Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for

Five different pseudo-polymorphs of 4-aminoarylphosphate: Supramolecular aggregation in organophosphates

Kamna Sharma, Alok Ch. Kalita and Ramaswamy Murugavel*

Department of Chemistry, Indian Institute of Technology-Bombay, Powai, Mumbai-400076, India. Fax: +91 22 2576 7152; Tel: +91 22 2576 7163; E-mail: rmv@chem.iitb.ac.in

Contents

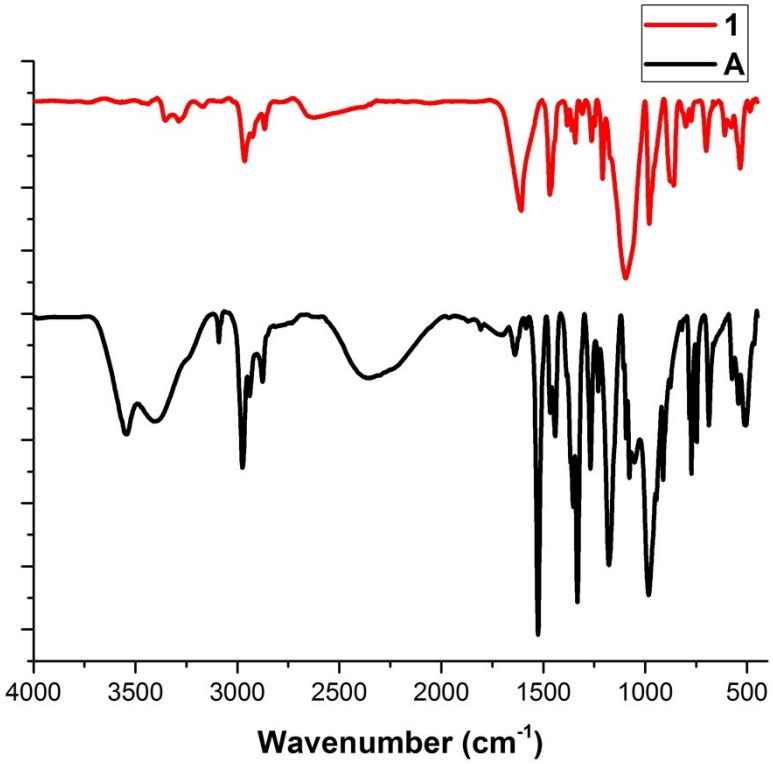

Fig. S1 FT-IR spectra of ndippH_2 **(A)** and **1** (as KBr disc)

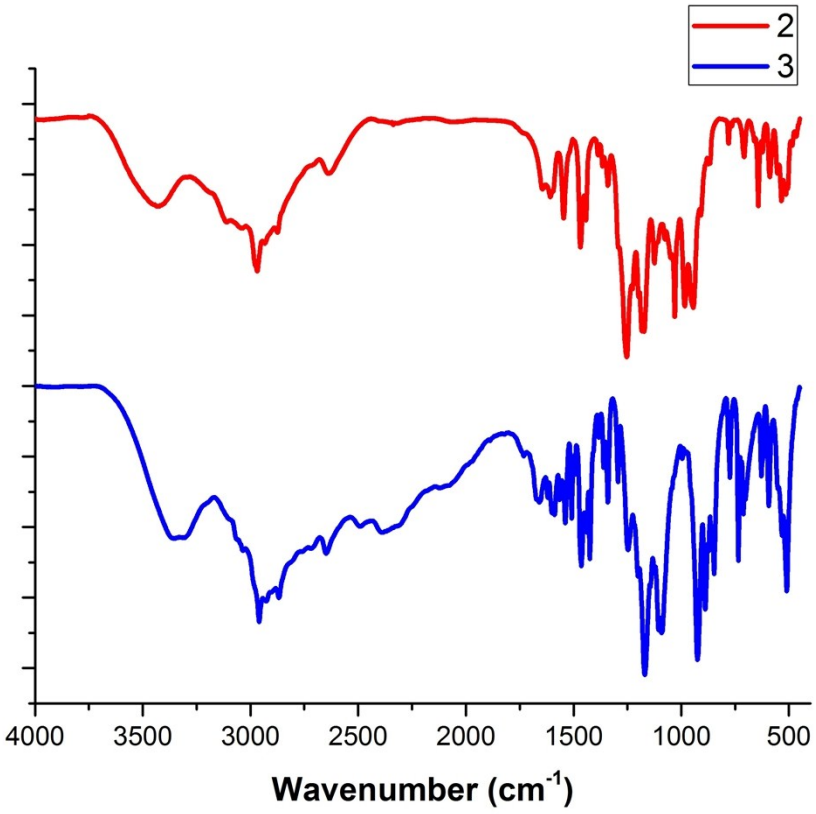

Fig. S2 FT-IR spectra of **2** and **3** (as KBr disc).

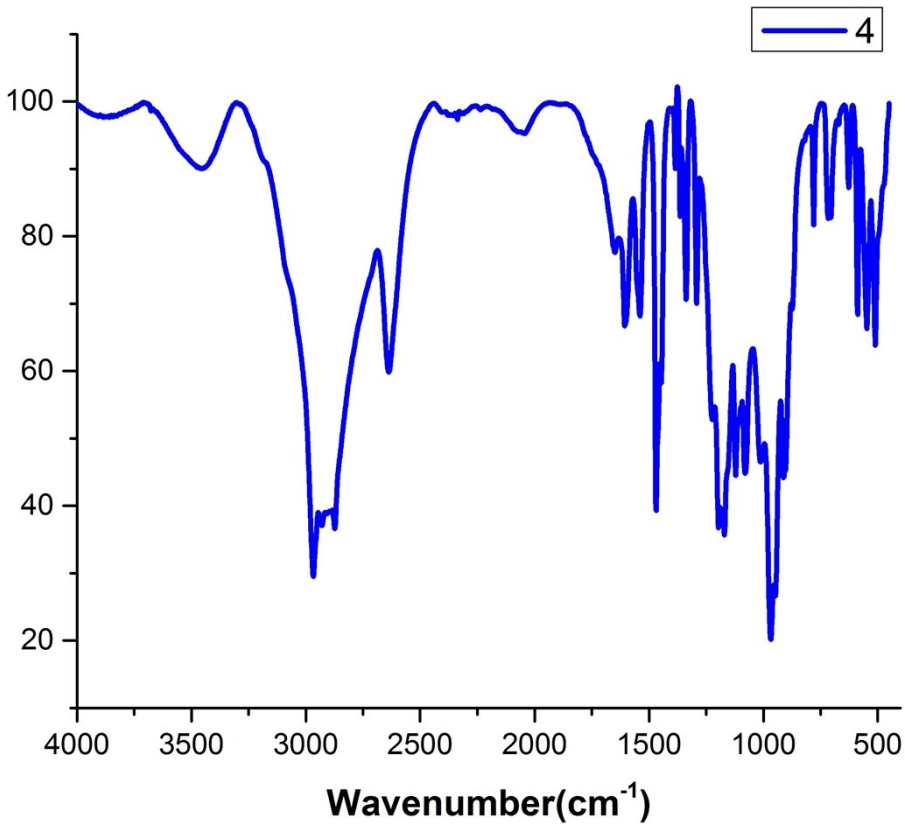

Fig. S3 FT-IR spectra of **4** (as KBr disc).

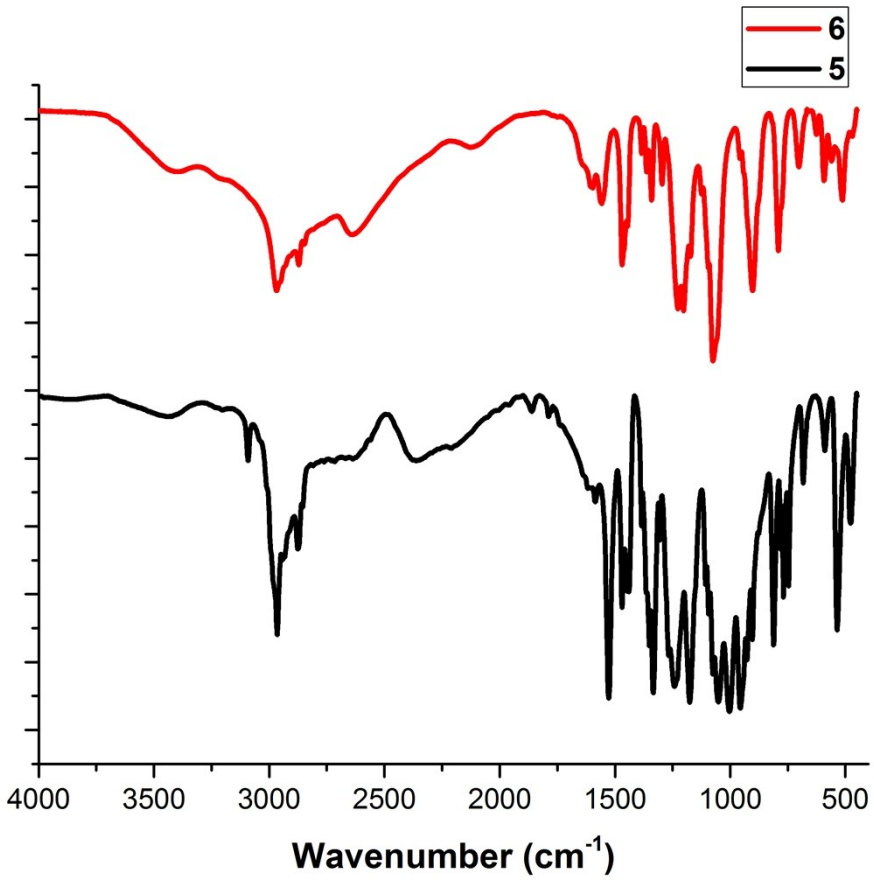

Fig. S4 FT-IR spectra of **5** and **6** (as KBr disc).

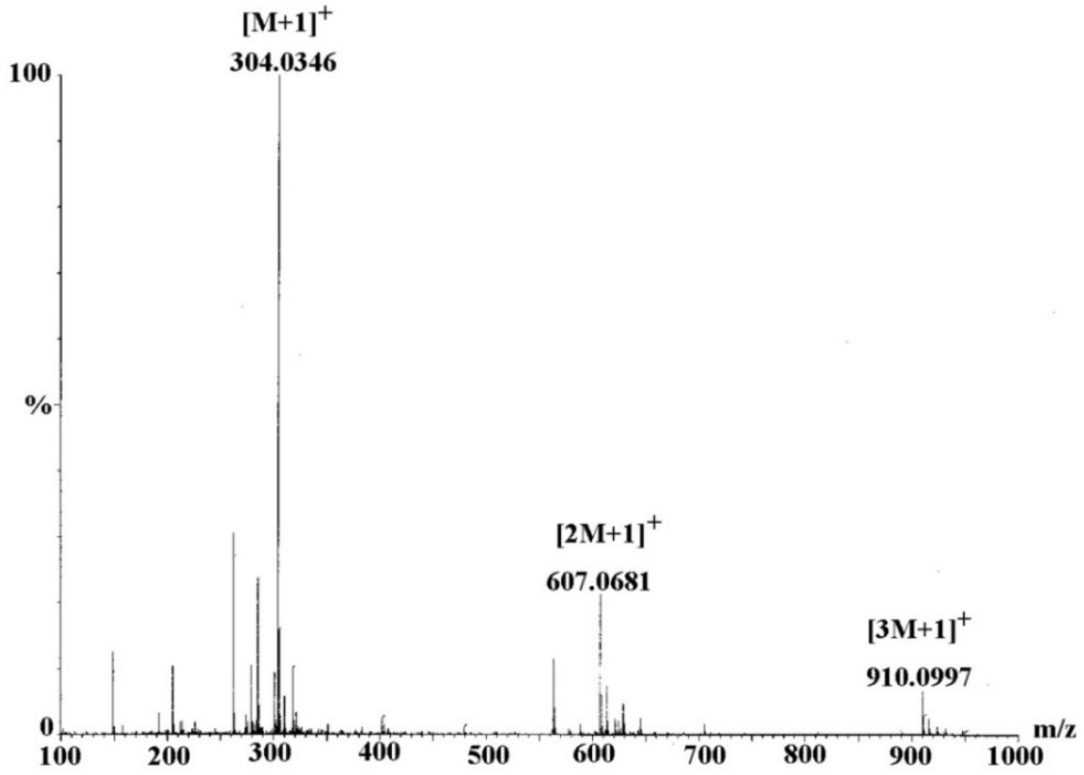

Fig. S5 ESI-MS of ndippH$_2$ (**A**) in positive ion mode in methanol.

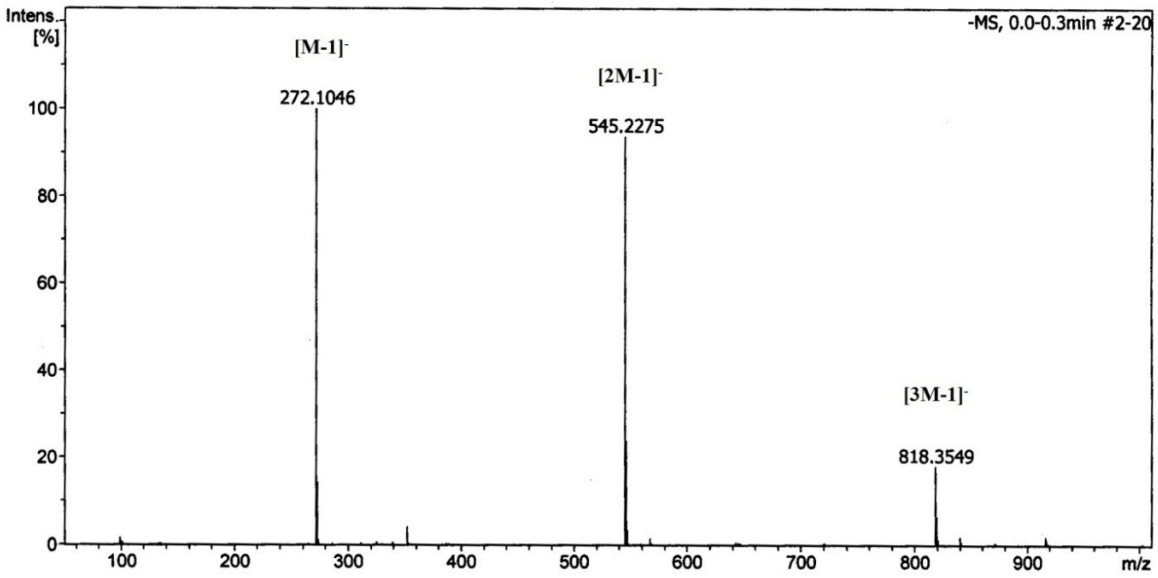

Fig. S6 ESI-MS of adippH$_2$ (**1**) in negative ion mode in methanol.

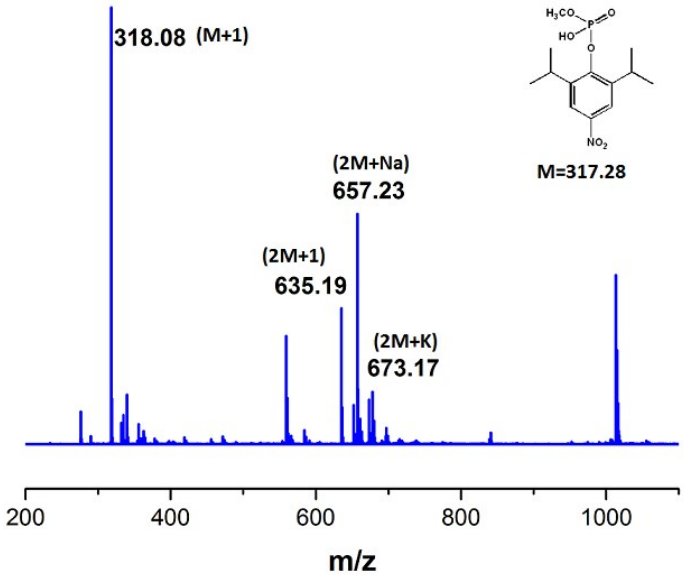

Fig. S7. ESI-MS of compound **5** in positive ion mode in methanol.

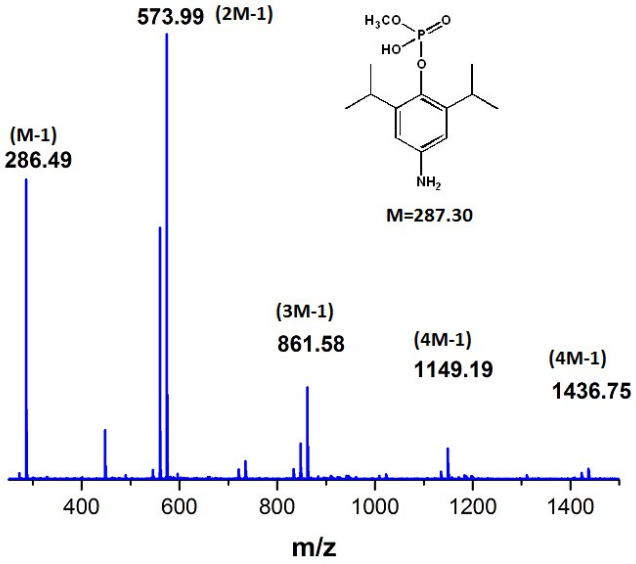

Fig. S8. ESI-MS of compound **6** in negative ion mode in methanol.

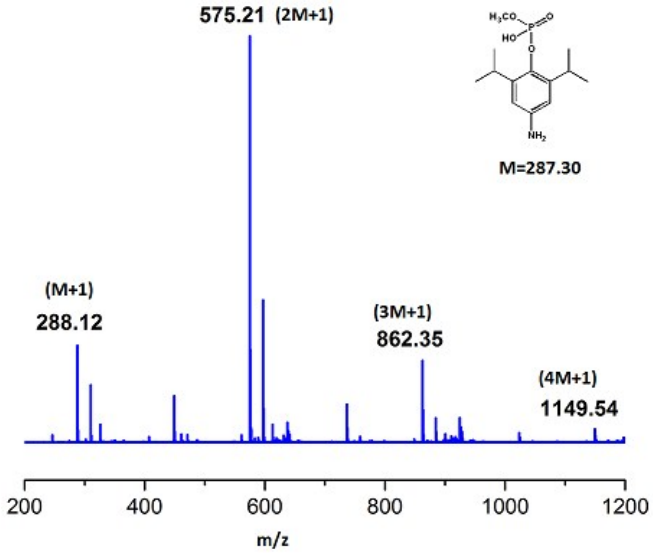

Fig. S9. ESI-MS of compound **6** in positive ion mode in methanol.

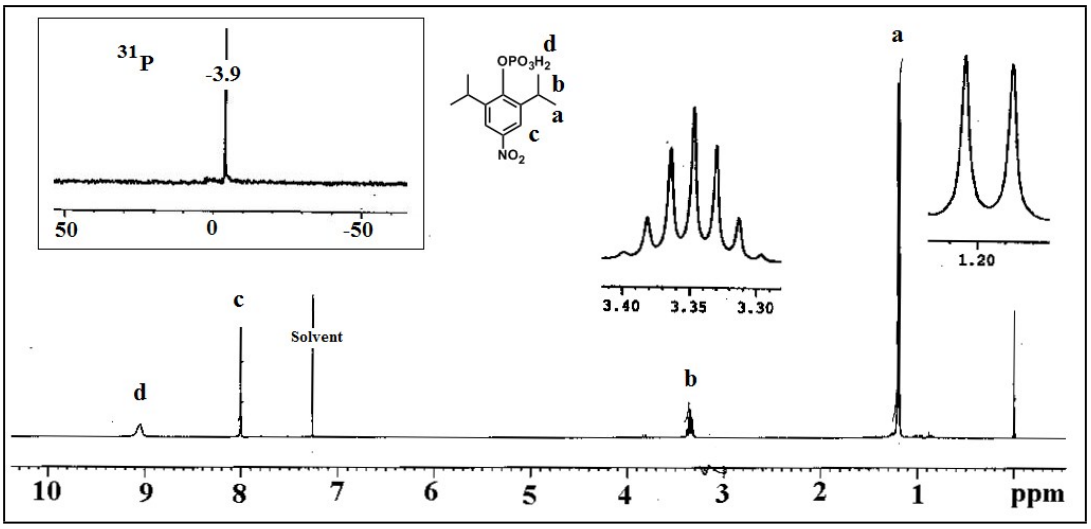

Fig. S10 ^{1}H, and ^{31}P NMR spectra of compound ndippH$_2$ (**A**) in CDCl$_3$.

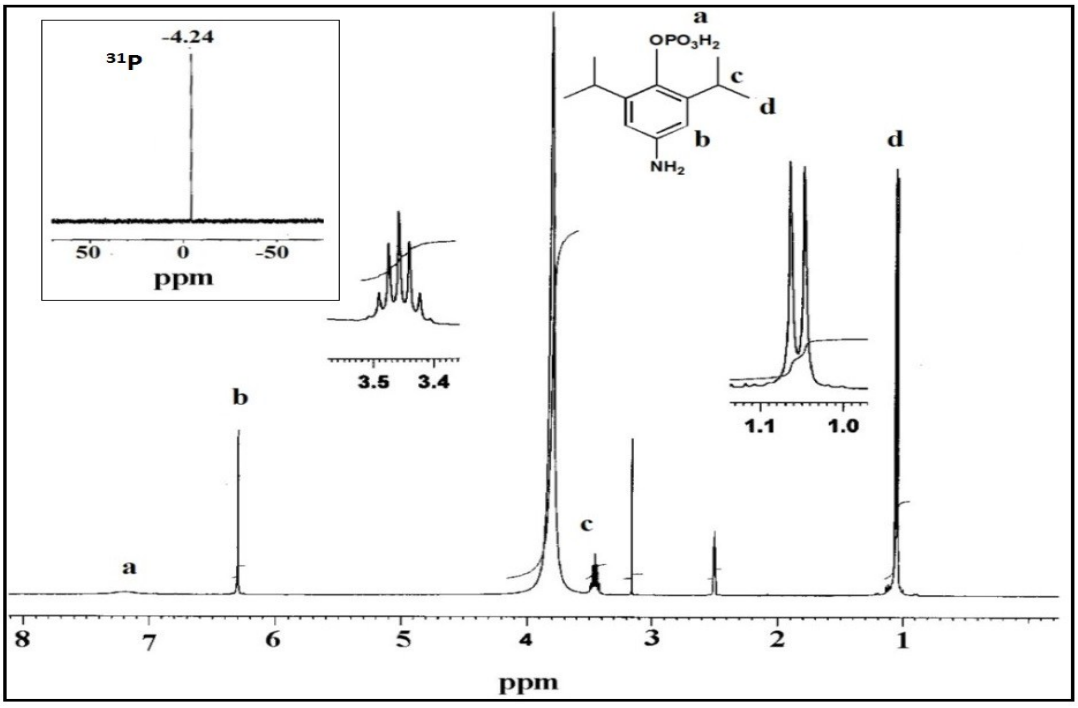

Fig. S11 ^{1}H, and ^{31}P NMR spectra of compound adippH$_2$ (**1**) in CD$_3$OD.

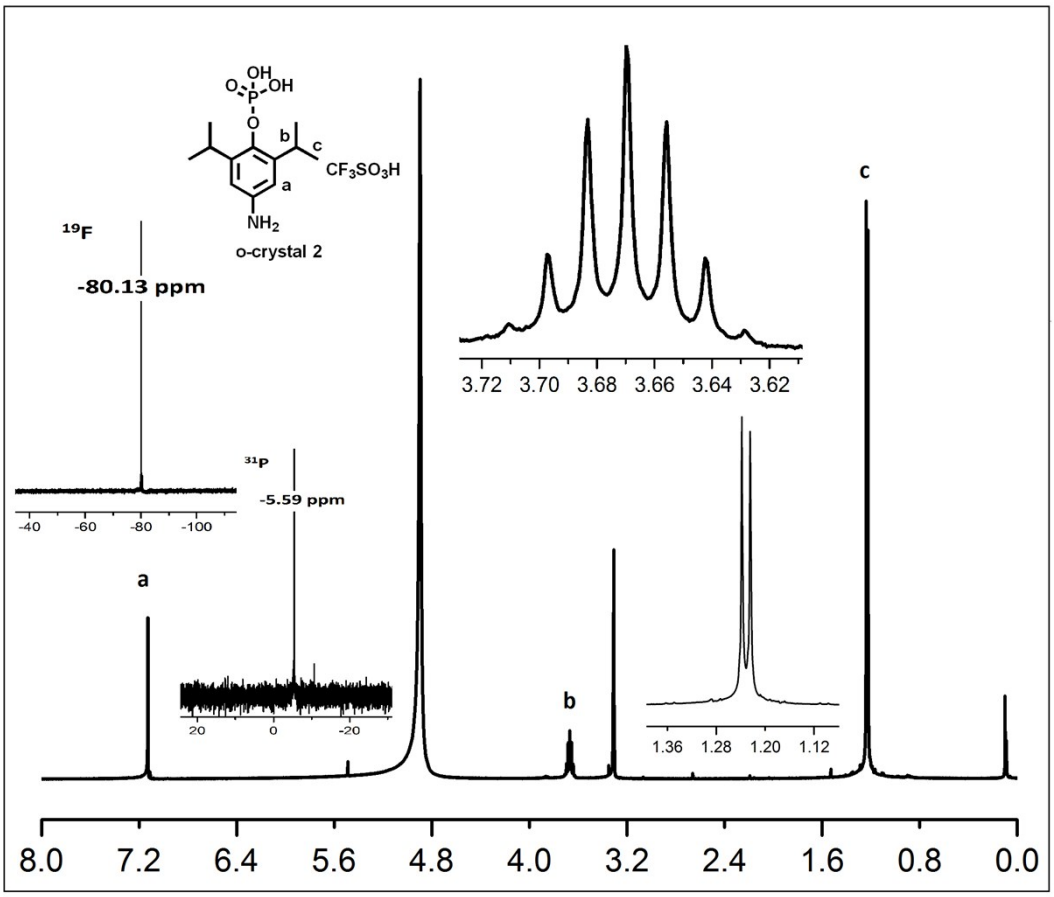

Fig. S12 ^{1}H, ^{19}F and ^{31}P NMR spectra of compound **2** in CD_3OD.

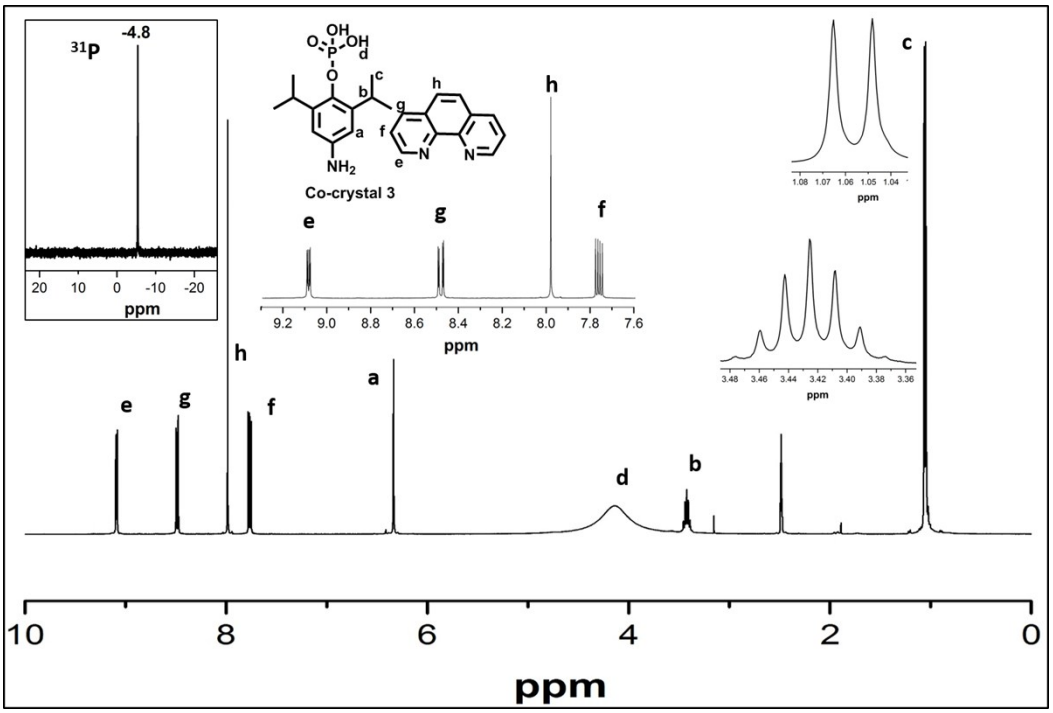

Fig. S13 ^{1}H, and ^{31}P NMR spectra of compound **3** in CD_3OD.

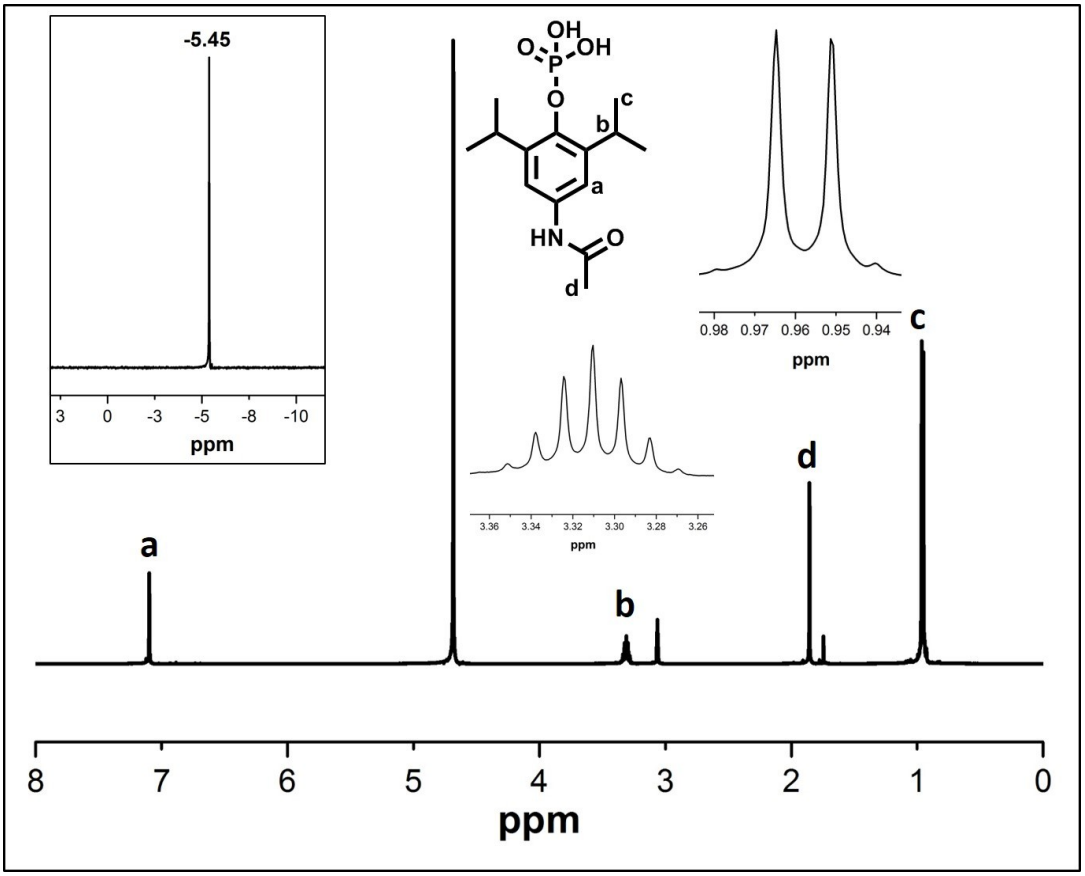

Fig. S14 ^{1}H, and ^{31}P NMR spectra of compound **4** in CD_3OD.

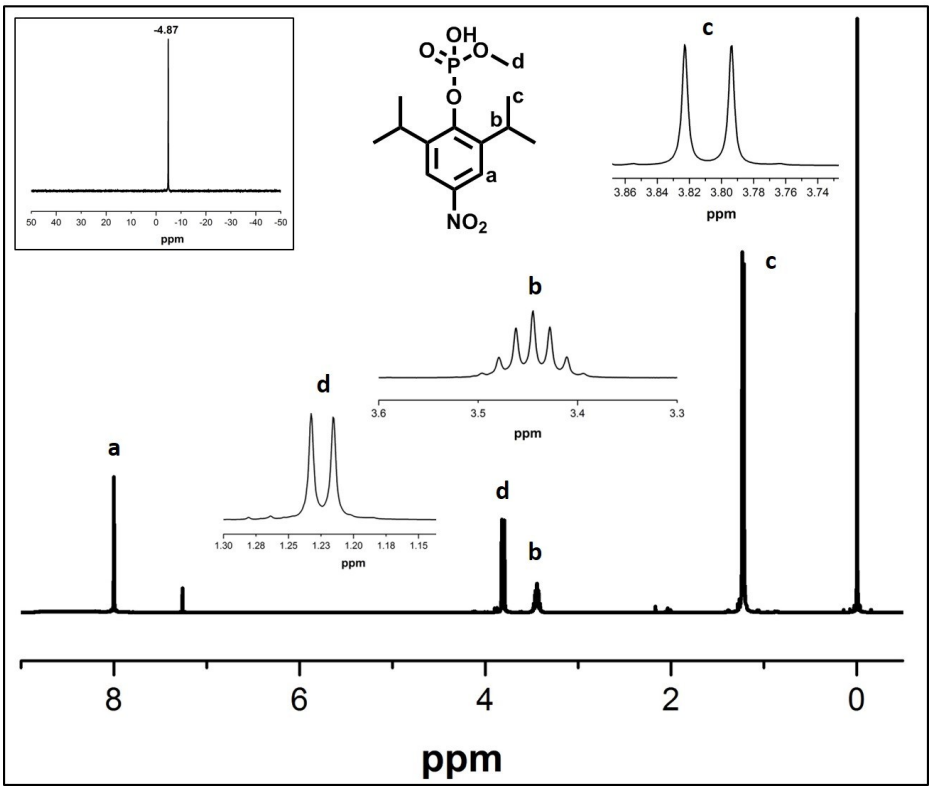

Fig. S15 ^{1}H, and ^{31}P NMR spectra of compound **5** in $CDCl_3$.

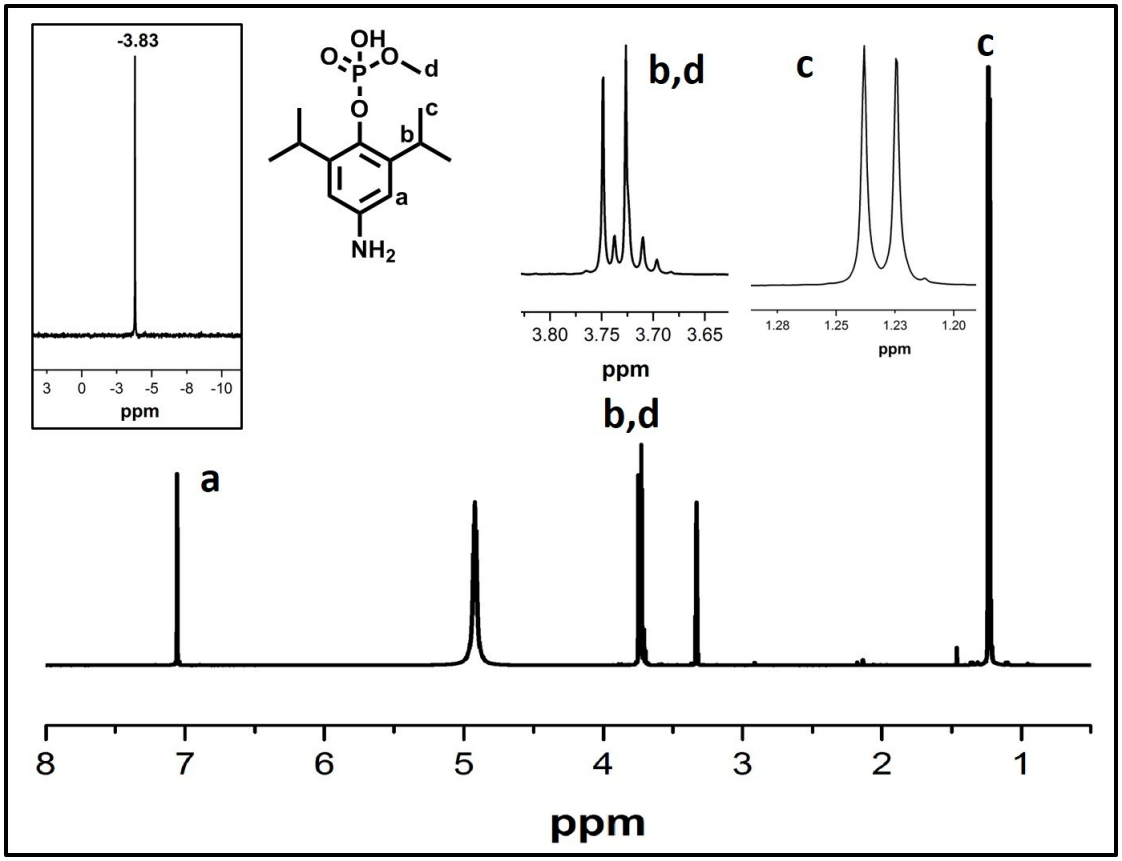

Fig. S16 ^{1}H, and ^{31}P NMR spectra of compound **6** in CD_3OD.

Photophysical studies.

UV-Visible spectroscopy has been investigated for all phosphate ligands in solid as well as in solution. The solid state absorption spectra for all phosphate ligands is shown in Fig. S17. Compound **A** gives two absorption maxima at 300 and 374 nm but for adippH$_2$ maxima appears at 220 and 270 nm. Three absorption maxima have been observed for co-crystal **2** at 249, 300 and 353 nm but co-crystal **3** showed absorption at 217, 255, 300 and 341 nm. Compound **4** and **6** show similar kind of U.V. spectra as **1**, showing the absorption maxima at 236, 283 nm for **4** and 218, 270 nm for **6**. Two absorption maxima has been observed for compound **5** at 257 and 320 nm.

Compound **A** (ndippH$_2$) shows absorption at 210, 290 and 413 nm in solution but does not show any fluorescence properties. Compound **1** has been reported showing two strong absorptions at 207 and 291 nm and emission at 350 nm. Co-crystal **2** showed λ_{max} at 203 nm and emission at 349 nm. Co-crystal **3** results absorption at 202, 229 and 263 nm but does show emission. Compound **4** and **5** show absorption at 207, 245 nm for **4**, 210 and 291 nm for **5**. Compound **6** shows absorption at 204 nm and emission at 350 nm.

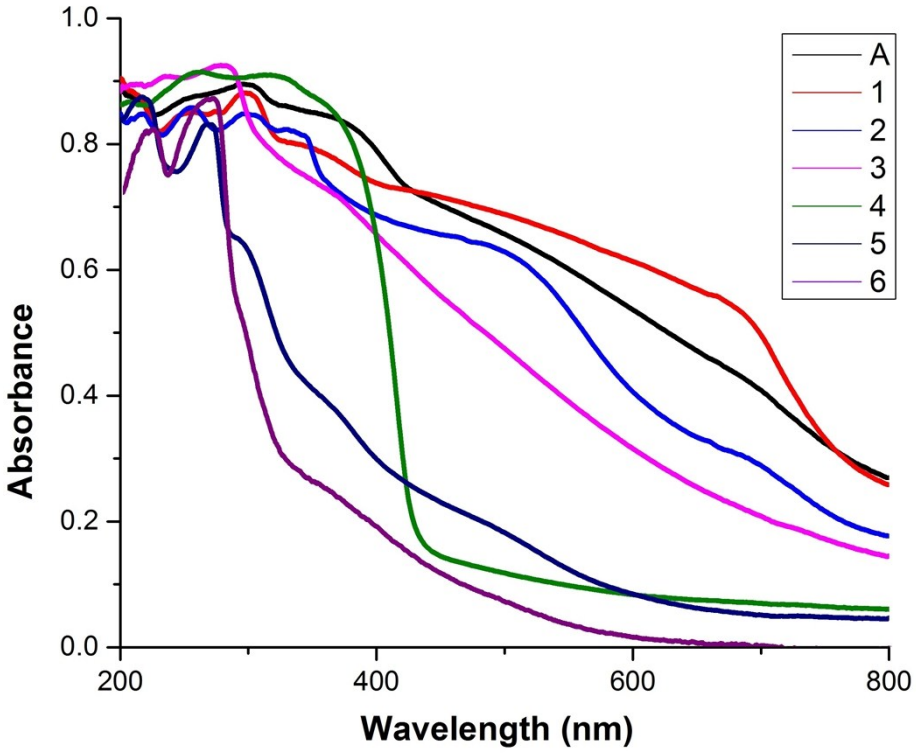

Fig. S17 DRUV-Vis spectrum of **A** and **1-6**.

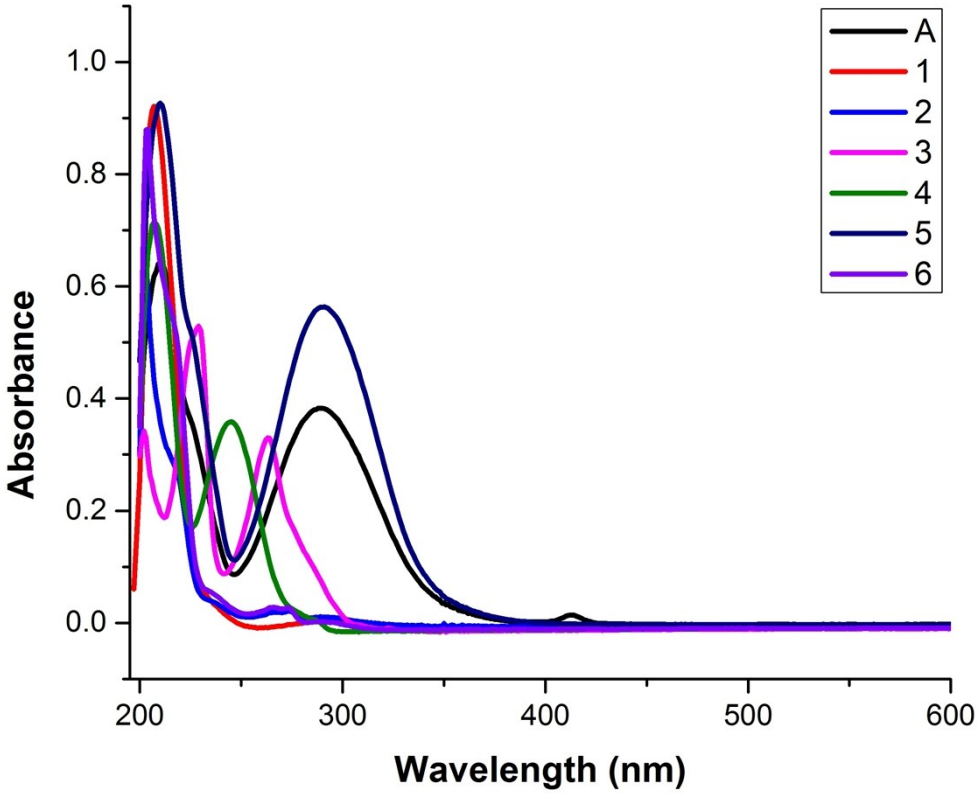

Fig. S18 UV-Uis spectrum of **A** and **1-6** in methanol.

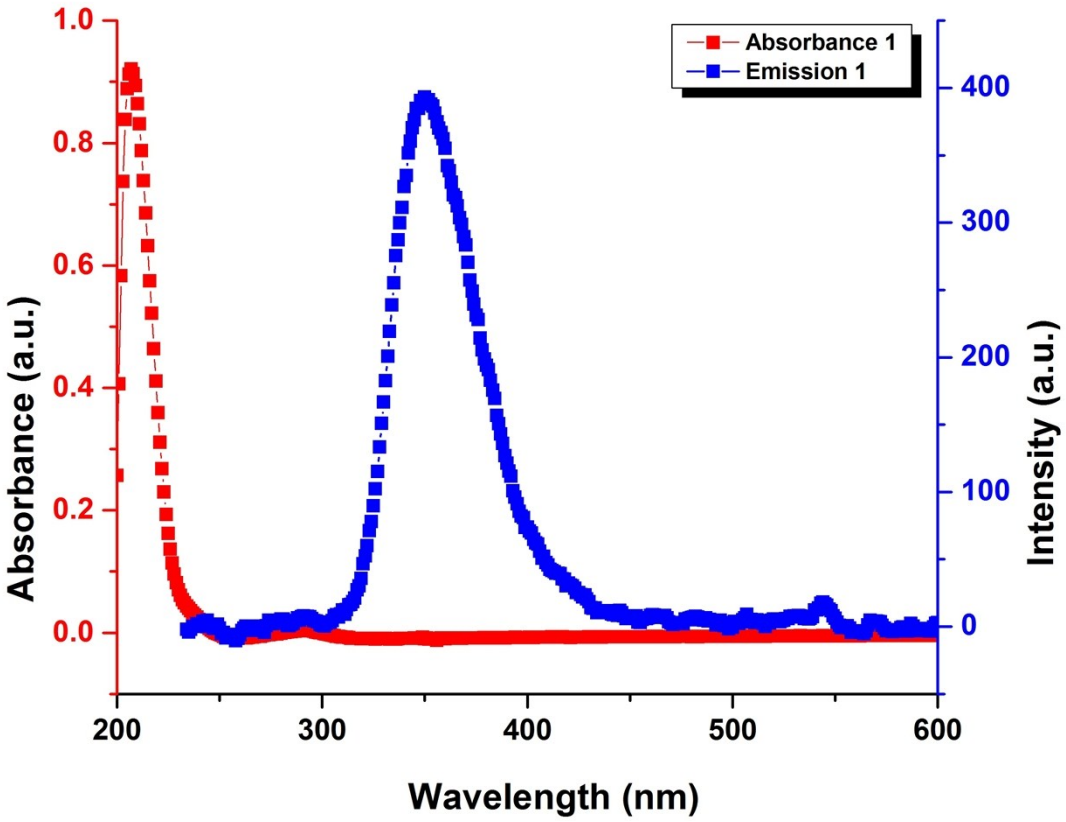

Fig. S19 Absorbance and emission spectrum of **1**.

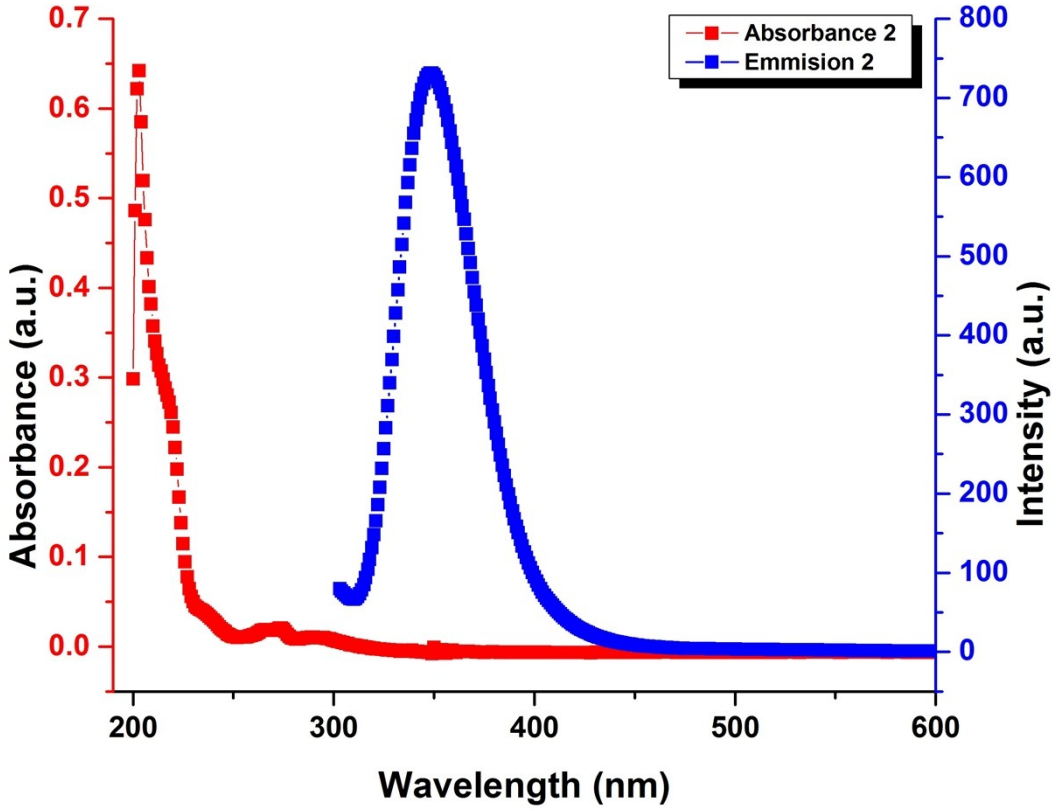

Fig. S20 Absorbance and emission spectrum of **2**.

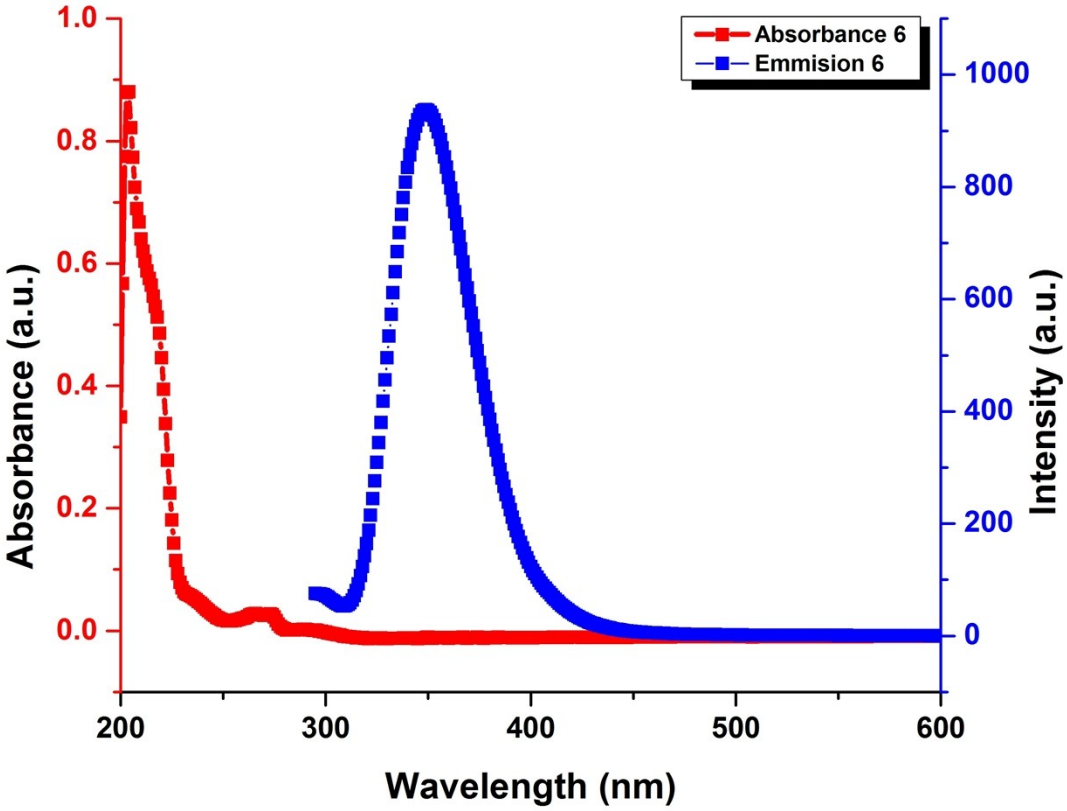

Fig. S21 Absorbance and emission spectrum of **6**.

Table S1. Bond distance and bond angle for ndippH_2 (**A**) [Å and °].

Bond distances		Bond angle	
O(1)-P(1)	1.5846(10)	O(4)-P(1)-O(3)	114.40(6)
O(2)-P(1)	1.5390(11)	O(4)-P(1)-O(2)	113.82(6)
O(3)-P(1)	1.5384(10)	O(3)-P(1)-O(2)	107.74(6)
O(4)-P(1)	1.4847(12)	O(4)-P(1)-O(1)	111.74(6)
		O(3)-P(1)-O(1)	101.49(6)
		O(2)-P(1)-O(1)	106.70(6)

Table S2. Hydrogen bond table for ndippH_2 (**A**) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...O(5)#1	0.93	2.53	3.4331(19)	165.1
O(2)-H(2)...O(7)	0.82	1.73	2.5156(15)	160.0
O(3)-H(3A)...O(4)#2	0.82	1.81	2.5791(15)	154.5
O(7)-H(7A)...O(4)#3	0.82	1.95	2.7425(15)	160.8

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x+1,y-1/2,-z+3/2 #3 -x+1,-y+1,-z+1

Table S3. Bond distance and bond angle for **1a** [Å and °].

Bond distances		Bond angle	
P(1)-O(3)	1.494(2)	O(3)-P(1)-O(1)	114.81(12)
P(1)-O(1)	1.509(2)	O(3)-P(1)-O(2)	110.88(15)
P(1)-O(2)	1.529(2)	O(1)-P(1)-O(2)	111.53(13)
P(1)-O(4)	1.6101(19)	O(3)-P(1)-O(4)	110.45(11)
		O(1)-P(1)-O(4)	105.78(11)
		O(2)-P(1)-O(4)	102.57(12)

Table S4. Hydrogen bond table for **1a** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13C)...O(2)#1	0.98	1.97	2.940(8)	170.1
C(14)-H(14B)...O(6)#2	0.98	2.38	3.06(2)	125.9
N(1)-H(1A)...O(1)#1	0.8894(19)	1.8448(16)	2.732(3)	174.52(13)
N(1)-H(1B)...O(3)#3	0.846(2)	1.8597(19)	2.697(3)	170.17(14)
N(1)-H(1C)...O(3)#4	0.8783(19)	2.0765(17)	2.893(3)	154.23(14)

Symmetry transformations used to generate equivalent atoms:

#1 x-y,x-1,-z+1 #2 x,x-y-1,-z+3/2 #3 -x+1,-y,-z+1

#4 x-y,-y,z+1/2

Table S5. Bond distance and bond angle for **1b** [Å and °].

Bond distances		Bond angle		Bond angle	
P(1)-O(3)	1.518(4)	O(3)-P(1)-O(4)	114.1(3)	O(11)-P(3)-O(10)	116.2(3)
P(1)-O(4)	1.535(5)	O(3)-P(1)-O(2)	114.9(3)	O(11)-P(3)-O(12)	110.5(2)
P(1)-O(2)	1.542(5)	O(4)-P(1)-O(2)	109.7(3)	O(10)-P(3)-O(12)	111.5(3)
P(1)-O(1)	1.621(4)	O(3)-P(1)-O(1)	110.2(2)	O(11)-P(3)-O(9)	105.9(2)
P(2)-O(7)	1.447(6)	O(4)-P(1)-O(1)	104.6(2)	O(10)-P(3)-O(9)	110.8(2)
P(2)-O(6)	1.500(4)	O(2)-P(1)-O(1)	102.2(2)	O(12)-P(3)-O(9)	100.8(2)
P(2)-O(8)	1.567(8)	O(7)-P(2)-O(6)	119.5(3)		
P(2)-O(5)	1.615(4)	O(7)-P(2)-O(8)	104.7(5)		
P(3)-O(11)	1.512(5)	O(6)-P(2)-O(8)	110.5(4)		
P(3)-O(10)	1.514(4)	O(7)-P(2)-O(5)	107.3(3)		
P(3)-O(12)	1.571(5)	O(6)-P(2)-O(5)	110.0(2)		
P(3)-O(9)	1.614(4)	O(8)-P(2)-O(5)	103.5(3)		

Table S6. Hydrogen bond table for **1b** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(8)-H(8)...O(13)	0.84	1.87	2.694(8)	166.8
O(12)-H(12)...O(7)#1	0.84	1.87	2.619(7)	147.7
N(3)-H(3A)...O(7)#2	0.895(5)	2.009(8)	2.826(9)	151.0(4)
N(3)-H(3A)...O(8)#2	0.895(5)	2.600(11)	3.391(12)	147.8(3)
N(1)-H(1A)...O(11)#3	0.915(5)	1.869(4)	2.781(6)	174.2(3)
N(2)-H(2A)...O(6)#4	0.925(5)	1.865(4)	2.774(7)	167.1(3)
N(2)-H(2B)...O(4)	0.940(5)	1.779(5)	2.717(7)	175.2(3)
N(3)-H(3B)...O(10)#5	1.050(5)	1.758(4)	2.802(6)	171.9(3)
N(2)-H(2C)...O(3)#6	1.096(5)	1.790(4)	2.816(7)	154.0(3)
N(3)-H(3C)...O(10)#2	0.880(5)	2.012(4)	2.812(7)	150.6(3)
N(1)-H(1B)...O(3)#7	0.999(5)	1.808(4)	2.797(7)	170.0(3)
N(1)-H(1C)...O(6)#8	0.989(5)	1.787(4)	2.740(6)	160.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2 #2 -x+2,-y,-z+1 #3 x-1,y,z

#4 -x+3/2,-y+1/2,-z+1 #5 x,-y,z-1/2 #6 -x+1,y,-z+1/2

#7 -x+1/2,-y+1/2,-z+1 #8 -x+1,y,-z+3/2

Table S7. Bond distance and bond angle for **1c** [Å and °].

Bond distances		Bond angle		Bond angle	
P(1)-O(3)	1.498(3)	O(3)-P(1)-O(2)	114.05(18)	O(10)-P(3)-O(12)	115.29(18)
P(1)-O(2)	1.507(3)	O(3)-P(1)-O(4)	111.24(19)	O(10)-P(3)-O(11)	109.5(2)
P(1)-O(4)	1.542(3)	O(2)-P(1)-O(4)	112.62(17)	O(12)-P(3)-O(11)	112.46(18)
P(1)-O(1)	1.621(3)	O(3)-P(1)-O(1)	109.64(16)	O(10)-P(3)-O(9)	109.55(16)
P(2)-O(6)	1.495(3)	O(2)-P(1)-O(1)	105.52(18)	O(12)-P(3)-O(9)	106.39(17)
P(2)-O(7)	1.526(3)	O(4)-P(1)-O(1)	102.97(18)	O(11)-P(3)-O(9)	102.78(19)
P(2)-O(8)	1.529(3)	O(6)-P(2)-O(7)	111.8(2)		
P(2)-O(5)	1.614(3)	O(6)-P(2)-O(8)	115.23(17)		
P(3)-O(10)	1.490(3)	O(7)-P(2)-O(8)	110.34(19)		
P(3)-O(12)	1.517(3)	O(6)-P(2)-O(5)	110.86(18)		
P(3)-O(11)	1.541(3)	O(7)-P(2)-O(5)	103.63(18)		
P(3)-O(9)	1.609(3)	O(8)-P(2)-O(5)	104.06(17)		

Table S8. Hydrogen bond table for **1c** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(3)#1	0.91	2.12	2.931(5)	148.6
N(1)-H(1A)...O(4)#1	0.91	2.53	3.257(5)	137.3
N(1)-H(1B)...O(12)#2	0.91	1.85	2.743(4)	165.7
N(1)-H(1C)...O(3)#2	0.91	1.77	2.674(5)	176.5
N(3)-H(3A)...O(6)#3	0.91	2.14	2.971(5)	152.0
N(3)-H(3A)...O(7)#3	0.91	2.52	3.115(5)	123.5
N(3)-H(3B)...O(8)#4	0.91	1.89	2.796(5)	174.7
N(3)-H(3C)...O(10)#5	0.91	1.77	2.668(5)	168.0
O(13)-H(13A)...O(8)#6	0.85(2)	1.87(2)	2.717(5)	170(7)
O(13)-H(13B)...O(2)#2	0.86(2)	1.89(3)	2.735(5)	167(7)
O(11)-H(11)...O(4)#7	0.84(2)	1.62(2)	2.412(4)	156(5)
N(2)-H(2A)...O(2)	0.81(4)	1.95(4)	2.745(5)	167(4)
N(2)-H(2B)...O(10)#7	1.00(5)	2.05(5)	2.931(6)	145(3)
N(2)-H(2B)...O(11)#7	1.00(5)	2.51(4)	3.238(6)	129(3)
N(2)-H(2C)...O(6)#8	1.07(5)	1.65(5)	2.693(5)	162(4)

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z-1/2 #2 -x+1,-y+1,-z+1 #3 -x+1,y,-z+1/2

#4 x-1,y,z #5 -x+1/2,-y+1/2,-z+1 #6 x-1/2,y+1/2,z

#7 -x+1,y,-z+3/2 #8 -x+3/2,-y+1/2,-z+1

Table S9. Bond distance and bond angle for **1d** [Å and °].

Bond distances		Bond angle		Bond angle	
P(1)-O(2)	1.4902(12)	O(2)-P(1)-O(4)	117.78(6)	O(6)-P(2)-O(7)	117.66(6)
P(1)-O(4)	1.5003(11)	O(2)-P(1)-O(3)	107.71(7)	O(6)-P(2)-O(8)	107.28(7)
P(1)-O(3)	1.5611(12)	O(4)-P(1)-O(3)	110.88(6)	O(7)-P(2)-O(8)	109.87(7)
P(1)-O(1)	1.6160(12)	O(2)-P(1)-O(1)	110.87(6)	O(6)-P(2)-O(5)	111.02(6)
P(2)-O(6)	1.4905(12)	O(4)-P(1)-O(1)	103.52(6)	O(7)-P(2)-O(5)	105.47(6)
P(2)-O(7)	1.5002(11)	O(3)-P(1)-O(1)	105.41(6)	O(8)-P(2)-O(5)	104.82(7)
P(2)-O(8)	1.5668(13)				
P(2)-O(5)	1.6024(11)				

Table S10. Hydrogen bond table for **1d** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(17)-H(17)...O(4)#1	0.982(16)	2.585(16)	3.2380(19)	124.0(12)
N(1)-H(1A)...O(2)#2	0.88(2)	2.09(2)	2.936(2)	162.2(18)
N(1)-H(1A)...O(8)#3	0.88(2)	2.52(2)	3.019(2)	117.2(15)
N(2)-H(2A)...O(4)#1	0.86(2)	1.94(2)	2.7911(19)	169.5(17)
N(1)-H(1B)...O(7)#4	0.90(2)	1.92(2)	2.7953(19)	162.4(18)
N(2)-H(2B)...O(6)#5	0.89(2)	1.92(2)	2.771(2)	159.4(17)
N(2)-H(2C)...O(7)#6	0.96(2)	1.81(2)	2.7598(19)	172.1(17)
O(8)-H(8)...O(2)#7	0.75(2)	1.90(3)	2.6007(18)	155(3)
O(9)-H(9D)...O(6)#8	0.90(3)	1.87(3)	2.7403(19)	163(2)
O(9)-H(9E)...O(1)#1	0.87(3)	1.99(3)	2.8504(18)	167(2)
O(3)-H(3)...O(4)#1	0.85(2)	1.75(2)	2.5997(17)	178(2)
N(1)-H(1C)...O(9)#2	0.96(2)	1.76(2)	2.675(2)	159.3(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1/2,y+1/2,-z+1/2 #3 x,y+1,z

#4 -x+1,-y+1,-z #5 -x+3/2,y+1/2,-z+1/2 #6 x+1/2,-y+1/2,z+1/2

#7 -x+1/2,y-1/2,-z+1/2 #8 x-1/2,-y+1/2,z+1/2

Table S11. Bond distance and bond angle for **1e** [Å and °].

Bond distances		Bond angle	
P(1)-O(3)	1.4949(18)	O(3)-P(1)-O(4)	116.33(10)
P(1)-O(4)	1.5050(18)	O(3)-P(1)-O(2)	113.08(11)
P(1)-O(2)	1.5570(18)	O(4)-P(1)-O(2)	109.72(11)
P(1)-O(1)	1.6083(16)	O(3)-P(1)-O(1)	105.39(9)
		O(4)-P(1)-O(1)	109.89(9)
		O(2)-P(1)-O(1)	101.22(10)

Table S12. Hydrogen bond table for **1e** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(8)	0.89	1.97	2.835(3)	162.3
N(1)-H(1B)...O(4)#1	0.89	1.89	2.759(3)	166.1
N(1)-H(1C)...O(10)#2	0.89	1.81	2.695(3)	175.4
N(2)-H(2A)...O(8)#3	0.89	1.89	2.769(3)	169.0
N(2)-H(2B)...O(3)#4	0.89	1.95	2.835(3)	173.1
N(2)-H(2C)...O(9)	0.89	1.90	2.787(3)	175.0
O(9)-H(9)...O(3)#5	0.82	1.88	2.692(3)	171.8
O(10)-H(10A)...O(7)#6	0.82	1.83	2.634(3)	165.8
O(2)-H(2)...O(7)#1	0.93(4)	1.60(4)	2.523(2)	170(3)
O(6)-H(6)...O(4)#7	0.77(4)	1.83(4)	2.583(3)	167(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+2,-z+1 #2 -x+1,-y+1,-z+1 #3 -x+1,-y+1,-z

#4 -x+2,-y+1,-z #5 x-1,y,z-1 #6 x,y-1,z #7 x-1,y,z

Table S13. Bond distance and bond angle for **2** [Å and °].

Bond distances		Bond angle			
O(1)-P(1)	1.598(2)	O(4)-P(1)-O(3)	114.98(11)	O(11)-P(3)-O(12)	114.96(13)
O(2)-P(1)	1.556(2)	O(4)-P(1)-O(2)	111.29(12)	O(11)-P(3)-O(10)	112.62(12)
O(3)-P(1)	1.5062(19)	O(3)-P(1)-O(2)	111.35(11)	O(12)-P(3)-O(10)	109.22(12)
O(4)-P(1)	1.501(2)	O(4)-P(1)-O(1)	108.37(11)	O(11)-P(3)-O(9)	111.41(12)
O(5)-P(2)	1.596(2)	O(3)-P(1)-O(1)	108.32(11)	O(12)-P(3)-O(9)	103.04(12)
O(6)-P(2)	1.492(2)	O(2)-P(1)-O(1)	101.58(12)	O(10)-P(3)-O(9)	104.70(12)
O(7)-P(2)	1.5072(19)	O(6)-P(2)-O(7)	117.67(12)	O(16)-S(1)-O(15)	113.33(17)
O(8)-P(2)	1.562(2)	O(6)-P(2)-O(8)	107.68(12)	O(16)-S(1)-O(14)	114.52(14)
O(9)-P(3)	1.574(2)	O(7)-P(2)-O(8)	110.07(11)	O(15)-S(1)-O(14)	113.75(16)
O(10)-P(3)	1.552(2)	O(6)-P(2)-O(5)	110.38(11)	O(16)-S(1)-C(37)	103.30(17)
O(11)-P(3)	1.481(2)	O(7)-P(2)-O(5)	106.90(11)	O(15)-S(1)-C(37)	104.16(19)
O(12)-P(3)	1.540(2)	O(8)-P(2)-O(5)	103.20(12)	O(14)-S(1)-C(37)	106.33(17)

Table S14. Hydrogen bond table for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(3)-H(3)...O(16)#1	0.95	2.58	3.330(4)	135.9
C(29)-H(29)...O(15)	0.95	2.53	3.308(4)	138.9
N(1)-H(1A)...O(16)#1	0.91	2.01	2.801(3)	144.4
N(1)-H(1A)...S(1)#1	0.91	2.94	3.830(3)	166.3
N(1)-H(1B)...O(4)#2	0.91	1.86	2.770(3)	177.0
N(1)-H(1C)...O(6)#3	0.91	1.95	2.804(3)	156.0
N(1)-H(1C)...O(8)#3	0.91	2.66	3.290(3)	127.4
N(2)-H(2A)...O(14)#4	0.91	2.05	2.938(3)	166.5
N(2)-H(2A)...S(1)#4	0.91	2.79	3.566(2)	144.3
N(2)-H(2B)...O(6)#5	0.91	1.84	2.748(3)	175.3
N(2)-H(2C)...O(3)#6	0.91	1.89	2.801(3)	176.4
N(3)-H(3A)...O(11)#7	0.91	1.92	2.741(3)	149.9
N(3)-H(3B)...O(7)	0.91	1.91	2.784(3)	159.2
N(3)-H(3C)...O(15)	0.91	2.00	2.902(4)	173.8
N(3)-H(3C)...S(1)	0.91	2.81	3.641(3)	152.9
O(8)-H(8)...O(11)#7	0.84	1.81	2.628(3)	164.2
O(10)-H(10)...O(4)#8	0.84	1.71	2.551(3)	176.1
O(2)-H(2)...O(13)#7	0.84	3.15	3.423(8)	102.0
O(12)-H(12)...O(3)#8	0.84	1.71	2.536(3)	169.3

Symmetry transformations used to generate equivalent atoms:

#1 x,y-1,z-1 #2 -x+1,-y,-z #3 -x+1,-y,-z+1

#4 x-1,y,z #5 -x,-y+1,-z+2 #6 x-1,y,z+1 #7 -x+1,-y+1,-z+1

#8 -x+1,-y+1,-z

Table S15. Bond distance and bond angle for **3** [Å and °].

Bond distances		Bond angle	
P(1)-O(3)	1.4918(17)	O(3)-P(1)-O(2)	117.85(10)
P(1)-O(2)	1.5008(18)	O(3)-P(1)-O(4)	108.65(9)
P(1)-O(4)	1.5664(17)	O(2)-P(1)-O(4)	109.96(9)
P(1)-O(1)	1.6209(16)	O(3)-P(1)-O(1)	109.03(9)
		O(2)-P(1)-O(1)	105.83(9)
		O(4)-P(1)-O(1)	104.72(9)

Table S16. Hydrogen bond table for **3** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(2)#1	0.82	1.74	2.550(2)	167.2
N(1)-H(1A)...O(3)#2	0.89	1.81	2.677(3)	164.7
N(1)-H(1B)...N(3)#2	0.89	2.14	2.949(3)	150.7
N(1)-H(1C)...O(5)	0.89	1.87	2.761(3)	174.0
C(5)-H(5)...N(3)#2	0.93	2.69	3.429(3)	137.4
C(13)-H(13)...O(2)	0.93	2.63	3.434(3)	145.8
O(5)-H(5A)...N(2)#3	0.85	2.08	2.866(3)	154.6
O(5)-H(5B)...O(2)#3	0.78(4)	2.05(4)	2.809(3)	166(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1 #2 -x+1,-y,-z+2 #3 -x+2,-y,-z

Table S17. Bond distance and bond angle for **4** [Å and °].

Bond distances		Bond angle	
O(1)-P(1)	1.579(3)	O(3)-P(1)-O(2)	116.0(2)
O(2)-P(1)	1.527(3)	O(3)-P(1)-O(4)	112.36(18)
O(3)-P(1)	1.492(3)	O(2)-P(1)-O(4)	107.55(19)
O(4)-P(1)	1.542(3)	O(3)-P(1)-O(1)	106.55(18)
		O(2)-P(1)-O(1)	106.16(17)
		O(4)-P(1)-O(1)	107.82(17)

Table S18. Hydrogen bond table for **4** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(3)#1	0.88	1.93	2.776(5)	160.7
O(4)-H(4)...O(3)#2	0.84	1.71	2.548(4)	171.1
O(2)-H(2)...O(5)#3	0.93(7)	1.52(7)	2.449(5)	171(7)

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2,-y+3/2,-z+5/4 #2 y,x,-z+1 #3 x,y-1,z

Table S19. Bond distance and bond angle for **5** [Å and °].

Bond distances		Bond angle	
O(1)-P(1)	1.5815(10)	O(2)-P(1)-O(4)	116.45(6)
O(2)-P(1)	1.4943(11)	O(2)-P(1)-O(3)	108.98(6)
O(3)-P(1)	1.5601(10)	O(4)-P(1)-O(3)	109.18(6)
O(4)-P(1)	1.5204(10)	O(2)-P(1)-O(1)	111.37(6)
		O(4)-P(1)-O(1)	106.76(6)
		O(3)-P(1)-O(1)	103.27(5)

Table S20. Hydrogen bond table for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13B)...O(3)#1	0.98	2.66	3.420(2)	135.0
O(4)-H(4)...O(2)#2	0.89(3)	1.61(3)	2.4980(14)	176(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x,-y+1,-z+1

Table S21. Bond distance and bond angle for **6** [Å and °].

Bond distances		Bond angle	
O(1)-P(1)	1.619(4)	O(4)-P(1)-O(3)	118.8(2)
O(2)-P(1)	1.576(4)	O(4)-P(1)-O(2)	113.7(2)
O(3)-P(1)	1.480(4)	O(3)-P(1)-O(2)	104.3(2)
O(4)-P(1)	1.479(4)	O(4)-P(1)-O(1)	108.4(2)
		O(3)-P(1)-O(1)	110.6(2)
		O(2)-P(1)-O(1)	99.2(2)

Table S22. Hydrogen bond table for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13B)...O(5)#1	0.98	2.62	3.116(9)	111.3
C(14)-H(14C)...O(3)#2	0.98	2.62	3.581(9)	166.4
C(15)-H(15A)...O(2)	0.98	2.63	3.400(9)	135.2
N(1)-H(1A)...O(4)#3	0.91	1.78	2.680(5)	169.8
N(1)-H(1B)...O(3)#4	0.91	1.77	2.675(6)	173.7
N(1)-H(1C)...O(5)#5	0.91	1.86	2.756(6)	168.6

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+3/2,z+1/2 #2 -x,-y+1,-z #3 x+1,y,z

#4 -x+1,-y+1,-z+1 #5 x+1,y,z+1