

Table 1S. Positional Parameters and U(eq) Values for Compound (5)

atom	x	y	z	U(eq) ^a
P	0.8525(1)	0.8471(1)	0.0697(1)	0.021(1)
O11	0.7683(2)	1.0443(2)	0.0656(3)	0.027(1)
O12	0.7688(2)	0.7752(2)	-0.0426(2)	0.032(1)
O13	1.0344(2)	0.7975(2)	0.0729(3)	0.029(1)
O21	0.2747(2)	0.8601(2)	0.4583(2)	0.027(1)
O22	0.2962(2)	0.5917(2)	0.6691(2)	0.026(1)
O31	0.6030(2)	0.6955(2)	0.5770(2)	0.029(1)
O32	0.1876(2)	0.4851(2)	0.2112(2)	0.038(1)
N	0.5911(2)	0.7640(2)	0.2780(2)	0.020(1)
C11	0.7700(2)	0.7798(2)	0.2540(2)	0.021(1)
C21	0.4623(3)	0.9352(2)	0.2674(2)	0.026(1)
C22	0.2823(3)	0.9294(3)	0.3106(2)	0.029(1)
C23	0.1409(3)	0.7827(3)	0.4905(2)	0.025(1)
C24	0.1414(3)	0.7244(3)	0.6504(2)	0.025(1)
C25	0.3130(3)	0.5252(3)	0.8178(2)	0.026(1)
C26	0.4488(3)	0.3586(3)	0.8152(2)	0.024(1)

^aU(eq) is defined as one third the trace of the orthogonalized U_{ij} tensor.

Table 2S. Positional Parameters and Ueq Values for the Hydrogen Atoms

Atom	x	y	z	(Ueq) ^a
H11B	0.7814	0.8589	0.3221	0.025
H21A	0.4920	0.0090	0.3308	0.031
H2A	0.2041	0.0421	0.3032	0.031
H22B	0.2489	0.8604	0.2450	0.035
H23A	0.1591	0.6877	0.4299	0.030
H23B	0.0316	0.8626	0.4703	0.030
H24A	0.1369	0.8167	0.7105	0.031
H24B	0.0427	0.6837	0.6796	0.031
H25A	0.2051	0.5100	0.8606	0.032
H25B	0.3458	0.6016	0.8761	0.032
H26A	0.5571	0.3773	0.7779	0.029
H26B	0.4616	0.3097	0.9151	0.029
H111	0.8380	0.0938	0.0220	0.033
H311	0.6750	0.6306	0.6327	0.035
H312	0.5074	0.6759	0.6009	0.035
H321	0.1944	0.4084	0.1529	0.045
H1	0.5783	0.7266	0.3724	0.024
H11A	0.8481	0.6712	0.2810	0.025

^aU(eq) is defined as 1/3 the trace of the orthogonalized Uij tensor.

Table 3S. Torsion Angles (deg) for Compound (5).

C26-N-C11-P	59.5(2)	C21-N-C22-P	-68.89(19)
O12-P-C11-N	-36.16(17)	O13-P-C11-N	-162.92(14)
O11-P-C11-N	82.17(15)	C11-N-C21-C22	-172.25(16)
C26-N-C21-C22	57.6(2)	C23-O21-C22-C21	-154.62(17)
N-C-21-C22-O21	58.9(2)	C22-O21-C23-C24	-176.85(16)
C25-O22-C24-C23	179.71(16)	O21-C23-C24-O22	-67.1(2)
O24-O22-C25-C26	163.58(16)	O22-C25-C26-N	-57.8(2)

Table 4S. Crystallographic Data for Compound (6)

Empirical Formula	C ₁₄ H ₄₀ N ₂ O ₁₄ P ₂
Formula weight	522.42
Crystal System	Triclinic
<i>a</i> (Å)	8.1829(8)
<i>b</i> (Å)	8.3092(10)
<i>c</i> (Å)	9.1429(10)
$\alpha(^{\circ})$	85.286(9)
$\beta(^{\circ})$	84.736(9)
$\gamma(^{\circ})$	73.158(7)
<i>V</i> (Å ³)	591.47(11)
<i>Z</i>	1
Space Group	P $\bar{1}$ (#2)
<i>d</i> _{calc} (g/cm ⁻³)	1.467
Temp(C ^o)	20±2
μ	0.231
No. data(<i>I</i> >3.0 σ (<i>I</i>))	1762
No. of parameters	170
R ₁	0.032
wR ₂	0.082