

Experimental

General

The materials procured from Sigma-Aldrich and Merck, were used without further purification. IR spectra were obtained on Perkin Elmer FT-IR spectrometer spectrum-2000 using potassium bromide pellets or as liquid films between two sodium chloride pellets. Mass spectra were recorded in a TOF-mass spectrometer model no. KC455. ^1H NMR, ^{13}C NMR and ^{31}P NMR spectra (300 MHz) were recorded on a Bruker spectrosSpin 300 MHz. All NMR samples were run in CDCl_3 and chemical shifts are expressed as ppm relative to internal Me_4Si . Column Chromatography was carried out with the use of silica gel (100-200 mesh), purchased from Sisco Research Laboratories (SRL) Pvt. Ltd. Mumbai, India.

Typical Procedure for the synthesis of α -amino phosphonates

In a 50 ml round bottom flask, the mixture of aldehyde (1 mmol), amine (1.1 mmol) and diethyl phosphate (1 mmol) in acetonitrile (2 ml) were stirred at 50 °C under a nitrogen atmosphere. To this resulted reaction mixture, Cu-nanoparticles (10 mol %) were added. The progress of reaction was continuously monitored through TLC. On the completion of reaction, as indicated by TLC examination, an excess of water was added to the reaction mixture. The crude product was extracted with ethyl acetate and dried over anhydrous Na_2SO_4 . Solvent was removed under vacuo. Subsequently, the reaction mixture was purified by column chromatography using silica gel and hexane (90): ethyl acetate (10) as an eluent to get pure α -amino phosphonates (Table 1, entry 1-7). All the products were unambiguously established on the basis of their spectral analysis (IR, ^1H NMR, ^{13}C NMR, ^{31}P NMR and mass spectra).

1. IR ν_{max} (KBr) 3295 (s, NH), 1236 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.09 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.24 (3H, t, $j = 7.0$ Hz $-\text{OCH}_2\text{CH}_3$), 3.64-3.70 (1H, t, $j = 6.9$, OCH_2CH_3), 3.90-3.93 (1H, t, $j = 6.9$, $-\text{OCH}_2\text{CH}_3$), 4.09-4.13 (2H, t, $j = 6.9$, $-\text{OCH}_2\text{CH}_3$), 4.70 (1H, d, $j = 23.7$, CHP), 6.57-7.48 (10H, m, ϕ). ^{13}C NMR (300 MHz, TMS, CDCl_3): 16.15 (dd, $^3j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 56.10 (d, $^1j_{\text{c,p}} = 150.4$ Hz, CH), 63.05 (d, $^2j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 113.67, 118.18, 127.73-128.42, 135.77, 146.08-146.27 (C_6H_6). ^{31}P NMR (300 MHz, TMS, CDCl_3): 22.51. m/z (GC-MS, HRMS): 318.92 (M^+).
2. IR ν_{max} (KBr) 3288 (s, NH), 1235 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 0.89 (3H, t, $j = 6.68$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.25 (3H, t, $j = 6.68$ Hz, $-\text{OCH}_2\text{CH}_3$), 3.86-4.71 (4H, m, $-\text{OCH}_2\text{CH}_3$), 4.90 (1H, d, $j =$

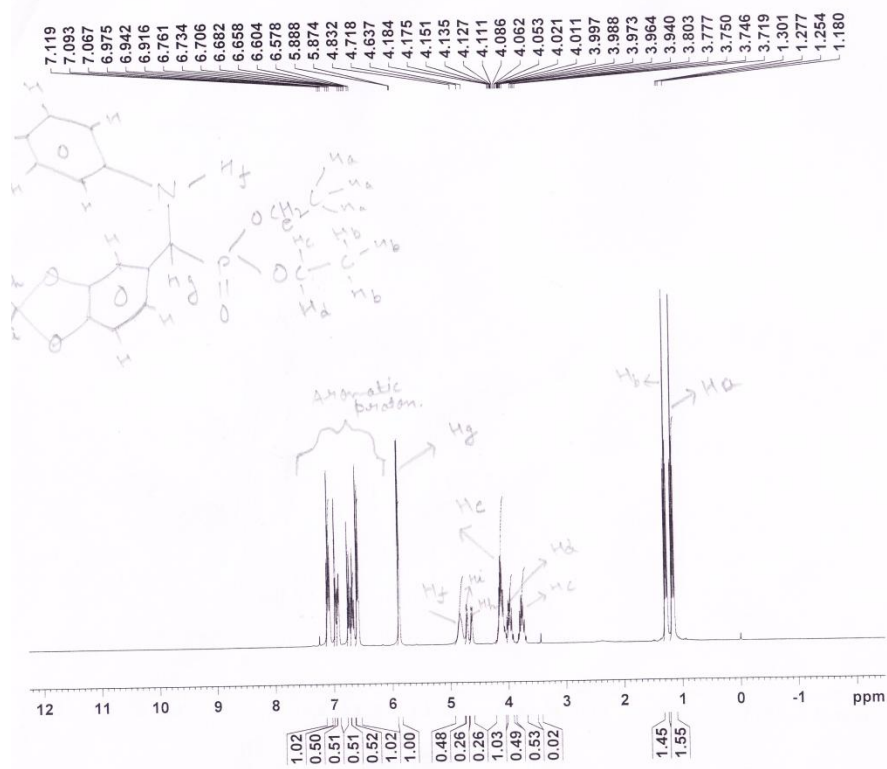
25.2, CHP), 6.52 (2H, d, $j = 7.7$ Hz, ϕ), 6.73 (1H, t, $j = 7.0$ Hz, ϕ), 7.11 (2H, t, $j = 7.0$ Hz, ϕ), 7.64-7.67(2H, dd, $j = 8.2$ Hz, ϕ), 8.18 (2H, d, $j = 7.7$ Hz, ϕ). m/z (GC-MS, HRMS): 364.09 (M^+).

3. IR ν_{\max} (KBr) 3276 (s, NH), 1222 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.13 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.25 (3H, t, $j = 7.0$ Hz, OCH_2CH_3), 3.77 (3H, s, ArOCH_3), 3.65-4.17 (4H, m, OCH_2CH_3), 4.66 (1H, d, $j = 23.7$, CHP), 6.57 (2H, d, $j = 7.2$ Hz, ϕ), 6.60 (1H, t, $j = 7.6$ Hz, ϕ), 6.84 (2H, d, $j = 7.2$ Hz, ϕ), 7.10 (2H, t, $j = 7.2$ Hz, ϕ), 7.38 (2H, dd, $j = 7.4$ Hz, ϕ). ^{13}C NMR (300 MHz, TMS, CDCl_3): 16.37 (dd, $^3j_{\text{c,p}} = 5.7$ Hz, OCH_2CH_3), 54.19-55.19 (d, $^1j_{\text{c,p}} = 150.4$ Hz, CH), 56.35 (s, OCH_3), 63.16 (d, $^2j_{\text{c,p}} = 5.7$ Hz, OCH_2CH_3), 113.86, 114.03, 118.31, 127.65, 128.95-129.43, 146.23-146.43, 159.28 (C_6H_6). m/z (GC-MS, HRMS): 349.09 (M^+).

4. IR ν_{\max} (KBr) 3571 (s, NH), 1231 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.07 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.23 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 2.15 (3H, s, ArOCH_3), 3.61-4.10 (4H, m, $-\text{OCH}_2\text{CH}_3$), 4.74 (1H, d, $j = 23.7$, CHP), 6.39-6.46 (4H, m, ϕ), 6.92 (1H, t, $j = 7.2$ Hz, ϕ), 7.25 (2H, dd, $j = 7.7$ Hz, ϕ), 7.47 (2H, d, $j = 7.0$ Hz, ϕ). ^{13}C NMR (300 MHz, TMS, CDCl_3): 15.36-15.68 (dd, $^3j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 20.75 (s, CH_3), 53.96-55.96 (d, $^1j_{\text{c,p}} = 152.4$ Hz, CH), 62.27-62.43 (t, $^2j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 109.56-109.97, 113.91, 117.32-118.27, 126.99-128.18, 135.44-137.86, 145.68-145.87 (C_6H_6). m/z (GC-MS, HRMS): 334.10 (M^+).

5. IR ν_{\max} (KBr) 3296 (s, NH), 1231 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.10 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.27 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 3.83 (3H, s, ArOCH_3), 3.60-4.23 (4H, m, $-\text{OCH}_2\text{CH}_3$), 4.84 (1H, d, $j = 23.7$, CHP), 6.92 (2H, d, $j = 7.0$ Hz, ϕ), 7.25 (2H, d, $j = 7.0$ Hz, ϕ), 7.46 (1H, t, $j = 6.9$ Hz, ϕ), 7.89 (2H, dd, $j = 7.5$ Hz, ϕ), 8.48 (2H, d, $j = 7.8$ Hz, ϕ). m/z (GC-MS, HRMS): 350.09 (M^+).

6. IR ν_{\max} (KBr) 3295 (s, NH), 1236 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.18 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.25 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 3.71-4.18 (4H, m, $-\text{OCH}_2\text{CH}_3$), 4.73(1H, d, $j = 23.7$, CHP), 4.83 (1H, br, NH), 5.87 (2H, s, CH_2), 6.57-6.91 (5H, m, ϕ), 6.97 (1H, s, ϕ), 7.09 (1H, t, $j = 6.9$ Hz, ϕ). ^{13}C NMR (300 MHz, TMS, CDCl_3): 16.06-16.28 (dd, $^3j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 54.52-56.53 (d, $^1j_{\text{c,p}} = 154.04$ Hz, CH), 63.01-63.10 (d, $^2j_{\text{c,p}} = 5.8$ Hz, OCH_2CH_3), 100.92 (s, CH_2), 108.00-108.08, 113.67, 118.21, 121.14-121.22, 128.95-129.54, 146.01-146.20, 147.15-147.80 (C_6H_6). ^{31}P NMR (300 MHz, TMS, CDCl_3): 22.40. m/z (GC-MS, HRMS): 360.74(M^+).

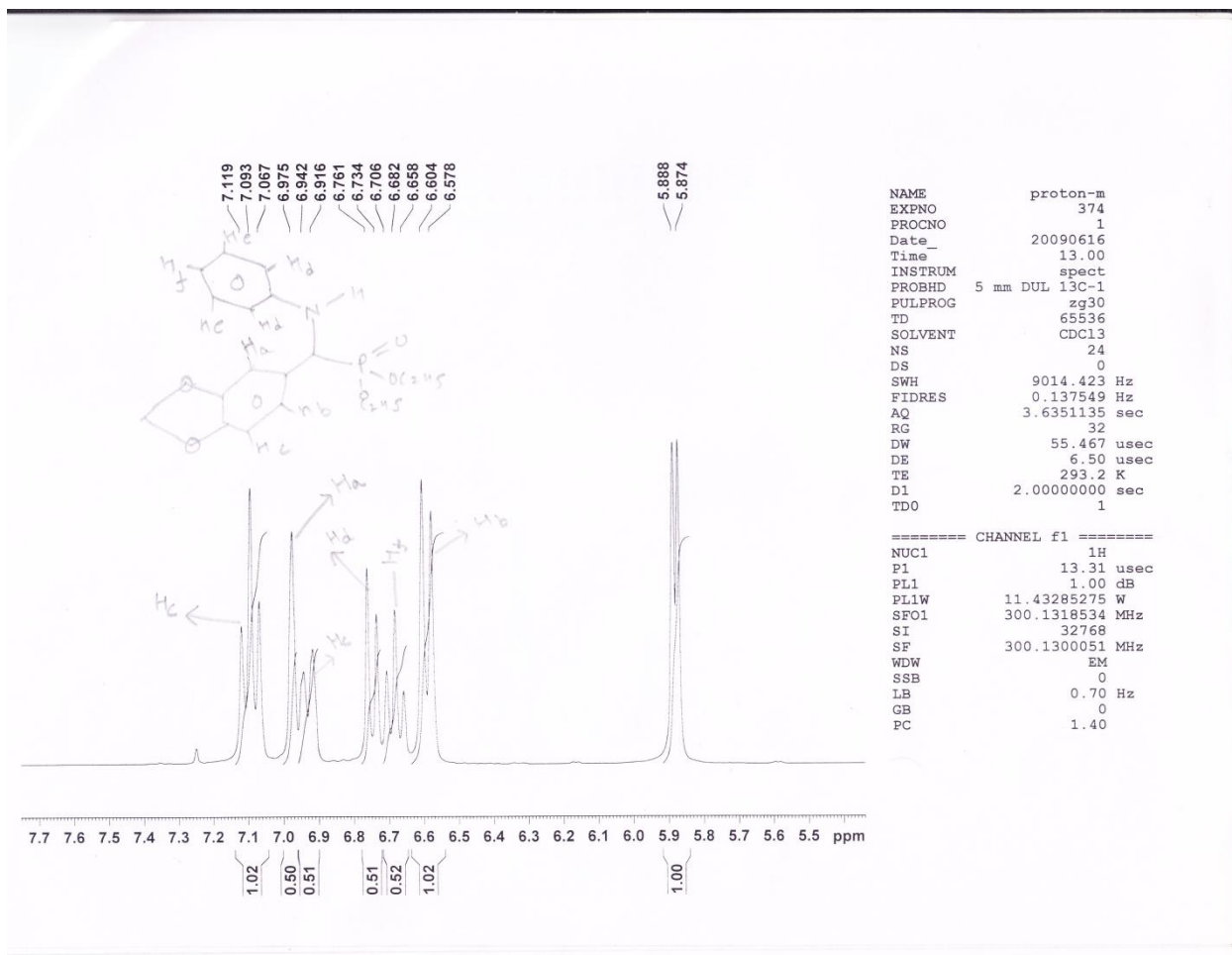


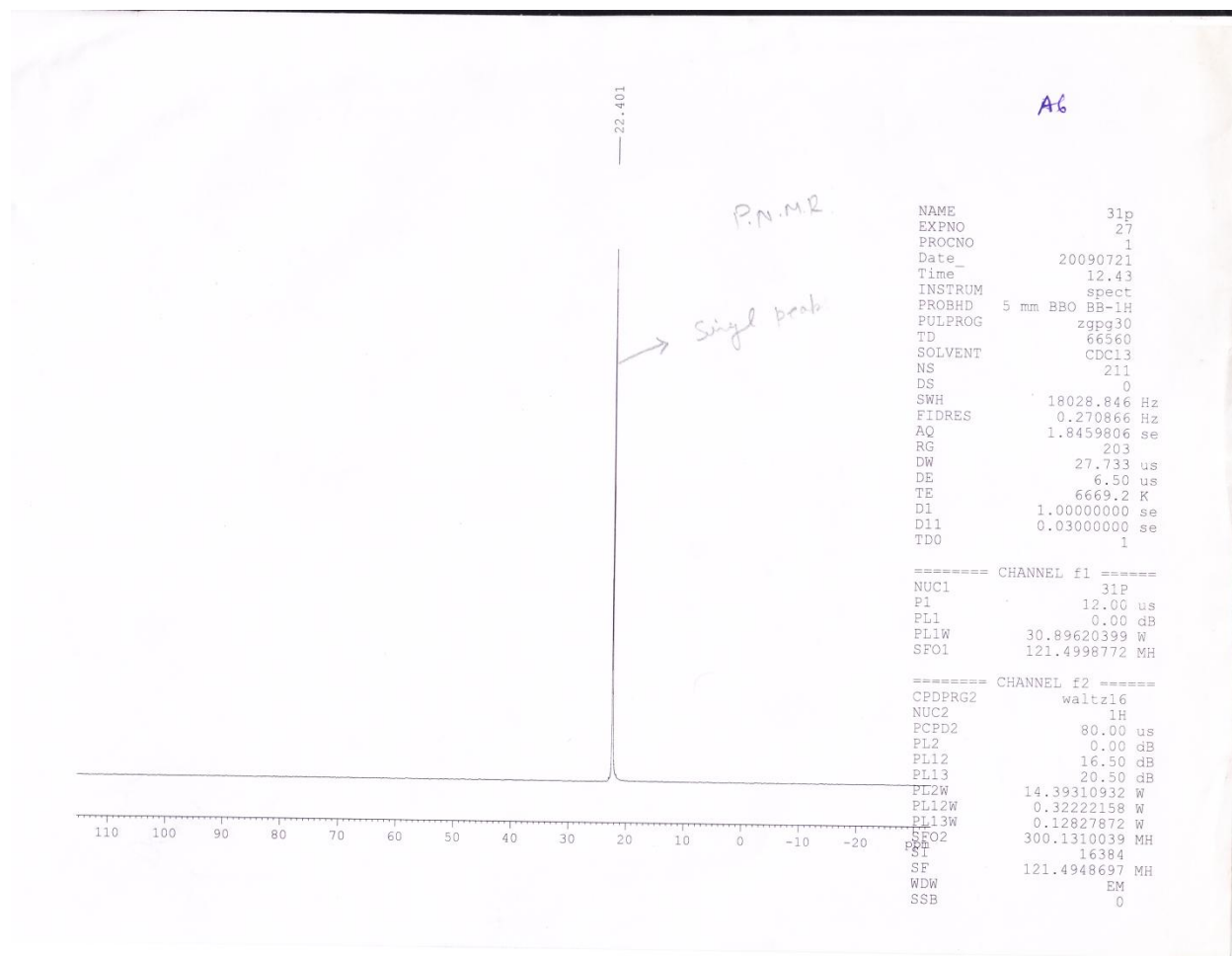
A-6

```

NAME          proton-m
EXPNO         374
PROCNO        1
Date_         20090616
Time          13.00
INSTRUM       spect
PROBHD        5 mm DUL 13C-1
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            24
DS            0
SWH           9014.423 Hz
FIDRES        0.137549 Hz
AQ            3.6351135 sec
RG            32
DW            55.467 usec
DE            6.50 usec
TE            293.2 K
D1            2.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          1H
P1            13.31 usec
PL1           1.00 dB
PL1W          11.43285275 W
SFO1          300.1318534 MHz
SI            32768
SF            300.1300051 MHz
WDW           EM
SSB           0
LB            0.70 Hz
GB            0
PC            1.40
    
```





7. IR ν_{\max} (KBr) 3456 (s, NH), 1224 (s, P=O). ^1H NMR (300 MHz, TMS, CDCl_3): δ 1.18 (3H, t, $j = 7.0$ Hz, $-\text{OCH}_2\text{CH}_3$), 1.23 (3H, t, $j = 6.96$, Hz $-\text{OCH}_2\text{CH}_3$), 3.60-4.23 (4H, m, $-\text{OCH}_2\text{CH}_3$), 4.75 (1H, d, $j = 23.7$, CHP), 4.84 (1H, d, CHP), 7.11 (1H, s), 6.57-7.10 (10H, m, ϕ), 7.90 (1H, s). m/z (GC-MS, HRMS): 353.09 (M^+).

Crystallographic data for the structural analysis have been deposited with in Cambridge Crystallographic Data Centre as supplementary publication number **CCDC 761136** for compound **3f**. Copies of this information may be obtained free of Charge from the Director,CCDC,12 Union road, Cambridge,CB2,IEZ,UK (E-mail:linstead@ccdc.cam.ac.uk or deposit @ccdc.cam .ac;Fax:44 1223 336033)

Table 1. Crystal data and structure refinement for 3f.

Identification code	shelxl
Empirical formula	C18 H22 N O5 P
Formula weight	363.34

Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 22.1091(11) Å	$\alpha = 90^\circ$.
	b = 10.4184(3) Å	$\beta = 118.495(6)^\circ$.
	c = 18.2639(8) Å	$\gamma = 90^\circ$.
Volume	3697.3(3) Å ³	
Z	8	
Density (calculated)	1.305 Mg/m ³	
Absorption coefficient	0.176 mm ⁻¹	
F(000)	1536	
Crystal size	0.24 x 0.18 x 0.12 mm ³	
Theta range for data collection	2.97 to 25.99°.	
Index ranges	-27<=h<=25, -12<=k<=10, -22<=l<=22	
Reflections collected	8459	
Independent reflections	3616 [R(int) = 0.0157]	
Completeness to theta = 25.99°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8728 and 0.8145	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3616 / 23 / 232	
Goodness-of-fit on F ²	1.071	

Final R indices [I>2sigma(I)] R1 = 0.0559, wR2 = 0.1791

R indices (all data) R1 = 0.0728, wR2 = 0.1892

Largest diff. peak and hole 0.758 and -0.491 e.Å⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$)

for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	6384(1)	3486(2)	6829(1)	35(1)
C(2)	6815(1)	2420(2)	7124(2)	43(1)
C(3)	7413(2)	2488(3)	7888(2)	54(1)
C(4)	7591(1)	3590(3)	8353(2)	55(1)
C(5)	7174(1)	4658(3)	8051(2)	49(1)
C(6)	6578(1)	4613(3)	7302(2)	41(1)
C(7)	5573(1)	2423(2)	5498(2)	35(1)
C(8)	5943(1)	2419(2)	4976(2)	37(1)
C(9)	5942(2)	3510(3)	4536(2)	53(1)
C(10)	6263(2)	3529(3)	4041(2)	62(1)
C(11)	6604(2)	2440(3)	4027(2)	51(1)
C(12)	7254(2)	993(4)	3844(2)	70(1)
C(13)	6608(1)	1359(3)	4455(2)	44(1)
C(14)	6282(1)	1301(2)	4933(2)	41(1)
C(15)	4447(3)	450(4)	3003(2)	94(1)
C(16)	4311(2)	1611(3)	3361(2)	74(1)
N(1)	5757(1)	3472(2)	6091(1)	40(1)
O(1)	6977(1)	405(2)	4324(2)	72(1)

O(2)	6957(1)	2229(2)	3591(2)	67(1)
O(3)	4472(1)	1355(2)	4216(1)	48(1)
O(5)	4389(1)	3758(2)	4490(1)	52(1)
P(1)	4642(1)	2486(1)	4851(1)	38(1)
O(4)	4342(1)	1931(2)	5409(1)	53(1)
C(17)	3993(3)	2703(5)	5740(4)	123(2)
C(18A)	4359(8)	2784(17)	6660(4)	164(5)
C(18B)	3974(14)	2231(19)	6493(10)	164(5)

Table 3. Bond lengths [Å] and angles [°] for 1.

C(1)-C(2)	1.395(4)
C(1)-N(1)	1.398(3)
C(1)-C(6)	1.398(3)
C(2)-C(3)	1.392(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.369(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.382(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.375(4)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-N(1)	1.453(3)
C(7)-C(8)	1.523(3)
C(7)-P(1)	1.820(2)
C(7)-H(7)	0.9800
C(8)-C(9)	1.391(4)
C(8)-C(14)	1.407(3)
C(9)-C(10)	1.389(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.370(4)

C(10)-H(10)	0.9300
C(11)-C(13)	1.368(4)
C(11)-O(2)	1.374(3)
C(12)-O(2)	1.419(4)
C(12)-O(1)	1.427(4)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.374(4)
C(13)-O(1)	1.377(3)
C(14)-H(14)	0.9300
C(15)-C(16)	1.473(3)
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-O(3)	1.451(4)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
N(1)-H(1)	0.8600
O(3)-P(1)	1.5687(19)
O(5)-P(1)	1.4678(19)
P(1)-O(4)	1.5681(19)
O(4)-C(17)	1.434(4)
C(17)-C(18B)	1.479(3)

C(17)-C(18A)	1.479(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18A)-H(18A)	0.9600
C(18A)-H(18B)	0.9600
C(18A)-H(18C)	0.9600
C(18B)-H(18D)	0.9600
C(18B)-H(18E)	0.9600
C(18B)-H(18F)	0.9600
C(2)-C(1)-N(1)	123.0(2)
C(2)-C(1)-C(6)	118.6(2)
N(1)-C(1)-C(6)	118.4(2)
C(3)-C(2)-C(1)	119.6(2)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(4)-C(3)-C(2)	121.3(3)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	119.2(3)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
C(6)-C(5)-C(4)	120.6(3)

C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	120.7(2)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
N(1)-C(7)-C(8)	115.1(2)
N(1)-C(7)-P(1)	106.56(16)
C(8)-C(7)-P(1)	111.87(16)
N(1)-C(7)-H(7)	107.7
C(8)-C(7)-H(7)	107.7
P(1)-C(7)-H(7)	107.7
C(9)-C(8)-C(14)	119.8(2)
C(9)-C(8)-C(7)	120.4(2)
C(14)-C(8)-C(7)	119.7(2)
C(10)-C(9)-C(8)	121.8(3)
C(10)-C(9)-H(9)	119.1
C(8)-C(9)-H(9)	119.1
C(11)-C(10)-C(9)	117.2(3)
C(11)-C(10)-H(10)	121.4
C(9)-C(10)-H(10)	121.4
C(13)-C(11)-C(10)	121.6(3)
C(13)-C(11)-O(2)	110.4(3)
C(10)-C(11)-O(2)	127.9(3)

O(2)-C(12)-O(1)	108.8(2)
O(2)-C(12)-H(12A)	109.9
O(1)-C(12)-H(12A)	109.9
O(2)-C(12)-H(12B)	109.9
O(1)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3
C(11)-C(13)-C(14)	122.5(2)
C(11)-C(13)-O(1)	109.8(2)
C(14)-C(13)-O(1)	127.8(3)
C(13)-C(14)-C(8)	117.0(2)
C(13)-C(14)-H(14)	121.5
C(8)-C(14)-H(14)	121.5
C(16)-C(15)-H(15A)	109.5
C(16)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(16)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(3)-C(16)-C(15)	109.2(3)
O(3)-C(16)-H(16A)	109.8
C(15)-C(16)-H(16A)	109.8
O(3)-C(16)-H(16B)	109.8
C(15)-C(16)-H(16B)	109.8

H(16A)-C(16)-H(16B)	108.3
C(1)-N(1)-C(7)	121.6(2)
C(1)-N(1)-H(1)	119.2
C(7)-N(1)-H(1)	119.2
C(13)-O(1)-C(12)	105.1(2)
C(11)-O(2)-C(12)	105.0(2)
C(16)-O(3)-P(1)	120.47(19)
O(5)-P(1)-O(4)	115.90(12)
O(5)-P(1)-O(3)	116.09(11)
O(4)-P(1)-O(3)	100.19(11)
O(5)-P(1)-C(7)	113.27(11)
O(4)-P(1)-C(7)	105.23(11)
O(3)-P(1)-C(7)	104.58(11)
C(17)-O(4)-P(1)	123.2(2)
O(4)-C(17)-C(18B)	117.7(9)
O(4)-C(17)-C(18A)	113.4(8)
C(18B)-C(17)-C(18A)	37.4(8)
O(4)-C(17)-H(17A)	108.9
C(18B)-C(17)-H(17A)	72.8
C(18A)-C(17)-H(17A)	108.9
O(4)-C(17)-H(17B)	108.9
C(18B)-C(17)-H(17B)	130.6
C(18A)-C(17)-H(17B)	108.9

H(17A)-C(17)-H(17B)	107.7
C(17)-C(18A)-H(18A)	109.5
C(17)-C(18A)-H(18B)	109.5
H(18A)-C(18A)-H(18B)	109.5
C(17)-C(18A)-H(18C)	109.5
H(18A)-C(18A)-H(18C)	109.5
H(18B)-C(18A)-H(18C)	109.5
C(17)-C(18B)-H(18D)	109.5
C(17)-C(18B)-H(18E)	109.5
H(18D)-C(18B)-H(18E)	109.5
C(17)-C(18B)-H(18F)	109.5
H(18D)-C(18B)-H(18F)	109.5
H(18E)-C(18B)-H(18F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic

displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(1)	39(1)	35(1)	2(1)	19(1)	0(1)
C(2)	41(1)	40(2)	44(1)	-4(1)	18(1)	2(1)
C(3)	40(2)	52(2)	55(2)	2(1)	12(1)	12(1)
C(4)	39(2)	64(2)	47(2)	-9(1)	9(1)	-1(1)
C(5)	45(2)	49(2)	51(2)	-14(1)	22(1)	-7(1)
C(6)	43(1)	37(1)	44(1)	0(1)	22(1)	3(1)
C(7)	37(1)	32(1)	35(1)	3(1)	14(1)	1(1)
C(8)	34(1)	36(1)	38(1)	0(1)	16(1)	-2(1)
C(9)	68(2)	38(2)	70(2)	9(1)	45(2)	9(1)
C(10)	86(2)	47(2)	74(2)	13(2)	54(2)	3(2)
C(11)	53(2)	58(2)	51(2)	-8(1)	32(1)	-11(1)
C(12)	60(2)	96(3)	66(2)	-7(2)	41(2)	5(2)
C(13)	42(1)	44(2)	48(1)	-7(1)	22(1)	1(1)
C(14)	42(1)	35(1)	43(1)	3(1)	18(1)	1(1)
C(15)	126(4)	104(3)	61(2)	8(2)	54(2)	32(3)
C(16)	93(3)	76(2)	38(2)	2(2)	18(2)	15(2)
N(1)	42(1)	36(1)	36(1)	-1(1)	13(1)	7(1)
O(1)	89(2)	58(1)	98(2)	0(1)	68(2)	14(1)

O(2)	79(2)	71(2)	75(1)	-6(1)	57(1)	-5(1)
O(3)	50(1)	45(1)	41(1)	-3(1)	16(1)	-4(1)
O(5)	49(1)	40(1)	56(1)	8(1)	17(1)	7(1)
P(1)	36(1)	37(1)	39(1)	2(1)	16(1)	1(1)
O(4)	56(1)	49(1)	68(1)	4(1)	42(1)	2(1)
C(17)	205(6)	89(3)	165(5)	22(3)	161(5)	34(3)
C(18A)	265(16)	144(11)	173(7)	-39(6)	176(10)	-50(8)
C(18B)	265(16)	144(11)	173(7)	-39(6)	176(10)	-50(8)

Table 5. Torsion angles [°] for 1.

N(1)-C(1)-C(2)-C(3)	-176.4(2)
C(6)-C(1)-C(2)-C(3)	2.1(4)
C(1)-C(2)-C(3)-C(4)	-0.9(5)
C(2)-C(3)-C(4)-C(5)	-0.9(5)
C(3)-C(4)-C(5)-C(6)	1.5(5)
C(4)-C(5)-C(6)-C(1)	-0.3(4)
C(2)-C(1)-C(6)-C(5)	-1.5(4)
N(1)-C(1)-C(6)-C(5)	177.0(2)
N(1)-C(7)-C(8)-C(9)	-52.5(3)
P(1)-C(7)-C(8)-C(9)	69.4(3)
N(1)-C(7)-C(8)-C(14)	128.1(2)
P(1)-C(7)-C(8)-C(14)	-110.0(2)
C(14)-C(8)-C(9)-C(10)	0.8(4)
C(7)-C(8)-C(9)-C(10)	-178.6(3)
C(8)-C(9)-C(10)-C(11)	-2.4(5)
C(9)-C(10)-C(11)-C(13)	2.4(5)
C(9)-C(10)-C(11)-O(2)	-179.9(3)
C(10)-C(11)-C(13)-C(14)	-1.0(5)
O(2)-C(11)-C(13)-C(14)	-179.0(3)
C(10)-C(11)-C(13)-O(1)	179.1(3)
O(2)-C(11)-C(13)-O(1)	1.0(3)

C(11)-C(13)-C(14)-C(8)	-0.7(4)
O(1)-C(13)-C(14)-C(8)	179.3(3)
C(9)-C(8)-C(14)-C(13)	0.8(4)
C(7)-C(8)-C(14)-C(13)	-179.8(2)
C(2)-C(1)-N(1)-C(7)	-12.0(4)
C(6)-C(1)-N(1)-C(7)	169.5(2)
C(8)-C(7)-N(1)-C(1)	-75.0(3)
P(1)-C(7)-N(1)-C(1)	160.38(18)
C(11)-C(13)-O(1)-C(12)	4.9(3)
C(14)-C(13)-O(1)-C(12)	-175.1(3)
O(2)-C(12)-O(1)-C(13)	-8.9(3)
C(13)-C(11)-O(2)-C(12)	-6.5(3)
C(10)-C(11)-O(2)-C(12)	175.6(3)
O(1)-C(12)-O(2)-C(11)	9.5(3)
C(15)-C(16)-O(3)-P(1)	157.2(3)
C(16)-O(3)-P(1)-O(5)	21.8(3)
C(16)-O(3)-P(1)-O(4)	147.4(2)
C(16)-O(3)-P(1)-C(7)	-103.7(3)
N(1)-C(7)-P(1)-O(5)	51.8(2)
C(8)-C(7)-P(1)-O(5)	-74.86(19)
N(1)-C(7)-P(1)-O(4)	-75.80(18)
C(8)-C(7)-P(1)-O(4)	157.56(17)
N(1)-C(7)-P(1)-O(3)	179.12(15)

C(8)-C(7)-P(1)-O(3)	52.47(18)
O(5)-P(1)-O(4)-C(17)	-16.2(4)
O(3)-P(1)-O(4)-C(17)	-142.0(4)
C(7)-P(1)-O(4)-C(17)	109.7(4)
P(1)-O(4)-C(17)-C(18B)	-156.7(11)
P(1)-O(4)-C(17)-C(18A)	-115.3(8)

Symmetry transformations used to generate equivalent atoms: