Experimental procedures

General. The urethane protected *N*-carboxyanhydrides (UNCAs) were obtained as a gift from Propeptide, Inc. Chiral HPLC analyses were carried out using a Waters M-6000 solvent pump and a Schoeffel Instrument Corp. UV detector. A Daicel Chemical Co. "Chiracel OD" column was used to detect the enantiomers at a flow rate of 1.5 mL/min, (214 nm).

General procedure of preparation and chiral HPLC analysis of L- and DL- standard Boc-amino acid benzyl amides.

The L-standard. A Boc-L-amino acid NCA was dissolved in toluene at a concentration of 0.33 M and the resulting solution was stirred at rt. Benzylamine (1.0 equiv) was added and the reaction mixture was stirred for 30 min. The reaction mixture was washed with 5% $NaHSO_4$ and dried over Na_2SO_4. The solvent was removed under reduced pressure to give the product.

The D,L-standard. The procedure for the L-standard was followed except that prior to the addition of the benzylamine, TEA (1.0 equiv) was added to the UNCA solution in toluene for 15 min in order to racemize the UNCA.

Chiral HPLC analysis. Solutions of L-and D,L-standards in 50:50 hexanes:IPA were prepared at the concentration of 1 mg/mL. Aliquots of 5-10 μL were injected to the chiral HPLC. The amino acids studied, the mobile phase used and the retention times for L and D-benzyl amides are presented in Figure 1.

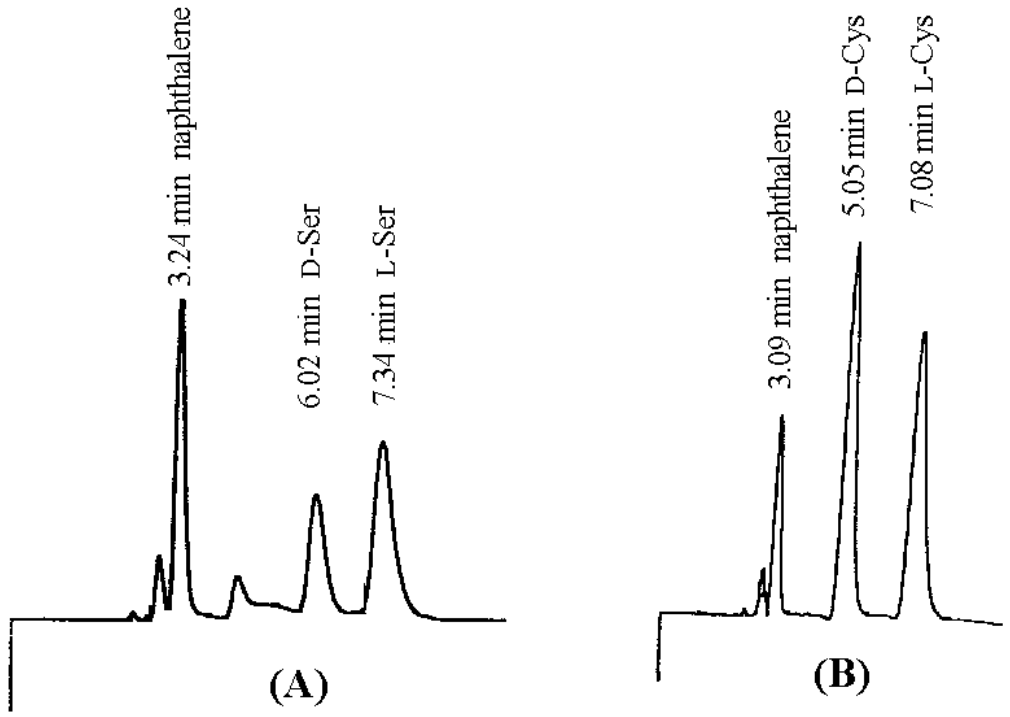


Figure 1. Chiral HPLC analysis of (A) Boc-L-Ser(OBzl)-NHBzl and Boc-D-Ser(OBzl)-NHBzl, mobile phase: hexane:IPA = 90:10. (B) Boc-L-Cys(4MB)-NHBzl and Boc-D-Cys(4MB)-NHBzl, mobile phase: hexane:IPA = 92:8.

The general protocol for the measurement of racemization (with yields).

Calibration. A standard solution containing Boc-DL-Ser(OBzl)-NHBzl (127 mg, 0.33 mmol) and naphthalene (1.04 mg) in DCM (10 mL) was mixed in a 100 mL volumetric flask. The solution was diluted with 50:50 hexanes : IPA to the mark and 5 injections (10 μL each) were analyzed by chiral HPLC using the conditions described above. The peak areas for each of the five runs were averaged and a ratio of peak area to concentration was established for each component of the mixture.

An illustrative procedure for activation *in situ.* To Boc-Ser(OBzl)-OH (97 mg, 0.33 mmol), naphthalene (1.04 mg) and DEPBT (98.6 mg, 0.33 mmol) in DCM (1.0 mL) at 20 °C was added DIEA (115 μL, 0.66 mmol). The resulting solution was stirred for 60 min (the delay time) and benzylamine (50 μL, 0.46 mmol) was added. After a further 5 min of stirring, the reaction mixture was diluted with DCM (9 mL) and washed with 5% $NaHSO_4$ (3×1 mL), brine (3×1 mL) and 10% Na_2CO_3 (3×1 mL) and dried over Na_2SO_4. To 1 mL of this solution was added 9 mL of 50:50 hexanes:IPA and a 10 μL aliquot was analyzed by chiral HPLC. The naphthalene peak from the analysis was divided by the standard naphthalene peak area to obtain the correction factor. The peak areas for the benzyl amide products were multiplied by this correction factor prior to calculating the concentration from the calibration values.

An illustrative procedure for pre-activated intermediates. To a solution of Boc-Cys(4MB)-OOBt (132 mg, 0.33 mmol) in THF (1 mL) containing naphthalene (1.04 mg) was added DIEA (57.5 μL, 0.33 mmol). After stirring for 30 min at 20 °C, benzylamine (50 μL, 0.46 mmol) was added. After a further 5 min of stirring, the reaction mixture was diluted with DCM (9 mL) and washed with 5% $NaHSO_4$ (3×1 mL), brine (3×1 mL) and 10% Na_2CO_3 (3×1 mL) and dried over Na_2SO_4. To 1 mL of this solution was added 9 mL of 50:50 hexanes:IPA and a 10 μl aliqot was analyzed by chiral HPLC for yield and optical purity.

Boc-Cys(4MB)-OAt To a solution of Boc-Cys(4MB)-OH (3.25 g, 10 mmol) and HOAt (1.36 g, 10 mmol) in THF (30 mL) at rt was added DCC (2.06 g, 10 mmol). A white precipitate formed immediately. After being stirred for 30 min, the mixture was filtered

and the filtrate was taken to dryness to give a colorless oil. The oil was triturated with ether (50 mL) and a solid white mass formed. The solid was dissolved in EtOAc (50 mL), filtered to remove insoluble material and diluted with petroleum ether (450 mL). After standing at room temperature for 30 min, the crystals formed were collected by filtration, washed with petroleum ether and dried under vacuum to give the product as a white powder (3.0 g, 68%). mp: 90-91 °C. ^{1}H NMR (360 MHz, $CDCl_3$): δ 1.47 (s, 9H); 2.31 (s, 2H); 3.10 (d, 2H, *J* = 5 Hz); 3.86 (s, 3H); 5.05 (m, 1H); 5.36 (d, 1H, *J* = 7.9 Hz); 7.11 (d, 2H, *J* = 7.6 Hz); 7.25 (d, 2H, *J* = 7.9 Hz); 7.42 (dd, 1H, *J* = 8.3, 4.3 Hz); 8.40 (d, 1H, *J* = 8.6 Hz); 8.69 (d, 1H, *J* = 4.3 Hz). HR-MS (FAB): calcd.: 576.0682 $(M + Cs)^+$; found 576.0695, Δ = 2.3 ppm .

Boc-Cys(4MB)-OOBt To a solution of Boc-Cys(4MB)-OH (3.25 g, 10 mmol) and HOOBt (1.63 g, 10 mmol) in THF (30 mL) at rt was added DCC (2.06 g, 10 mmol). A white precipitate formed immediately. After being stirred for 2 h, the mixture was filtered and the filtrate was taken to dryness to give a yellow oil. The oil was dissolved in ethyl ether (25 mL) and petroleum ether (100 mL) was added. After standing at rt for overnight, the crystals formed were collected by filtration, washed with petroleum ether and dried under vacuum to give the product as a white powder (3.8 g, 80%). mp: 96-97.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.45 (s, 9H); 2.31 (s, 2H); 3.10 (m, 2H); 3.86 (s, 3H); 4.97 (m, 1H); 5.31 (d, 1H, *J* = 10.0 Hz); 7.11 (d, 2H, *J* = 8.0 Hz); 7.25 (d, 2H, *J* = 7.9 Hz); 7.83 (m, 1H); 8.01 (m, 1H); 8.22 (m, 1H); 8.35 (m, 1H). FAB-MS *m/z*: 471 $(M + H)^+$, 493 $(M + Na)^+$. Anal. Calc. For C, 58.70; H, 5.57; N, 11.91; Found: C, 58.56; H, 5.78; N, 11.84.

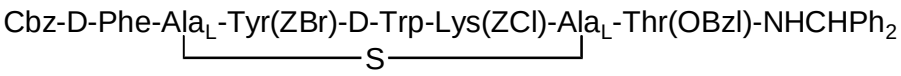
General procedure for peptide synthesis using DEPBT as the coupling reagent

To a solution of equal molar *N*-protected amino acids, amino acid ester and DEPBT in DMF (or CH_2Cl_2, THF), two equivalents of TEA was added. The reaction mixture was stirred at room temperature for 2-4 h (for peptide cyclizations, 24-48 h was used). Saturated NaCl solution was added. The peptide was extracted with EtOAc (3×10 ml). The combined organic layer was washed with 1N HCl, water, 5% Na_2CO_3, brine and dried over $MgSO_4$. The solvent was removed under reduced pressure to give the crude peptide, which was then recrystallized from a suitable solvent.

Cbz-Ala-Phe-OMe Yield: 94%; FAB-MS *m/z*: 385 $(M + H)^+$; mp: 101-102 ºC; $[\alpha]_D$: -11.5 (c = 1, EtOH).

Boc-Ile-Tyr-OMe Yield: 91%; FAB-MS *m/z*: 409 $(M + H)^+$; mp: 144-146 ºC; $[\alpha]_D$: -17 (c = 1, EtOH).

Boc-Trp-Lys(Cbz)-Gly-Gly-OMe Yield: 82%; mp: 150-151 ºC; $[\alpha]_D$: +28.7 (c = 1, MeOH); Anal. Calc. For C, 59.99; H, 6.61; N, 12.33; Found: C, 60.49; H, 6.94; N, 11.92.



Yield: 70%. R_f = 0.4 ($CHCl_3$:MeOH:HOAc = 100:5:1). Since this compound has very bad solubility in all common solvents, it was deprotected by HF to yield **compound 1**, which was characterized by NMR and HR-MS. Electrospray MS *m/z* 915 $(M + H)^+$, 937 $(M + Na)^+$. FT-MALDI-MS *m/z* expected 915.4187 $(M + H)^+$, found 915.4189, Δ = 0.2 ppm. The NMR assignments of **compound 1** are shown in Table 1.

Table 1. The ^{1}H chemical shifts of **compound 1**

Residue	(δ in ppm)	**Compound 1**
D-Phe[1]	α	4.21
	β	3.01, 2.90
	others	7.30, 7.25, 7.12
Ala_L[2]	NH	8.55
	α	4.59
	β	2.75, 2.52
Tyr[3]	NH	8.50
	α	4.69
	β	2.65, 2.50
	OH	9.18
	others	6.90, 6.58
D-Trp[4]	NH	8.61
	α	4.3
	β	3.07, 2.81
	others	10.80, 7.17
		7.54, 6.97
		7.05, 7.30
Lys[5]	NH	8.32
	α	4.1
	β	1.56, 1.32
	γ, δ	0.96, 1.38
	ε	2.65
Ala_L[6]	NH	7.99
	α	4.3
	β	2.72, 2.66
Thr[7]	NH	7.56
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	OH	4.83

X-ray diffraction analysis of DEPBT

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C6A 0.031(3) 0.029(4) 0.032(3) -0.007(3) 0.005(3) -0.002(3)
C7A 0.041(3) 0.031(3) 0.032(3) -0.005(2) 0.011(3) -0.001(3)
O1B 0.036(3) 0.044(3) 0.068(4) 0.019(3) 0.006(2) -0.006(2)
N1B 0.037(3) 0.040(3) 0.035(2) 0.009(2) 0.009(2) -0.002(2)
N2B 0.036(3) 0.035(3) 0.033(3) 0.009(3) 0.008(2) 0.003(2)
N3B 0.031(3) 0.053(3) 0.029(3) 0.008(3) 0.008(2) -0.001(3)
C1B 0.030(4) 0.025(3) 0.030(3) -0.006(2) 0.004(3) -0.002(3)
C2B 0.028(4) 0.040(4) 0.042(4) -0.005(3) 0.006(4) -0.004(4)
C3B 0.033(4) 0.042(6) 0.064(7) -0.014(4) 0.004(4) 0.001(4)
C4B 0.035(4) 0.047(6) 0.054(5) -0.004(4) 0.000(4) 0.008(4)
C5B 0.043(5) 0.040(4) 0.034(4) 0.002(3) 0.000(3) 0.001(3)
C6B 0.028(3) 0.028(3) 0.028(4) -0.004(3) 0.007(2) -0.001(3)
C7B 0.034(3) 0.033(3) 0.036(3) -0.001(2) 0.004(2) 0.000(2)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters are
only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
;

loop_
 _geom_bond_atom_site_label_1
 _geom_bond_atom_site_label_2
 _geom_bond_distance
 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
P1 O5 1.455(2) . ?
P1 O4 1.549(2) . ?
P1 O3 1.552(2) . ?
P1 O2 1.635(2) . ?
O2 N3A 1.360(3) . ?
```

```
O2 N3B 1.427(3) . ?
O3 C4 1.433(4) . ?
O4 C2 1.475(3) . ?
C1 C2 1.499(4) . ?
C3 C4 1.458(5) . ?
O1A C7A 1.21 . ?
N1A N2A 1.28 . ?
N1A C1A 1.40 . ?
N2A N3A 1.37 . ?
N3A C7A 1.41 . ?
C1A C2A 1.40 . ?
C1A C6A 1.40 . ?
C2A C3A 1.37 . ?
C3A C4A 1.39 . ?
C4A C5A 1.37 . ?
C5A C6A 1.40 . ?
C6A C7A 1.45 . ?
O1B C7B 1.21 . ?
N1B N2B 1.28 . ?
N1B C1B 1.40 . ?
N2B N3B 1.37 . ?
N3B C7B 1.41 . ?
C1B C2B 1.40 . ?
C1B C6B 1.40 . ?
C2B C3B 1.37 . ?
C3B C4B 1.39 . ?
C4B C5B 1.37 . ?
C5B C6B 1.40 . ?
C6B C7B 1.45 . ?

loop_
 _geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
O5 P1 O4 118.98(12) . . ?
O5 P1 O3 119.33(13) . . ?
O4 P1 O3 98.74(12) . . ?
O5 P1 O2 104.80(12) . . ?
O4 P1 O2 107.02(12) . . ?
O3 P1 O2 107.10(12) . . ?
N3A O2 P1 117.4(2) . . ?
N3B O2 P1 123.4(2) . . ?
C4 O3 P1 122.7(2) . . ?
C2 O4 P1 121.6(2) . . ?
O4 C2 C1 106.7(2) . . ?
O3 C4 C3 110.8(3) . . ?
N2A N1A C1A 120.6 . . ?
N1A N2A N3A 117.7 . . ?
O2 N3A N2A 111.2(2) . . ?
O2 N3A C7A 117.2(2) . . ?
N2A N3A C7A 129.5 . . ?
C2A C1A N1A 117.7 . . ?
C2A C1A C6A 119.9 . . ?
```

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N1A C1A C6A 122.4 . . ?
C3A C2A C1A 119.7 . . ?
C2A C3A C4A 120.3 . . ?
C5A C4A C3A 121.3 . . ?
C4A C5A C6A 119.0 . . ?
C5A C6A C1A 119.7 . . ?
C5A C6A C7A 120.8 . . ?
C1A C6A C7A 119.5 . . ?
O1A C7A N3A 120.7 . . ?
O1A C7A C6A 129.2 . . ?
N3A C7A C6A 110.1 . . ?
N2B N1B C1B 120.6 . . ?
N1B N2B N3B 117.7 . . ?
N2B N3B C7B 129.5 . . ?
N2B N3B O2 113.0(2) . . ?
C7B N3B O2 117.4(2) . . ?
C2B C1B N1B 117.7 . . ?
C2B C1B C6B 119.9 . . ?
N1B C1B C6B 122.4 . . ?
C3B C2B C1B 119.8 . . ?
C2B C3B C4B 120.2 . . ?
C5B C4B C3B 121.3 . . ?
C4B C5B C6B 119.1 . . ?
C5B C6B C1B 119.7 . . ?
C5B C6B C7B 120.8 . . ?
C1B C6B C7B 119.5 . . ?
O1B C7B N3B 120.7 . . ?
O1B C7B C6B 129.2 . . ?
N3B C7B C6B 110.1 . . ?

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_refine_diff_density_min   -0.736
_refine_diff_density_rms    0.064

     Then comes the original report file
&N&9&9&_STRUCTURE& DETERMINATION& SUMMARY&/
&H&N&-Crystal Data&/&H&N&5Empirical Formula&9&4
C&V11&0 H&V14&0 N&V3&0 O&V5&0 P
&H&5Color; Habit&9&9
colorless plate
&H&5Crystal size (mm)&5&90.25 x 0.5 x 0.7
&H&5Crystal System&6&9&2Monoclinic
&H&5Space Group&6&9&5P2&V1&0/c
&H&5Unit Cell Dimensions&6&5&-a&/ =& 14.688(7) &GA&H
&9&9&9&9&-b&/ =& 11.808(5) &GA&H
&9&9&9&9&-c&/ =& 7.843(5) &GA&H
&9&9&9&9&-&Gb&/ =& 97.63(4)&^o&0&H
&5Volume&9&9&71348.2(11) &GA&^3&0&H
&5Z&9&9&9&34&H
&5Formula weight&8&8       299.2 &H
&5Density(calc.)&8&8   1.474 Mg/m&^3&0&H
&5Absorption Coefficient&8    0.227 mm&^-1&0&H
&5F(000)&7&9&9624 &H
&F&N&-Data Collection&/&H&N&5Diffractometer Used&2&9
Siemens R3m/V&H&5Radiation&4&9&9MoK&Ga (&Gl = 0.71073 &GA)&H
&5Temperature (K)&2&9&4  178&H
&5Monochromator&9&9Highly oriented graphite crystal&H
```

&52&Gq Range&5&9&8   3.0 to 55.0&^o&0&H
&5Scan Type&4&9&9Wyckoff&H
&5Scan& Speed&3&9&9Constant;   10.19&^o&0/min. in &Gw&H
&5Scan Range (&Gw)&6&9&1   0.60&^o&0 &H
&5Background Measurement&9Stationary crystal and stationary &N
&9&9&9&9counter at beginning and end of&N
&9&9&9&9scan, each for   0.5% of total&N
&9&9&9&9scan time&H
&5Standard Reflections&9&1   3 measured every   197 reflections&H
&5Index Ranges&9&9 -19 &G< h& &G< 18,   0 &G< k &G< 15&N
&9&9&9&9   0 &G< l &G< 10&H
&5Reflections Collected& &8   3327
&H&5Independent Reflections&6&1   3099 (R&Vint&0 =   1.33%)&H
&5Observed Reflections&2&8   2332 (F& &_>&/   4.0&Gs(F))&H
&5Absorption Correction&9&1N/A&H
&F&N&-Solution and Refinement&/&H
&N&5System Used&2&9&9Siemens SHELXTL PLUS (PC Version)&H
&5Solution&5&9&9Direct Methods&H
&5Refinement Method&5&9Full-Matrix Least-Squares&H
&5Quantity Minimized&4&8 &GSw(F&vo&0-F&vc&0)&^2&0&H
&5Absolute Structure&4&9N/A&H
&5Extinction Correction&2&8N/A&H
&5Hydrogen Atoms&9&8Riding model, fixed isotropic U&H
&5Weighting Scheme&7&8w&^-1&0 = &Gs&^2&0(F) +   0.0010F&^2&0&H
&5Number of Parameters Refined&2 229&H
&5Final R Indices (obs. data)&4R =   6.03 %, wR =   8.36 %&H
&5R Indices (all data)&7&4R =   7.82 %, wR =   8.76 %&H
&5Goodness-of-Fit&7&8   1.87&H
&5Largest and Mean &GD/&Gs&2&8   0.057,   0.006&H
&5Data-to-Parameter Ratio&7 10.2:1&H
&5Largest Difference Peak&7   0.80 e&GA&^-3&0&H
&5Largest Difference Hole&7   -0.73 e&GA&^-3&0&H&F
Table 1. Atomic coordinates (x10&^4&0) and equivalent isotropic&N
&9displacement coefficients (&GA&^2&0x10&^3&0)&J2&H
&9&3x&9&2y&9&2z&9&1U(eq)&N
&C

P(1)	3606(1)	479(1)	2165(1)	32(1)
O(2)	2838(1)	1201(2)	3040(3)	36(1)
O(3)	3357(2)	582(2)	187(3)	47(1)
O(4)	3382(1)	-790(2)	2367(3)	36(1)
O(5)	4485(1)	909(2)	2978(3)	42(1)
C(1)	3692(2)	-2611(3)	3628(4)	46(1)
C(2)	3597(2)	-1384(3)	4026(4)	39(1)
C(3)	3704(3)	990(3)	-2625(4)	49(1)
C(4)	3815(4)	1347(4)	-834(5)	75(2)
O(1A)	1570(2)	-189(4)	3997(5)	45(2)
N(1A)	988	2308	449	47(2)
N(2A)	1815	2095	1090	53(3)
N(3A)	1963	1201	2213	28(2)
C(1A)	260	1666	922	35(2)
C(2A)	-625	1924	139	46(3)
C(3A)	-1359	1310	551	47(4)
C(4A)	-1222	424	1725	47(4)
C(5A)	-358	151	2515	37(3)
C(6A)	398	775	2112	29(2)
C(7A)	1319	508	2905	35(2)
O(1B)	1698(3)	2420(4)	765(6)	49(2)

N(1B)	764	-202	3414	37(2)
N(2B)	1618	43	3577	34(2)
N(3B)	1876	976	2712	36(2)
C(1B)	124	446	2348	28(2)
C(2B)	-801	152	2263	36(3)
C(3B)	-1455	769	1247	45(4)
C(4B)	-1199	1695	324	46(3)
C(5B)	-294	2006	384	39(3)
C(6B)	381	1379	1410	26(2)
C(7B)	1342	1684	1520	33(2)

&E
&N* Equivalent isotropic U defined as one third of the&N
&2trace of the orthogonalized U&Vij&0 tensor
&F
Table 2. Bond lengths (&GA)&J2&N&N
&D

P(1)-O(2)	1.636 (2)
P(1)-O(3)	1.551 (2)
P(1)-O(4)	1.546 (2)
P(1)-O(5)	1.453 (2)
O(2)-N(3A)	1.361 (4)
O(2)-N(3B)	1.427 (4)
O(3)-C(4)	1.433 (5)
O(4)-C(2)	1.475 (4)
C(1)-C(2)	1.493 (5)
C(3)-C(4)	1.455 (5)

&E
&N&N
Table 3. Bond angles (&^o&0)&N&N
&D

O(2)-P(1)-O(3)	107.1(1)
O(2)-P(1)-O(4)	107.1(1)
O(3)-P(1)-O(4)	98.8(1)
O(2)-P(1)-O(5)	104.8(1)
O(3)-P(1)-O(5)	119.3(1)
O(4)-P(1)-O(5)	118.9(1)
P(1)-O(2)-N(3A)	117.4(2)
P(1)-O(2)-N(3B)	123.2(2)
N(3A)-O(2)-N(3B)	20.6(3)
P(1)-O(3)-C(4)	122.9(2)
P(1)-O(4)-C(2)	121.8(2)
O(4)-C(2)-C(1)	107.0(2)
O(3)-C(4)-C(3)	110.8(4)
O(2)-N(3A)-N(2A)	111.4(2)
O(2)-N(3A)-C(7A)	117.0(2)
O(2)-N(3B)-N(2B)	113.1(2)
O(2)-N(3B)-C(7B)	117.4(2)

&E
&J3
&N&N
Table 5. H-Atom coordinates (x10&^4&0) and isotropic&N
&9displacement coefficients (&GA&^2&0x10&^3&0)&J2&H
&9&3x&9&2y&9&2z&9&2U&N
&C

H(1A)	3837	-3031	4677	60
H(1B)	3124	-2881	3019	60
H(1C)	4174	-2711	2925	60

H(2A)	3116	-1269	4725	40
H(2B)	4162	-1100	4632	40
H(3A)	4018	1498	-3304	60
H(3B)	3943	238	-2709	60
H(3C)	3059	993	-3043	60
H(4A)	4459	1351	-409	40
H(4B)	3582	2101	-740	40
H(2A)	-715	2532	-677	50
H(3A)	-1970	1507	49	50
H(4A)	-1734	-33	1943	50
H(5A)	-273	-434	3371	50
H(2B)	-975	-485	2910	50
H(3B)	-2088	547	1151	50
H(4B)	-1665	2152	-318	50
H(5B)	-121	2620	-308	50

&E
&F
Table 4. Anisotropic displacement coefficients (&GA&^2&0x10&^3&0)&H
&9&4U&V11&0&7U&V22&0&7U&V33&0&7U&V12&0&7U&V13&0&7U&V23&0&J2&H
&C

P(1)	29(1)	39(1)	26(1)	0(1)	0(1)	2(1)
O(2)	30(1)	40(1)	36(1)	-1(1)	-1(1)	-7(1)
O(3)	45(1)	66(2)	27(1)	-4(1)	1(1)	7(1)
O(4)	44(1)	34(1)	27(1)	2(1)	-3(1)	1(1)
O(5)	30(1)	56(1)	40(1)	-5(1)	-1(1)	2(1)
C(1)	56(2)	42(2)	40(2)	3(2)	7(2)	7(2)
C(2)	45(2)	42(2)	28(2)	5(1)	1(1)	5(1)
C(3)	62(2)	50(2)	38(2)	12(2)	16(2)	8(2)
C(4)	131(4)	54(2)	36(2)	-40(3)	-2(2)	13(2)
O(1A)	42(3)	58(4)	34(3)	0(3)	7(2)	16(3)
N(1A)	39(3)	41(3)	59(4)	3(3)	2(3)	14(3)
N(2A)	46(4)	64(5)	44(4)	-7(4)	-9(3)	27(4)
N(3A)	20(3)	60(4)	6(2)	1(2)	4(2)	-10(3)
C(1A)	44(4)	31(4)	28(4)	-4(3)	2(3)	1(3)
C(2A)	54(6)	45(5)	38(4)	7(5)	0(5)	-3(4)
C(3A)	30(4)	64(9)	45(6)	7(5)	-7(4)	-20(5)
C(4A)	32(5)	61(8)	51(7)	-11(5)	15(5)	-16(6)
C(5A)	29(5)	46(4)	38(4)	-4(4)	9(4)	-5(3)
C(6A)	28(4)	29(4)	30(4)	-2(3)	4(3)	-6(3)
C(7A)	42(4)	31(3)	34(3)	0(3)	12(3)	-6(3)
O(1B)	36(3)	43(3)	66(4)	-6(2)	5(3)	17(3)
N(1B)	35(3)	38(3)	38(3)	-3(2)	9(2)	11(2)
N(2B)	32(4)	34(4)	35(4)	2(3)	5(3)	10(3)
N(3B)	31(3)	48(4)	31(4)	-2(3)	7(2)	8(3)
C(1B)	28(4)	27(4)	28(3)	-3(3)	5(3)	-6(3)
C(2B)	26(5)	40(4)	43(5)	-4(4)	7(4)	-8(3)
C(3B)	31(4)	48(7)	58(8)	2(4)	7(4)	-16(5)
C(4B)	39(5)	43(6)	56(5)	10(4)	7(5)	-1(4)
C(5B)	40(5)	39(4)	37(5)	1(3)	2(4)	6(3)
C(6B)	28(3)	24(4)	26(4)	-2(3)	7(3)	-3(3)
C(7B)	32(3)	33(3)	34(3)	2(3)	4(3)	-1(3)

&E
&N&J3The anisotropic displacement exponent takes the form:&N
-2&Gp&^2&0(h&^2&0a*&^2&0U&v11&0 + ... + 2hka*b*U&v12&0)

Finally a report file that comes with the CIF file
Table 1. Crystal data and structure refinement for PON&:

&N
&HEmpirical formula&9&6 C&v11&0H&v14&0N&v3&0O&v5&0P
&HFormula weight&9&9 299.22
&HTemperature&3&9&9 178(2) K
&HWavelength&4&9&9 0.71073 &GA
&HCrystal system&9&9 Monoclinic
&HSpace group&6&9&6 P2&v1&0/c
&HUnit cell dimensions&6&6
&Ia&: =& 14.688(7) &GA&2 alpha =& 90&^o&0
&N&9&9&9&6&Ib&: =& 11.808(5) &GA&2 beta =& 97.63(4)&^o&0
&N&9&9&9&6&Ic&: =& 7.843(5) &GA&2 gamma =& 90&^o&0
&HVolume, Z, F(000)&6&9 1348.2(12) &GA&^3&0, 4, 624
&HDensity (calculated)&3&9 1.474 Mg/m&^3&0
&HAbsorption coefficient&9&1 0.227 mm&^-1&0
&HCrystal size&5&6&9 0.70 x 0.50 x 0.25 mm
&H&Gq range for data collection&5 2.22 to 27.49&^o&0
&HLimiting indices&9&7 -19 &G< &Ih&: &G< 18, 0 &G< &Ik&: &G<
15, 0 &G< &Il&: &G< 10
&HReflections collected&2&9 3327, 2395 observed [I>2&Gs(I)]
&HIndependent reflections&9 3099 (R&Vint&0 = 0.0145)
&HRefinement method&6&9 Full-matrix least-squares on F&^2&0
&HData / restraints / parameters&2 3098 / 0 / 229
&HGoodness-of-fit on F&^2&0&9&2 1.051
&HFinal R indices [I>2&Gs(I)]&8R1 = 0.0605, wR2 = 0.1529
&HR indices (all data)&7&6R1 = 0.0791, wR2 = 0.1693
&HLargest diff. peak and hole&5 0.772 and -0.736 e&GA&^-3&0
&HScan speed, range, type&9 10&^o&0/minute, 0.6&^o&0, Wyckoff
&HBackground range, % time&8 0.6&^o&0, 25% each side
&F
&W64
Table 2. Atomic coordinates [x 10&^4&0] and equivalent isotropic
displacement parameters [&GA&^2&0 x 10&^3&0] for PON U(eq) is defined
as
one third of the trace of the orthogonalized &IU&vij&0&: tensor.&N
&C

&E
&J2
&C

	x	y	z	U(eq)	occupancy
&E					
&C					
P(1)	3606(1)	479(1)	2165(1)	33(1)	
O(2)	2838(1)	1201(2)	3038(2)	37(1)	
O(3)	3356(2)	581(2)	185(3)	48(1)	
O(4)	3380(1)	-791(2)	2367(2)	37(1)	
O(5)	4486(1)	911(2)	2979(3)	43(1)	
C(1)	3691(2)	-2615(3)	3626(4)	47(1)	
C(2)	3599(2)	-1382(3)	4029(4)	39(1)	
C(3)	3704(2)	990(3)	-2628(4)	49(1)	
C(4)	3813(4)	1349(4)	-834(5)	75(1)	
O(1A)	1568(2)	-191(3)	3997(5)	45(2)	

N(1A)	989(2)	2307(3)	448(5)	48(1)	
N(2A)	1816(2)	2092(3)	1089(5)	52(2)	
N(3A)	1963(2)	1199(3)	2212(4)	29(1)	
C(1A)	261(2)	1666(3)	922(4)	37(2)	0.5
C(2A)	-624(2)	1925(4)	140(6)	46(2)	0.5
C(3A)	-1359(2)	1314(5)	554(7)	50(3)	0.5
C(4A)	-1223(2)	429(4)	1728(7)	46(3)	0.5
C(5A)	-359(2)	153(3)	2517(5)	38(2)	0.5
C(6A)	397(2)	775(2)	2113(3)	31(2)	0.5
C(7A)	1318(2)	507(3)	2905(3)	34(1)	0.5
O(1B)	1696(2)	2423(3)	765(5)	50(2)	0.5
N(1B)	763(2)	-200(3)	3415(4)	37(1)	0.5
N(2B)	1618(2)	45(3)	3577(5)	34(1)	0.5
N(3B)	1876(2)	978(3)	2712(4)	38(2)	0.5
C(1B)	123(2)	448(2)	2349(4)	29(2)	0.5
C(2B)	-802(2)	153(3)	2264(6)	37(2)	0.5
C(3B)	-1456(2)	770(4)	1248(7)	46(3)	0.5
C(4B)	-1200(2)	1696(4)	325(7)	46(2)	0.5
C(5B)	-295(2)	2007(3)	385(6)	39(2)	0.5
C(6B)	380(2)	1381(2)	1411(4)	28(2)	0.5
C(7B)	1341(2)	1686(3)	1520(4)	34(1)	0.5

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&E
&J2
&F
&W76
Table 3. Bond lengths [&GA] and angles [&^o&0] for PON&H
&C

_____

&E
&D

P(1)-O(5)	1.455(2)
P(1)-O(4)	1.549(2)
P(1)-O(3)	1.552(2)
P(1)-O(2)	1.635(2)
O(2)-N(3A)	1.360(3)
O(2)-N(3B)	1.427(3)
O(3)-C(4)	1.433(4)
O(4)-C(2)	1.475(3)
C(1)-C(2)	1.499(4)
C(3)-C(4)	1.458(5)
O(1A)-C(7A)	1.21
N(1A)-N(2A)	1.28
N(1A)-C(1A)	1.40
N(2A)-N(3A)	1.37
N(3A)-C(7A)	1.41
C(1A)-C(2A)	1.40
C(1A)-C(6A)	1.40
C(2A)-C(3A)	1.37
C(3A)-C(4A)	1.39
C(4A)-C(5A)	1.37
C(5A)-C(6A)	1.40
C(6A)-C(7A)	1.45
O(1B)-C(7B)	1.21
N(1B)-N(2B)	1.28

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N(1B)-C(1B)          1.40
N(2B)-N(3B)          1.37
N(3B)-C(7B)          1.41
C(1B)-C(2B)          1.40
C(1B)-C(6B)          1.40
C(2B)-C(3B)          1.37
C(3B)-C(4B)          1.39
C(4B)-C(5B)          1.37
C(5B)-C(6B)          1.40
C(6B)-C(7B)          1.45
&E
&D
O(5)-P(1)-O(4)           118.98(12)
O(5)-P(1)-O(3)           119.33(13)
O(4)-P(1)-O(3)            98.74(12)
O(5)-P(1)-O(2)           104.80(12)
O(4)-P(1)-O(2)           107.02(12)
O(3)-P(1)-O(2)           107.10(12)
N(3A)-O(2)-P(1)          117.4(2)
N(3B)-O(2)-P(1)          123.4(2)
C(4)-O(3)-P(1)           122.7(2)
C(2)-O(4)-P(1)           121.6(2)
O(4)-C(2)-C(1)           106.7(2)
O(3)-C(4)-C(3)           110.8(3)
N(2A)-N(1A)-C(1A)        120.6
N(1A)-N(2A)-N(3A)        117.7
O(2)-N(3A)-N(2A)         111.2(2)
O(2)-N(3A)-C(7A)         117.2(2)
N(2A)-N(3A)-C(7A)        129.5
C(2A)-C(1A)-N(1A)        117.7
C(2A)-C(1A)-C(6A)        119.9
N(1A)-C(1A)-C(6A)        122.4
C(3A)-C(2A)-C(1A)        119.7
C(2A)-C(3A)-C(4A)        120.3
C(5A)-C(4A)-C(3A)        121.3
C(4A)-C(5A)-C(6A)        119.0
C(5A)-C(6A)-C(1A)        119.7
C(5A)-C(6A)-C(7A)        120.8
C(1A)-C(6A)-C(7A)        119.5
O(1A)-C(7A)-N(3A)        120.7
O(1A)-C(7A)-C(6A)        129.2
N(3A)-C(7A)-C(6A)        110.1
N(2B)-N(1B)-C(1B)        120.6
N(1B)-N(2B)-N(3B)        117.7
N(2B)-N(3B)-C(7B)        129.5
N(2B)-N(3B)-O(2)         113.0(2)
C(7B)-N(3B)-O(2)         117.4(2)
C(2B)-C(1B)-N(1B)        117.7
C(2B)-C(1B)-C(6B)        119.9
N(1B)-C(1B)-C(6B)        122.4
C(3B)-C(2B)-C(1B)        119.8
C(2B)-C(3B)-C(4B)        120.2
C(5B)-C(4B)-C(3B)        121.3
C(4B)-C(5B)-C(6B)        119.1
C(5B)-C(6B)-C(1B)        119.7
C(5B)-C(6B)-C(7B)        120.8
C(1B)-C(6B)-C(7B)        119.5
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O(1B)-C(7B)-N(3B) 120.7
O(1B)-C(7B)-C(6B) 129.2
N(3B)-C(7B)-C(6B) 110.1
&E
&J0
&C

&E
&J3
&HSymmetry transformations used to generate equivalent atoms:&N
&C
&E
&F
&W72
Table 4. Anisotropic displacement parameters [&GA&^2&0 x 10&^3&0] for PON&NThe anisotropic displacement factor exponent takes the form:&N -2&Gp&^2&0 [(ha&^*&0)&^2&0U&v11&0 + ... + 2hka&^*&0b&^*&0U&v12&0]&N
&C

&E
&J2
&C

	U11	U22	U33	U23	U13	U12
&E						
&C						
P(1)	30(1)	41(1)	26(1)	2(1)	0(1)	-1(1)
O(2)	31(1)	41(1)	37(1)	-7(1)	-2(1)	-1(1)
O(3)	47(1)	67(2)	28(1)	8(1)	0(1)	-5(1)
O(4)	45(1)	36(1)	28(1)	0(1)	-4(1)	2(1)
O(5)	31(1)	57(1)	40(1)	2(1)	0(1)	-5(1)
C(1)	57(2)	41(2)	42(2)	6(1)	9(1)	3(1)
C(2)	46(2)	42(2)	29(1)	4(1)	2(1)	6(1)
C(3)	60(2)	52(2)	37(2)	8(1)	14(1)	11(2)
C(4)	132(4)	53(2)	37(2)	11(2)	1(2)	-38(2)
O(1A)	43(3)	59(3)	35(3)	14(2)	7(2)	-1(2)
N(1A)	41(3)	43(3)	57(3)	15(3)	2(2)	2(2)
N(2A)	46(4)	58(5)	48(4)	26(3)	-7(3)	-7(3)
N(3A)	21(2)	59(4)	8(2)	-9(2)	4(2)	2(2)
C(1A)	40(4)	38(4)	31(4)	-1(3)	0(3)	-3(3)
C(2A)	52(6)	43(4)	40(4)	-6(3)	-6(4)	5(4)
C(3A)	28(3)	62(8)	56(6)	-25(5)	-5(4)	5(4)
C(4A)	35(5)	54(7)	51(6)	-11(5)	16(4)	-6(5)
C(5A)	32(4)	46(4)	38(3)	-4(3)	8(4)	-6(4)
C(6A)	31(3)	29(4)	32(3)	-7(3)	5(3)	-2(3)
C(7A)	41(3)	31(3)	32(3)	-5(2)	11(3)	-1(3)
O(1B)	36(3)	44(3)	68(4)	19(3)	6(2)	-6(2)
N(1B)	37(3)	40(3)	35(2)	9(2)	9(2)	-2(2)
N(2B)	36(3)	35(3)	33(3)	9(3)	8(2)	3(2)
N(3B)	31(3)	53(3)	29(3)	8(3)	8(2)	-1(3)
C(1B)	30(4)	25(3)	30(3)	-6(2)	4(3)	-2(3)
C(2B)	28(4)	40(4)	42(4)	-5(3)	6(4)	-4(4)
C(3B)	33(4)	42(6)	64(7)	-14(4)	4(4)	1(4)
C(4B)	35(4)	47(6)	54(5)	-4(4)	0(4)	8(4)
C(5B)	43(5)	40(4)	34(4)	2(3)	0(3)	1(3)

C(6B)	28(3)	28(3)	28(4)	-4(3)	7(2)	-1(3)
C(7B)	34(3)	33(3)	36(3)	-1(2)	4(2)	0(2)

&E
&J3
&F
&W64
Table 5. Hydrogen coordinates (x 10&^4&0) and isotropic displacement parameters (&GA&^2&0 x 10&^3&0) for PON&H
&C

&E
&J2
&C

	x	y	z	U(eq)
H(1A)	3835(2)	-3035(3)	4675(4)	60
H(1B)	3122(2)	-2884(3)	3017(4)	60
H(1C)	4173(2)	-2714(3)	2923(4)	60
H(2A)	3118(2)	-1267(3)	4728(4)	40
H(2B)	4163(2)	-1098(3)	4635(4)	40
H(3A)	4018(2)	1498(3)	-3307(4)	60
H(3B)	3943(2)	238(3)	-2712(4)	60
H(3C)	3059(2)	994(3)	-3045(4)	60
H(4A)	4457(4)	1352(4)	-408(5)	40
H(4B)	3579(4)	2103(4)	-739(5)	40
H(2A)	-714(3)	2534(4)	-677(7)	50
H(3A)	-1970(2)	1512(6)	52(9)	50
H(4A)	-1736(2)	-28(5)	1947(8)	50
H(5A)	-275(2)	-431(4)	3374(6)	50
H(2B)	-975(2)	-484(4)	2911(6)	50
H(3B)	-2089(2)	548(5)	1153(9)	50
H(4B)	-1666(2)	2153(5)	-317(9)	50
H(5B)	-122(3)	2621(4)	-307(7)	50

&E
&J3
&L120
&W72
&H&-Experimental&/
R1=(&GS&GB&GBF&Vo&0&GB-&GBF&Vc&0&GB&GB/&GS&GBF&Vo&0&GB),
& wR2=&GSw(F&Vo&0&^2&0-
F&Vc&0&^2&0)&^2&0/&GSw[(F&Vo&0&^2&0)&^2&0]&^&Gh&0,
& S=[&GSw(F&Vo&0&^2&0-F&Vc&0&^2&0)&^2&0/(n-p)]&^&Gh&0

&NRigid body heterorings with 50% occupancy were used to refine the disorder.

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