0.9672	5.6198
H(20)	0.2004	-0.1315	0.7347	4.9900
H(21)	0.1472	-0.1824	0.5030	4.8610
H(22)	0.1197	-0.2342	0.2645	5.6237
H(23)	0.0773	-0.1684	0.0483	4.8569
H(24)	0.0694	-0.0456	0.0828	3.6326



9

Table 2. Atomic coordinates and  $B_{eq}$  for H-atoms (continued)

atom	x	y	z	$B_{eq}$
H(25)	0.5647	0.0649	0.2251	8.4260
H(26)	0.5003	0.0099	0.1339	8.4260
H(27)	0.4326	0.0877	0.1763	8.4260
H(28)	0.3515	-0.0060	0.2905	5.0107
H(29)	0.6441	0.0506	0.4916	4.4286
H(30)	-0.0156	0.3422	0.7841	13.9227
H(31)	0.0245	0.3848	0.6876	13.9227
H(32)	0.1113	0.3417	0.8235	13.9227
H(33)	0.1811	0.4174	1.0471	9.6300
H(34)	-0.1527	0.4844	0.7938	9.9748

20

Table 3. Anisotropic Displacement Parameters

atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
P(1)	0.032(2)	0.038(2)	0.032(3)	-0.010(2)	0.009(2)	0.007(2)
P(2)	0.033(2)	0.029(2)	0.027(2)	-0.006(2)	0.007(2)	0.003(2)
P(3)	0.035(2)	0.024(2)	0.034(3)	-0.010(2)	0.004(2)	0.004(2)
O(1)	0.032(6)	0.064(7)	0.043(7)	-0.020(5)	0.011(5)	-0.006(5)
O(2)	0.032(6)	0.055(7)	0.035(6)	-0.017(5)	0.012(5)	0.006(5)
O(3)	0.031(6)	0.033(6)	0.042(6)	-0.001(5)	0.000(5)	-0.010(5)
O(4)	0.029(5)	0.049(6)	0.021(5)	-0.003(5)	-0.008(4)	0.008(5)
O(5)	0.041(6)	0.020(5)	0.035(6)	-0.015(4)	0.006(4)	-0.002(4)
O(6)	0.040(6)	0.023(5)	0.035(6)	-0.004(4)	0.001(4)	0.000(4)
N(1)	0.041(8)	0.040(8)	0.062(9)	-0.018(6)	0.021(6)	-0.002(6)
N(2)	0.029(7)	0.018(6)	0.037(7)	-0.011(5)	0.001(5)	0.000(5)
N(3)	0.029(7)	0.044(8)	0.055(8)	0.006(6)	0.022(6)	0.013(6)
C(1)	0.047(10)	0.020(8)	0.040(10)	-0.011(7)	0.016(8)	0.012(7)
C(2)	0.039(10)	0.039(9)	0.045(11)	0.000(7)	0.013(8)	0.014(8)
C(3)	0.048(10)	0.059(11)	0.047(12)	-0.006(8)	0.018(9)	0.004(9)
C(4)	0.057(12)	0.050(11)	0.052(12)	-0.002(9)	0.017(9)	0.014(8)
C(5)	0.086(14)	0.055(12)	0.071(14)	0.001(10)	0.056(12)	0.012(10)
C(6)	0.055(11)	0.068(12)	0.065(13)	-0.007(9)	0.043(10)	0.014(10)
C(7)	0.035(9)	0.055(10)	0.037(10)	-0.014(8)	0.016(8)	-0.003(8)
C(8)	0.021(8)	0.033(9)	0.064(12)	-0.005(7)	0.019(8)	0.010(8)
C(9)	0.038(10)	0.031(9)	0.070(13)	0.002(8)	0.014(9)	0.020(8)
C(10)	0.021(9)	0.058(11)	0.087(15)	-0.007(8)	0.005(9)	0.017(10)
C(11)	0.037(10)	0.063(11)	0.044(11)	-0.019(8)	-0.003(8)	-0.003(8)
C(12)	0.021(8)	0.063(11)	0.048(11)	-0.017(8)	0.002(7)	0.008(8)

Table 3. Anisotropic Displacement Parameters (continued)

atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
C(13)	0.030(9)	0.024(8)	0.043(10)	-0.005(7)	0.004(8)	0.014(7)
C(14)	0.035(9)	0.029(8)	0.041(11)	-0.012(7)	0.021(8)	-0.001(7)
C(15)	0.031(9)	0.038(9)	0.036(10)	-0.008(7)	0.006(7)	0.012(7)
C(16)	0.033(9)	0.029(9)	0.042(10)	-0.003(7)	0.001(7)	0.009(7)
C(17)	0.045(10)	0.049(10)	0.033(10)	-0.002(8)	-0.015(7)	0.008(8)
C(18)	0.068(13)	0.064(13)	0.055(12)	0.005(10)	-0.003(10)	0.013(10)
C(19)	0.057(12)	0.081(14)	0.038(12)	0.012(10)	-0.003(9)	0.023(10)
C(20)	0.054(11)	0.060(11)	0.035(11)	0.010(9)	-0.006(8)	0.013(9)
C(21)	0.037(10)	0.027(9)	0.062(12)	-0.003(7)	0.013(8)	0.000(8)
C(22)	0.051(11)	0.045(10)	0.053(12)	-0.016(9)	0.021(9)	-0.007(9)
C(23)	0.038(10)	0.059(12)	0.060(12)	0.002(9)	-0.001(9)	-0.001(10)
C(24)	0.072(14)	0.040(11)	0.081(14)	-0.013(10)	0.018(11)	-0.015(10)
C(25)	0.063(12)	0.060(12)	0.044(11)	-0.020(9)	0.020(9)	-0.022(9)
C(26)	0.040(9)	0.040(10)	0.049(11)	-0.011(8)	0.011(8)	-0.001(8)
C(27)	0.026(8)	0.036(9)	0.031(9)	-0.007(7)	0.007(7)	-0.005(7)
C(28)	0.034(9)	0.026(8)	0.024(9)	-0.008(7)	0.009(7)	0.001(6)
C(29)	0.022(8)	0.019(8)	0.044(10)	-0.007(6)	0.004(6)	0.005(7)
C(30)	0.023(8)	0.045(10)	0.043(11)	0.003(7)	0.013(7)	0.007(8)
C(31)	0.040(10)	0.053(11)	0.054(12)	-0.004(8)	0.011(8)	0.010(9)
C(32)	0.042(10)	0.046(11)	0.051(12)	-0.001(8)	0.013(8)	0.006(9)
C(33)	0.062(12)	0.085(14)	0.027(11)	0.001(10)	0.015(8)	0.024(10)
C(34)	0.059(11)	0.040(10)	0.063(12)	0.010(8)	0.032(9)	0.033(9)
C(35)	0.034(9)	0.016(8)	0.043(10)	0.003(6)	0.013(7)	0.007(7)
C(36)	0.023(8)	0.042(10)	0.050(11)	-0.005(7)	0.011(7)	0.001(8)

26

Table 3. Anisotropic Displacement Parameters (continued)

atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
C(37)	0.073(12)	0.017(9)	0.061(12)	-0.011(8)	0.014(9)	0.009(8)
C(38)	0.078(13)	0.021(9)	0.068(13)	-0.015(8)	-0.006(10)	0.003(9)
C(39)	0.044(10)	0.039(10)	0.055(12)	-0.008(8)	-0.004(8)	-0.011(8)
C(40)	0.027(9)	0.036(9)	0.041(10)	-0.004(7)	-0.005(7)	0.001(8)
C(41)	0.030(8)	0.033(9)	0.034(10)	-0.009(7)	0.005(7)	-0.003(7)
C(42)	0.038(9)	0.030(8)	0.014(8)	-0.012(7)	0.005(6)	-0.003(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

2

Table 4. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
P(1)	O(1)	1.624(9)	P(1)	O(2)	1.606(9)
P(1)	N(1)	1.576(11)	P(1)	N(3)	1.570(10)
P(2)	O(3)	1.626(8)	P(2)	O(4)	1.615(9)
P(2)	N(1)	1.553(11)	P(2)	N(2)	1.537(9)
P(3)	O(5)	1.615(8)	P(3)	O(6)	1.605(8)
P(3)	N(2)	1.614(10)	P(3)	N(3)	1.572(10)
O(1)	C(1)	1.394(14)	O(2)	C(14)	1.402(13)
O(3)	C(15)	1.406(14)	O(4)	C(28)	1.409(13)
O(5)	C(29)	1.401(13)	O(6)	C(42)	1.406(13)
C(1)	C(2)	1.43(2)	C(1)	C(14)	1.33(2)
C(2)	C(3)	1.39(2)	C(2)	C(7)	1.43(2)
C(3)	C(4)	1.36(2)	C(4)	C(5)	1.37(2)
C(5)	C(6)	1.38(2)	C(6)	C(7)	1.40(2)
C(7)	C(8)	1.48(2)	C(8)	C(9)	1.40(2)
C(8)	C(13)	1.39(2)	C(9)	C(10)	1.37(2)
C(10)	C(11)	1.40(2)	C(11)	C(12)	1.39(2)
C(12)	C(13)	1.40(2)	C(13)	C(14)	1.40(2)
C(15)	C(16)	1.45(2)	C(15)	C(28)	1.34(2)
C(16)	C(17)	1.41(2)	C(16)	C(21)	1.41(2)
C(17)	C(18)	1.38(2)	C(18)	C(19)	1.38(2)
C(19)	C(20)	1.33(2)	C(20)	C(21)	1.46(2)
C(21)	C(22)	1.44(2)	C(22)	C(23)	1.41(2)
C(22)	C(27)	1.44(2)	C(23)	C(24)	1.34(2)
C(24)	C(25)	1.41(2)	C(25)	C(26)	1.37(2)

Table 4. Bond Lengths( $\text{\AA}$ ) (continued)

atom	atom	distance	atom	atom	distance
C(26)	C(27)	1.39(2)	C(27)	C(28)	1.40(2)
C(29)	C(30)	1.44(2)	C(29)	C(42)	1.31(2)
C(30)	C(31)	1.42(2)	C(30)	C(35)	1.44(2)
C(31)	C(32)	1.33(2)	C(32)	C(33)	1.37(2)
C(33)	C(34)	1.36(2)	C(34)	C(35)	1.43(2)
C(35)	C(36)	1.42(2)	C(36)	C(37)	1.41(2)
C(36)	C(41)	1.45(2)	C(37)	C(38)	1.33(2)
C(38)	C(39)	1.40(2)	C(39)	C(40)	1.37(2)
C(40)	C(41)	1.38(2)	C(41)	C(42)	1.38(2)
C(43)	C(44)	1.52(2)	C(44)	C(45)	1.36(2)
C(44)	C(46)	1.39(2)	C(45)	C(46)	1.34(2)
C(47)	C(48)	1.48(3)	C(48)	C(49)	1.46(2)
C(48)	C(50)	1.37(2)	C(49)	C(50)	1.37(2)

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	P(1)	O(2)	96.9(5)	O(1)	P(1)	N(1)	110.7(5)
O(1)	P(1)	N(3)	109.6(6)	O(2)	P(1)	N(1)	111.8(5)
O(2)	P(1)	N(3)	110.3(5)	N(1)	P(1)	N(3)	115.9(6)
O(3)	P(2)	O(4)	97.2(4)	O(3)	P(2)	N(1)	111.0(6)
O(3)	P(2)	N(2)	108.5(5)	O(4)	P(2)	N(1)	109.8(6)
O(4)	P(2)	N(2)	110.6(5)	N(1)	P(2)	N(2)	117.8(6)
O(5)	P(3)	O(6)	96.3(4)	O(5)	P(3)	N(2)	110.2(5)
O(5)	P(3)	N(3)	112.3(5)	O(6)	P(3)	N(2)	111.9(5)
O(6)	P(3)	N(3)	108.5(6)	N(2)	P(3)	N(3)	116.0(5)
P(1)	O(1)	C(1)	107.8(8)	P(1)	O(2)	C(14)	109.2(8)
P(2)	O(3)	C(15)	107.6(8)	P(2)	O(4)	C(28)	107.9(7)
P(3)	O(5)	C(29)	108.2(8)	P(3)	O(6)	C(42)	109.7(7)
P(1)	N(1)	P(2)	123.9(7)	P(2)	N(2)	P(3)	122.3(6)
P(1)	N(3)	P(3)	123.6(6)	O(1)	C(1)	C(2)	122(1)
O(1)	C(1)	C(14)	113(1)	C(2)	C(1)	C(14)	123(1)
C(1)	C(2)	C(3)	125(1)	C(1)	C(2)	C(7)	114(1)
C(3)	C(2)	C(7)	119(1)	C(2)	C(3)	C(4)	121(1)
C(3)	C(4)	C(5)	118(1)	C(4)	C(5)	C(6)	122(1)
C(5)	C(6)	C(7)	119(1)	C(2)	C(7)	C(6)	117(1)
C(2)	C(7)	C(8)	120(1)	C(6)	C(7)	C(8)	121(1)
C(7)	C(8)	C(9)	121(1)	C(7)	C(8)	C(13)	119(1)
C(9)	C(8)	C(13)	118(1)	C(8)	C(9)	C(10)	120(1)
C(9)	C(10)	C(11)	122(1)	C(10)	C(11)	C(12)	117(1)
C(11)	C(12)	C(13)	121(1)	C(8)	C(13)	C(12)	120(1)

Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(8)	C(13)	C(14)	118(1)	C(12)	C(13)	C(14)	121(1)
O(2)	C(14)	C(1)	111(1)	O(2)	C(14)	C(13)	124(1)
C(1)	C(14)	C(13)	123(1)	O(3)	C(15)	C(16)	123(1)
O(3)	C(15)	C(28)	112(1)	C(16)	C(15)	C(28)	123(1)
C(15)	C(16)	C(17)	121(1)	C(15)	C(16)	C(21)	113(1)
C(17)	C(16)	C(21)	124(1)	C(16)	C(17)	C(18)	117(1)
C(17)	C(18)	C(19)	119(1)	C(18)	C(19)	C(20)	123(1)
C(19)	C(20)	C(21)	121(1)	C(16)	C(21)	C(20)	113(1)
C(16)	C(21)	C(22)	122(1)	C(20)	C(21)	C(22)	123(1)
C(21)	C(22)	C(23)	123(1)	C(21)	C(22)	C(27)	120(1)
C(23)	C(22)	C(27)	116(1)	C(22)	C(23)	C(24)	121(1)
C(23)	C(24)	C(25)	122(1)	C(24)	C(25)	C(26)	117(1)
C(25)	C(26)	C(27)	121(1)	C(22)	C(27)	C(26)	119(1)
C(22)	C(27)	C(28)	115(1)	C(26)	C(27)	C(28)	124(1)
O(4)	C(28)	C(15)	112(1)	O(4)	C(28)	C(27)	123(1)
C(15)	C(28)	C(27)	123(1)	O(5)	C(29)	C(30)	123(1)
O(5)	C(29)	C(42)	114(1)	C(30)	C(29)	C(42)	122(1)
C(29)	C(30)	C(31)	124(1)	C(29)	C(30)	C(35)	115(1)
C(31)	C(30)	C(35)	120(1)	C(30)	C(31)	C(32)	123(1)
C(31)	C(32)	C(33)	118(1)	C(32)	C(33)	C(34)	120(1)
C(33)	C(34)	C(35)	124(1)	C(30)	C(35)	C(34)	112(1)
C(30)	C(35)	C(36)	120(1)	C(34)	C(35)	C(36)	127(1)
C(35)	C(36)	C(37)	122(1)	C(35)	C(36)	C(41)	120(1)
C(37)	C(36)	C(41)	116(1)	C(36)	C(37)	C(38)	121(1)



Table 5. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(37)	C(38)	C(39)	123(1)	C(38)	C(39)	C(40)	117(1)
C(39)	C(40)	C(41)	122(1)	C(36)	C(41)	C(40)	119(1)
C(36)	C(41)	C(42)	115(1)	C(40)	C(41)	C(42)	125(1)
O(6)	C(42)	C(29)	111(1)	O(6)	C(42)	C(41)	123(1)
C(29)	C(42)	C(41)	125(1)	C(43)	C(44)	C(45)	122(1)
C(43)	C(44)	C(46)	121(1)	C(45)	C(44)	C(46)	116(1)
C(44)	C(45)	C(46*)	121(1)	C(44)	C(46)	C(45*)	121(1)
C(47)	C(48)	C(49)	124(2)	C(47)	C(48)	C(50**)	123(2)
C(49)	C(48)	C(50)	112(1)	C(48)	C(49)	C(50)	126(1)
C(48)	C(50)	C(49**)	121(2)				

Symmetry operations: \* = 1-x, -y, 1-z; \*\* = -x, 1-y, 2-z

Table 6. Important Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
P(1)	O(1)	C(1)	C(2)	179.4(9)	P(1)	O(1)	C(1)	C(14)	5(1)
P(1)	O(2)	C(14)	C(1)	2(1)	P(1)	O(2)	C(14)	C(13)	-179.7(10)
P(1)	N(1)	P(2)	O(3)	-130.2(8)	P(1)	N(1)	P(2)	O(4)	123.5(8)
P(1)	N(1)	P(2)	N(2)	-4(1)	P(1)	N(3)	P(3)	O(5)	-125.2(8)
P(1)	N(3)	P(3)	O(6)	129.6(8)	P(1)	N(3)	P(3)	N(2)	2(1)
P(2)	O(3)	C(15)	C(16)	173(1)	P(2)	O(3)	C(15)	C(28)	-7(1)
P(2)	O(4)	C(28)	C(15)	7(1)	P(2)	O(4)	C(28)	C(27)	-173(1)
P(2)	N(1)	P(1)	O(1)	124.8(8)	P(2)	N(1)	P(1)	O(2)	-128.4(8)
P(2)	N(1)	P(1)	N(3)	0(1)	P(2)	N(2)	P(3)	O(5)	120.9(7)
P(2)	N(2)	P(3)	O(6)	-133.3(7)	P(2)	N(2)	P(3)	N(3)	-8.1(10)
P(3)	O(5)	C(29)	C(30)	175.3(9)	P(3)	O(5)	C(29)	C(42)	-1(1)
P(3)	O(6)	C(42)	C(29)	4(1)	P(3)	O(6)	C(42)	C(41)	-172(1)
P(3)	N(2)	P(2)	O(3)	136.0(7)	P(3)	N(2)	P(2)	O(4)	-118.5(7)
P(3)	N(2)	P(2)	N(1)	8(1)	P(3)	N(3)	P(1)	O(1)	-124.6(8)
P(3)	N(3)	P(1)	O(2)	129.8(8)	P(3)	N(3)	P(1)	N(1)	1(1)
O(1)	P(1)	O(2)	C(14)	0.7(8)	O(1)	C(1)	C(2)	C(3)	6(2)
O(1)	C(1)	C(2)	C(7)	-176(1)	O(1)	C(1)	C(14)	O(2)	-4(1)
O(1)	C(1)	C(14)	C(13)	177(1)	O(2)	P(1)	O(1)	C(1)	-3.2(8)
O(2)	C(14)	C(1)	C(2)	-178(1)	O(2)	C(14)	C(13)	C(8)	-179(1)
O(2)	C(14)	C(13)	C(12)	0(1)	O(3)	P(2)	O(4)	C(28)	-10.8(8)
O(3)	C(15)	C(16)	C(17)	3(2)	O(3)	C(15)	C(16)	C(21)	178(1)
O(3)	C(15)	C(28)	O(4)	0(1)	O(3)	C(15)	C(28)	C(27)	-178(1)
O(4)	P(2)	O(3)	C(15)	10.7(8)	O(4)	C(28)	C(15)	C(16)	179(1)
O(4)	C(28)	C(27)	C(22)	179(1)	O(4)	C(28)	C(27)	C(26)	0(2)

Table 6. Important Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(5)	P(3)	O(6)	C(42)	-5.0(8)	O(5)	C(29)	C(30)	C(31)	3(1)
O(5)	C(29)	C(30)	C(35)	-177(1)	O(5)	C(29)	C(42)	O(6)	-1(1)
O(5)	C(29)	C(42)	C(41)	174(1)	O(6)	P(3)	O(5)	C(29)	4.0(8)
O(6)	C(42)	C(29)	C(30)	-178(1)	O(6)	C(42)	C(41)	C(36)	179(1)
O(6)	C(42)	C(41)	C(40)	0(2)	N(1)	P(1)	O(1)	C(1)	113.2(8)
N(1)	P(1)	O(2)	C(14)	-114.9(8)	N(1)	P(2)	O(3)	C(15)	-103.8(9)
N(1)	P(2)	O(4)	C(28)	104.7(8)	N(2)	P(2)	O(3)	C(15)	125.3(8)
N(2)	P(2)	O(4)	C(28)	-123.7(8)	N(2)	P(3)	O(5)	C(29)	120.1(8)
N(2)	P(3)	O(6)	C(42)	-119.7(8)	N(3)	P(1)	O(1)	C(1)	-117.7(8)
N(3)	P(1)	O(2)	C(14)	114.6(8)	N(3)	P(3)	O(5)	C(29)	-108.9(8)
N(3)	P(3)	O(6)	C(42)	111.0(8)	C(1)	C(2)	C(3)	C(4)	177(1)