Hard-and-soft phosphinoxide receptors for f-element binding: the influence of nature of ligand and counter-ion on the structure and photophysical properties of europium(III) complexes

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Supplementary data

List

PyPPO Structure

Table 1 Crystal data and structure refinement for PyPPO.

Identification code	a	
Empirical formula	C29 H25 N O3 P2	
Formula weight	497.44	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5163(7) Å	α= 100.1501(13)°.
	b = 10.9689(7) Å	β= 104.7237(14)°.
	c = 12.9195(8) Å	γ = 115.6149(12)°.
Volume	1227.77(14) $Å^3$	
Z	2	
Density (calculated)	1.346 Mg/m^3	
Absorption coefficient	0.210 mm^{-1}	
F(000)	520	
Crystal size	0.380 x 0.210 x 0.180 mm^3	
Theta range for data collection	1.725 to 30.155°.	
Index ranges	-14<=h<=14, -15<=k<=15, -18<=l<=18	
Reflections collected	16095	
Independent reflections	7220 [R(int) = 0.0363]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.969 and 0.912	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7220 / 0 / 318	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1017	
R indices (all data)	R1 = 0.0741, wR2 = 0.1140	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.467 and -0.353 e. $Å^{-3}$	

Table 2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PyPPO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	6049(1)	3241(1)	2173(1)	13(1)
P(2)	10774(1)	8480(1)	3118(1)	12(1)
N(1)	8287(2)	5968(2)	2768(1)	13(1)
O(1)	4522(1)	2472(1)	2233(1)	19(1)
O(1W)	7175(2)	7177(2)	6544(1)	28(1)
O(2)	11480(1)	10014(1)	3802(1)	17(1)
C(1)	6992(2)	5154(2)	2909(1)	12(1)
C(2)	6346(2)	5719(2)	3528(1)	15(1)
C(3)	7063(2)	7190(2)	4015(1)	16(1)
C(4)	8397(2)	8046(2)	3876(1)	14(1)
C(5)	8973(2)	7396(2)	3255(1)	12(1)
C(6)	5949(2)	3133(2)	745(1)	14(1)
C(7)	4768(2)	3216(2)	40(2)	20(1)
C(8)	4675(2)	3208(2)	-1050(2)	24(1)
C(9)	5728(2)	3084(2)	-1450(2)	25(1)
C(10)	6898(2)	2986(2)	-753(2)	27(1)
C(11)	7017(2)	3019(2)	347(2)	22(1)
C(12)	7313(2)	2618(2)	2727(1)	15(1)
C(13)	6787(2)	1156(2)	2288(2)	25(1)
C(14)	7725(2)	615(2)	2646(2)	29(1)
C(15)	9183(2)	1507(2)	3444(2)	22(1)
C(16)	9698(2)	2949(2)	3897(2)	22(1)
C(17)	8771(2)	3505(2)	3538(2)	19(1)
C(18)	10400(2)	8220(2)	1629(2)	15(1)
C(19)	9166(2)	7026(2)	756(2)	23(1)
C(20)	8968(2)	6946(2)	-365(2)	28(1)
C(21)	9985(2)	8046(2)	-622(2)	26(1)
C(22)	11220(2)	9225(2)	242(2)	26(1)
C(23)	11434(2)	9320(2)	1364(2)	21(1)
C(24)	11913(2)	7704(2)	3602(2)	15(1)
C(25)	13132(2)	8483(2)	4636(2)	20(1)
C(26)	13996(2)	7895(2)	5074(2)	25(1)
C(27)	13634(2)	6534(2)	4493(2)	25(1)
C(28)	12428(2)	5753(2)	3461(2)	23(1)
C(29)	11567(2)	6332(2)	3005(2)	19(1)

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

P(1)-O(1)	1.4877(13)	C(22)-H(22A)	0.9500
P(1)-C(12)	1.7945(18)	C(23)-H(23A)	0.9500
P(1)-C(6)	1.8003(18)	C(24)-C(25)	1.393(3)
P(1)-C(1)	1.8190(17)	C(24)-C(29)	1.402(2)
P(2)-O(2)	1.4923(12)	C(25)-C(26)	1.391(3)
P(2)-C(24)	1.7996(18)	C(25)-H(25A)	0.9500
P(2)-C(18)	1.8052(18)	C(26)-C(27)	1.380(3)
P(2)-C(5)	1.8243(17)	C(26)-H(26A)	0.9500
N(1)-C(5)	1.347(2)	C(27)-C(28)	1.385(3)
N(1)-C(1)	1.348(2)	C(27)-H(27A)	0.9500
O(1W)-H(1WB)	0.8257	C(28)-C(29)	1.389(3)
O(1W)-H(1WA)	0.8823	C(28)-H(28A)	0.9500
C(1)-C(2)	1.397(2)	C(29)-H(29A)	0.9500
C(2)-C(3)	1.385(2)		
C(2)-H(2A)	0.9500	O(1)-P(1)-C(12)	114.59(8)
C(3)-C(4)	1.389(2)	O(1)-P(1)-C(6)	112.36(8)
C(3)-H(3A)	0.9500	C(12)-P(1)-C(6)	106.32(8)
C(4)-C(5)	1.392(2)	O(1)-P(1)-C(1)	111.42(8)
C(4)-H(4A)	0.9500	C(12)-P(1)-C(1)	107.81(8)
C(6)-C(7)	1.390(2)	C(6)-P(1)-C(1)	103.60(8)
C(6)-C(11)	1.391(2)	O(2)-P(2)-C(24)	112.50(8)
C(7)-C(8)	1.385(3)	O(2)-P(2)-C(18)	112.46(8)
C(7)-H(7A)	0.9500	C(24)-P(2)-C(18)	108.62(8)
C(8)-C(9)	1.382(3)	O(2)-P(2)-C(5)	110.80(7)
C(8)-H(8A)	0.9500	C(24)-P(2)-C(5)	104.46(8)
C(9)-C(10)	1.386(3)	C(18)-P(2)-C(5)	107.58(8)
C(9)-H(9A)	0.9500	C(5)-N(1)-C(1)	117.30(14)
C(10)-C(11)	1.387(3)	H(1WB)-O(1W)-H(1WA)	106.0
C(10)-H(10A)	0.9500	N(1)-C(1)-C(2)	123.35(15)
C(11)-H(11A)	0.9500	N(1)-C(1)-P(1)	115.77(12)
C(12)-C(17)	1.389(2)	C(2)-C(1)-P(1)	120.80(13)
C(12)-C(13)	1.398(2)	C(3)-C(2)-C(1)	118.48(15)
C(13)-C(14)	1.383(3)	C(3)-C(2)-H(2A)	120.8
C(13)-H(13A)	0.9500	C(1)-C(2)-H(2A)	120.8
C(14)-C(15)	1.383(3)	C(2)-C(3)-C(4)	118.94(15)
C(14)-H(14A)	0.9500	C(2)-C(3)-H(3A)	120.5
C(15)-C(16)	1.382(3)	C(4)-C(3)-H(3A)	120.5
C(15)-H(15A)	0.9500	C(3)-C(4)-C(5)	118.95(16)
C(16)-C(17)	1.386(3)	C(3)-C(4)-H(4A)	120.5
C(16)-H(16A)	0.9500	C(5)-C(4)-H(4A)	120.5
C(17)-H(17A)	0.9500	N(1)-C(5)-C(4)	122.98(15)
C(18)-C(19)	1.392(3)	N(1)-C(5)-P(2)	116.91(12)
C(18)-C(23)	1.399(2)	C(4)-C(5)-P(2)	120.07(13)
C(19)-C(20)	1.391(3)	C(7)-C(6)-C(11)	119.88(17)
C(19)-H(19A)	0.9500	C(7)-C(6)-P(1)	117.20(13)
C(20)-C(21)	1.384(3)	C(11)-C(6)-P(1)	122.88(14)
C(20)-H(20A)	0.9500	C(8)-C(7)-C(6)	119.77(17)
C(21)-C(22)	1.381(3)	C(8)-C(7)-H(7A)	120.1
C(21)-H(21A)	0.9500	C(6)-C(7)-H(7A)	120.1
C(22)-C(23)	1.387(3)	C(9)-C(8)-C(7)	120.43(18)

C(9)-C(8)-H(8A)	119.8	C(18)-C(19)-H(19A)	120.1
C(7)-C(8)-H(8A)	119.8	C(20)-C(19)-H(19A)	120.1
C(8)-C(9)-C(10)	119.89(18)	C(21)-C(20)-C(19)	120.58(19)
C(8)-C(9)-H(9A)	120.1	C(21)-C(20)-H(20A)	119.7
C(10)-C(9)-H(9A)	120.1	C(19)-C(20)-H(20A)	119.7
C(11)-C(10)-C(9)	120.15(18)	C(22)-C(21)-C(20)	119.77(18)
C(11)-C(10)-H(10A)	119.9	C(22)-C(21)-H(21A)	120.1
C(9)-C(10)-H(10A)	119.9	C(20)-C(21)-H(21A)	120.1
C(10)-C(11)-C(6)	119.86(17)	C(21)-C(22)-C(23)	120.32(18)
C(10)-C(11)-H(11A)	120.1	C(21)-C(22)-H(22A)	119.8
C(6)-C(11)-H(11A)	120.1	C(23)-C(22)-H(22A)	119.8
C(17)-C(12)-C(13)	119.17(16)	C(22)-C(23)-C(18)	120.20(18)
C(17)-C(12)-P(1)	123.83(13)	C(22)-C(23)-H(23A)	119.9
C(13)-C(12)-P(1)	116.98(14)	C(18)-C(23)-H(23A)	119.9
C(14)-C(13)-C(12)	119.93(18)	C(25)-C(24)-C(29)	119.76(17)
C(14)-C(13)-H(13A)	120.0	C(25)-C(24)-P(2)	117.82(14)
C(12)-C(13)-H(13A)	120.0	C(29)-C(24)-P(2)	122.34(14)
C(15)-C(14)-C(13)	120.58(18)	C(24)-C(25)-C(26)	119.89(18)
C(15)-C(14)-H(14A)	119.7	C(24)-C(25)-H(25A)	120.1
C(13)-C(14)-H(14A)	119.7	C(26)-C(25)-H(25A)	120.1
C(16)-C(15)-C(14)	119.68(18)	C(27)-C(26)-C(25)	120.14(19)
C(16)-C(15)-H(15A)	120.2	C(27)-C(26)-H(26A)	119.9
C(14)-C(15)-H(15A)	120.2	C(25)-C(26)-H(26A)	119.9
C(15)-C(16)-C(17)	120.23(18)	C(26)-C(27)-C(28)	120.39(18)
C(15)-C(16)-H(16A)	119.9	C(26)-C(27)-H(27A)	119.8
C(17)-C(16)-H(16A)	119.9	C(28)-C(27)-H(27A)	119.8
C(16)-C(17)-C(12)	120.39(17)	C(27)-C(28)-C(29)	120.19(18)
C(16)-C(17)-H(17A)	119.8	C(27)-C(28)-H(28A)	119.9
C(12)-C(17)-H(17A)	119.8	C(29)-C(28)-H(28A)	119.9
C(19)-C(18)-C(23)	119.31(17)	C(28)-C(29)-C(24)	119.61(18)
C(19)-C(18)-P(2)	124.48(14)	C(28)-C(29)-H(29A)	120.2
C(23)-C(18)-P(2)	116.21(13)	C(24)-C(29)-H(29A)	120.2
C(18)-C(19)-C(20)	119.82(18)		

Symmetry transformations used to generate equivalent atoms:

Table 4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for PyPPO. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	12(1)	11(1)	14(1)	4(1)	5(1)	5(1)
P(2)	12(1)	10(1)	14(1)	3(1)	5(1)	5(1)
N(1)	13(1)	13(1)	14(1)	5(1)	5(1)	7(1)
O(1)	14(1)	17(1)	25(1)	6(1)	9(1)	5(1)
O(1W)	35(1)	21(1)	39(1)	12(1)	24(1)	15(1)
O(2)	18(1)	11(1)	20(1)	3(1)	7(1)	5(1)
C(1)	13(1)	12(1)	12(1)	5(1)	4(1)	7(1)
C(2)	14(1)	18(1)	15(1)	7(1)	7(1)	9(1)
C(3)	16(1)	20(1)	14(1)	5(1)	6(1)	12(1)
C(4)	16(1)	13(1)	12(1)	3(1)	4(1)	8(1)
C(5)	12(1)	12(1)	12(1)	5(1)	4(1)	6(1)
C(6)	15(1)	12(1)	15(1)	3(1)	5(1)	6(1)
C(7)	18(1)	22(1)	18(1)	5(1)	5(1)	12(1)
C(8)	24(1)	27(1)	18(1)	7(1)	2(1)	14(1)
C(9)	31(1)	25(1)	16(1)	6(1)	9(1)	13(1)
C(10)	31(1)	35(1)	23(1)	10(1)	16(1)	20(1)
C(11)	20(1)	28(1)	22(1)	9(1)	9(1)	16(1)
C(12)	18(1)	15(1)	14(1)	7(1)	6(1)	9(1)
C(13)	23(1)	14(1)	29(1)	5(1)	0(1)	7(1)
C(14)	36(1)	14(1)	34(1)	6(1)	5(1)	15(1)
C(15)	25(1)	22(1)	28(1)	14(1)	12(1)	16(1)
C(16)	17(1)	21(1)	26(1)	10(1)	4(1)	9(1)
C(17)	19(1)	12(1)	22(1)	6(1)	4(1)	8(1)
C(18)	16(1)	15(1)	16(1)	5(1)	8(1)	10(1)
C(19)	20(1)	24(1)	19(1)	7(1)	9(1)	5(1)
C(20)	24(1)	31(1)	16(1)	4(1)	4(1)	7(1)
C(21)	34(1)	33(1)	19(1)	13(1)	14(1)	20(1)
C(22)	35(1)	23(1)	28(1)	15(1)	21(1)	14(1)
C(23)	25(1)	15(1)	22(1)	6(1)	12(1)	8(1)
C(24)	12(1)	16(1)	19(1)	8(1)	8(1)	8(1)
C(25)	17(1)	21(1)	21(1)	8(1)	7(1)	8(1)
C(26)	18(1)	36(1)	23(1)	14(1)	7(1)	14(1)
C(27)	24(1)	38(1)	32(1)	25(1)	19(1)	23(1)
C(28)	27(1)	24(1)	32(1)	14(1)	18(1)	19(1)
C(29)	18(1)	18(1)	22(1)	7(1)	10(1)	10(1)

Table 5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for PyPPO.

	x	y	z	U(eq)
H(1WB)	7626	7987	6504	34(7)
H(1WA)	6602	7211	6930	55(9)
H(2A)	5436	5108	3613	18
H(3A)	6650	7608	4438	19
H(4A)	8908	9058	4199	17
H(7A)	4027	3279	305	24
H(8A)	3883	3289	-1525	29
H(9A)	5650	3065	-2203	29
H(10A)	7620	2897	-1029	32
H(11A)	7826	2963	827	26
H(13A)	5785	535	1743	30
H(14A)	7366	-379	2342	35
H(15A)	9827	1131	3678	27
H(16A)	10691	3561	4456	26
H(17A)	9134	4499	3849	22
H(19A)	8461	6268	926	27
H(20A)	8127	6129	-960	33
H(21A)	9834	7991	-1389	31
H(22A)	11928	9974	67	31
H(23A)	12285	10135	1954	25
H(25A)	13374	9415	5042	24
H(26A)	14836	8431	5775	30
H(27A)	14215	6130	4803	30
H(28A)	12189	4820	3064	27
H(29A)	10748	5802	2292	22

Table 6 Torsion angles [°] for PyPPO.

C(5)-N(1)-C(1)-C(2)	-0.1(2)		
C(5)-N(1)-C(1)-P(1)	176.70(12)	C(6)-P(1)-C(12)-C(13)	-70.80(16)
O(1)-P(1)-C(1)-N(1)	-171.02(12)	C(1)-P(1)-C(12)-C(13)	178.63(15)
C(12)-P(1)-C(1)-N(1)	62.42(14)	C(17)-C(12)-C(13)-C(14)	-1.2(3)
C(6)-P(1)-C(1)-N(1)	-50.00(14)	P(1)-C(12)-C(13)-C(14)	177.50(17)
O(1)-P(1)-C(1)-C(2)	5.86(17)	C(12)-C(13)-C(14)-C(15)	0.4(3)
C(12)-P(1)-C(1)-C(2)	-120.69(14)	C(13)-C(14)-C(15)-C(16)	0.9(3)
C(6)-P(1)-C(1)-C(2)	126.89(14)	C(14)-C(15)-C(16)-C(17)	-1.3(3)
N(1)-C(1)-C(2)-C(3)	0.5(3)	C(15)-C(16)-C(17)-C(12)	0.5(3)
P(1)-C(1)-C(2)-C(3)	-176.10(13)	C(13)-C(12)-C(17)-C(16)	0.8(3)
C(1)-C(2)-C(3)-C(4)	-0.4(2)	P(1)-C(12)-C(17)-C(16)	-177.84(14)
C(2)-C(3)-C(4)-C(5)	-0.2(2)	O(2)-P(2)-C(18)-C(19)	-145.76(15)
C(1)-N(1)-C(5)-C(4)	-0.5(2)	C(24)-P(2)-C(18)-C(19)	89.05(17)
C(1)-N(1)-C(5)-P(2)	177.05(12)	C(5)-P(2)-C(18)-C(19)	-23.48(18)
C(3)-C(4)-C(5)-N(1)	0.7(3)	O(2)-P(2)-C(18)-C(23)	33.51(16)
C(3)-C(4)-C(5)-P(2)	-176.80(13)	C(24)-P(2)-C(18)-C(23)	-91.68(15)
O(2)-P(2)-C(5)-N(1)	-173.69(12)	C(5)-P(2)-C(18)-C(23)	155.79(14)
C(24)-P(2)-C(5)-N(1)	-52.31(15)	C(23)-C(18)-C(19)-C(20)	-0.5(3)
C(18)-P(2)-C(5)-N(1)	63.01(15)	P(2)-C(18)-C(19)-C(20)	178.71(16)
O(2)-P(2)-C(5)-C(4)	3.97(16)	C(18)-C(19)-C(20)-C(21)	-0.2(3)
C(24)-P(2)-C(5)-C(4)	125.35(14)	C(19)-C(20)-C(21)-C(22)	0.9(3)
C(18)-P(2)-C(5)-C(4)	-119.33(14)	C(20)-C(21)-C(22)-C(23)	-0.9(3)
O(1)-P(1)-C(6)-C(7)	38.38(16)	C(21)-C(22)-C(23)-C(18)	0.2(3)
C(12)-P(1)-C(6)-C(7)	164.49(14)	C(19)-C(18)-C(23)-C(22)	0.6(3)
C(1)-P(1)-C(6)-C(7)	-82.01(15)	P(2)-C(18)-C(23)-C(22)	-178.74(15)
O(1)-P(1)-C(6)-C(11)	-143.74(15)	O(2)-P(2)-C(24)-C(25)	11.10(16)
C(12)-P(1)-C(6)-C(11)	-17.63(17)	C(18)-P(2)-C(24)-C(25)	136.26(14)
C(1)-P(1)-C(6)-C(11)	95.87(16)	C(5)-P(2)-C(24)-C(25)	-109.15(14)
C(11)-C(6)-C(7)-C(8)	-1.0(3)	O(2)-P(2)-C(24)-C(29)	-172.09(14)
P(1)-C(6)-C(7)-C(8)	176.92(14)	C(18)-P(2)-C(24)-C(29)	-46.92(16)
C(6)-C(7)-C(8)-C(9)	1.5(3)	C(5)-P(2)-C(24)-C(29)	67.66(16)
C(7)-C(8)-C(9)-C(10)	-0.9(3)	C(29)-C(24)-C(25)-C(26)	-0.3(3)
C(8)-C(9)-C(10)-C(11)	-0.2(3)	P(2)-C(24)-C(25)-C(26)	176.60(14)
C(9)-C(10)-C(11)-C(6)	0.7(3)	C(24)-C(25)-C(26)-C(27)	-0.9(3)
C(7)-C(6)-C(11)-C(10)	-0.1(3)	C(25)-C(26)-C(27)-C(28)	1.2(3)
P(1)-C(6)-C(11)-C(10)	-177.92(15)	C(26)-C(27)-C(28)-C(29)	-0.4(3)
O(1)-P(1)-C(12)-C(17)	-127.42(15)	C(27)-C(28)-C(29)-C(24)	-0.8(3)
C(6)-P(1)-C(12)-C(17)	107.83(16)	C(25)-C(24)-C(29)-C(28)	1.1(3)
C(1)-P(1)-C(12)-C(17)	-2.75(18)	P(2)-C(24)-C(29)-C(28)	-175.61(14)
O(1)-P(1)-C(12)-C(13)	53.95(17)		

Symmetry transformations used to generate equivalent atoms:

Table 7 Hydrogen bonds for PyPPO [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WB)...O(2)#1	0.83	2.14	2.955(2)	172
O(1W)-H(1WA)...O(1)#2	0.88	1.89	2.763(2)	173

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1 #2 -x+1,-y+1,-z+1

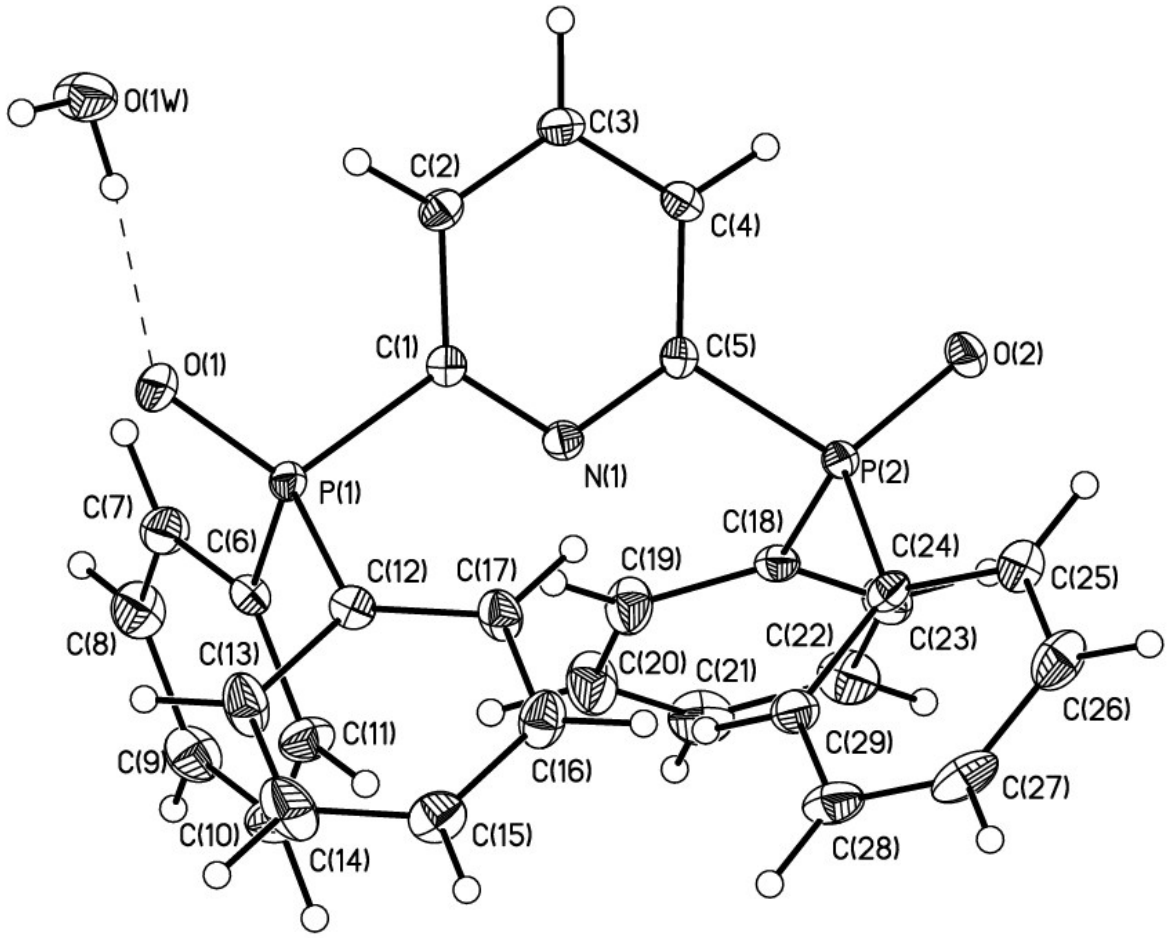

Figure 1 General view of the unit cell independent part of PyPPO structure with the representation of intermolecular O(1W)-H…O(1) hydrogen bond by a dash line. Non-hydrogen atoms are represented as probability ellipsoids of atomic displacements (p=0.5).

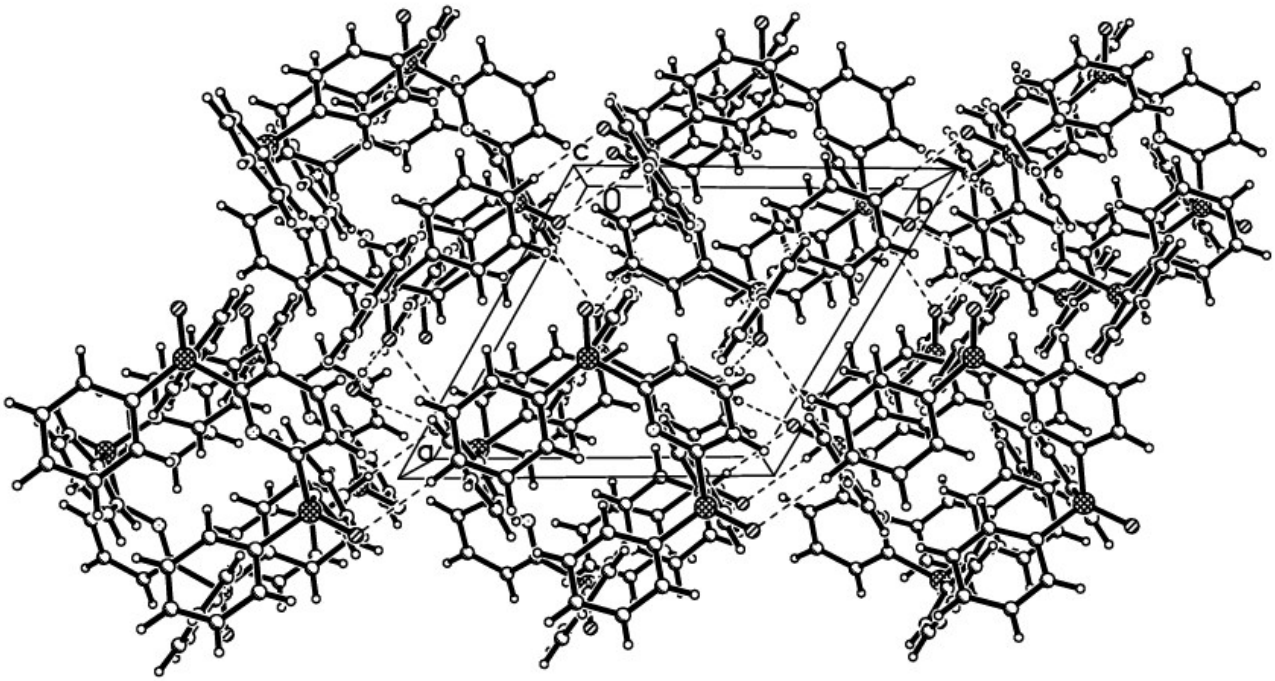

Figure 2 A fragment of PyPPO crystal packing along the *ab* plane of the unit cell.

DPPO Structure

Table 8 Crystal data and structure refinement for DPPO.

Identification code	a	
Empirical formula	C42 H42 N2 O6 P2	
Formula weight	732.71	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.6373(6) Å	α= 90°.
	b = 20.0602(14) Å	β= 106.8510(16)°.
	c = 11.4415(8) Å	γ = 90°.
Volume	1897.3(2) $Å^3$	
Z	2	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.165 mm^{-1}	
F(000)	772	
Crystal size	0.240 x 0.210 x 0.160 mm^3	
Theta range for data collection	2.030 to 27.999°.	
Index ranges	-11<=h<=11, -26<=k<=26, -15<=l<=15	
Reflections collected	21684	
Independent reflections	4582 [R(int) = 0.0589]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.988 and 0.950	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4582 / 12 / 254	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1442	
R indices (all data)	R1 = 0.0793, wR2 = 0.1608	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.686 and -0.420 e. $Å^{-3}$	

Table 9 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DPPO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	1482(1)	5977(1)	3686(1)	14(1)
O(1)	960(2)	5951(1)	4815(1)	19(1)
N(1)	671(2)	5396(1)	1467(2)	16(1)
C(1)	485(2)	5341(1)	2591(2)	16(1)
C(2)	-461(3)	4856(1)	2918(2)	18(1)
C(3)	-1268(3)	4408(1)	2022(2)	23(1)
C(4)	-1104(3)	4457(1)	854(2)	22(1)
C(5)	-112(2)	4960(1)	618(2)	16(1)
C(6)	936(2)	6748(1)	2852(2)	16(1)
C(7)	1679(3)	6968(1)	1986(2)	23(1)
C(8)	1161(3)	7554(1)	1348(2)	26(1)
C(9)	-89(3)	7918(1)	1562(2)	28(1)
C(10)	-822(3)	7704(1)	2418(2)	31(1)
C(11)	-314(3)	7118(1)	3066(2)	23(1)
C(12)	3634(3)	5872(1)	3987(2)	17(1)
C(13)	4386(3)	5726(1)	3090(2)	22(1)
C(14)	6064(3)	5683(1)	3402(2)	27(1)
C(15)	6991(3)	5780(1)	4598(2)	26(1)
C(16)	6250(3)	5915(1)	5491(2)	27(1)
C(17)	4572(3)	5962(1)	5195(2)	22(1)
O(1S)	4586(13)	8656(7)	4981(19)	64(2)
O(2S)	6901(5)	7855(2)	4235(4)	61(1)
C(1S)	6282(8)	8743(4)	5423(7)	66(2)
C(2S)	7239(8)	8528(3)	4601(7)	67(2)
C(3S)	5166(11)	7752(7)	3687(11)	82(2)
C(4S)	4660(20)	7957(11)	4765(17)	82(4)
O(1S')	4760(20)	8533(10)	5250(30)	64(2)
O(2S')	6329(7)	8354(3)	3533(6)	61(1)
C(1S')	5728(14)	9062(5)	5042(9)	66(2)
C(2S')	6094(12)	9014(4)	3882(9)	67(2)
C(3S')	5570(20)	7822(9)	3995(15)	82(2)
C(4S')	4230(30)	7949(16)	4540(30)	82(4)

Table 10 Bond lengths [Å] and angles [°] for DPPO.

P(1)-O(1)	1.4877(15)	O(1S')-C(1S')	1.410(9)
P(1)-C(12)	1.802(2)	O(1S')-C(4S')	1.425(10)
P(1)-C(6)	1.807(2)	O(2S')-C(2S')	1.413(8)
P(1)-C(1)	1.820(2)	O(2S')-C(3S')	1.433(10)
N(1)-C(5)	1.337(3)	C(1S')-C(2S')	1.454(8)
N(1)-C(1)	1.346(3)	C(1S')-H(1SC)	0.9900
C(1)-C(2)	1.390(3)	C(1S')-H(1SD)	0.9900
C(2)-C(3)	1.389(3)	C(2S')-H(2SC)	0.9900
C(2)-H(2A)	0.9500	C(2S')-H(2SD)	0.9900
C(3)-C(4)	1.388(3)	C(3S')-C(4S')	1.489(10)
C(3)-H(3A)	0.9500	C(3S')-H(3SC)	0.9900
C(4)-C(5)	1.399(3)	C(3S')-H(3SD)	0.9900
C(4)-H(4A)	0.9500	C(4S')-H(4SB)	0.9900
C(5)-C(5)#1	1.490(4)	C(4S')-H(4SC)	0.9900
C(6)-C(11)	1.390(3)		
C(6)-C(7)	1.399(3)	O(1)-P(1)-C(12)	112.64(10)
C(7)-C(8)	1.387(3)	O(1)-P(1)-C(6)	113.01(9)
C(7)-H(7A)	0.9500	C(12)-P(1)-C(6)	107.31(10)
C(8)-C(9)	1.384(3)	O(1)-P(1)-C(1)	111.74(9)
C(8)-H(8A)	0.9500	C(12)-P(1)-C(1)	107.84(9)
C(9)-C(10)	1.380(4)	C(6)-P(1)-C(1)	103.76(10)
C(9)-H(9A)	0.9500	C(5)-N(1)-C(1)	117.71(18)
C(10)-C(11)	1.391(3)	N(1)-C(1)-C(2)	123.86(19)
C(10)-H(10A)	0.9500	N(1)-C(1)-P(1)	115.84(15)
C(11)-H(11A)	0.9500	C(2)-C(1)-P(1)	120.23(16)
C(12)-C(13)	1.396(3)	C(3)-C(2)-C(1)	117.6(2)
C(12)-C(17)	1.396(3)	C(3)-C(2)-H(2A)	121.2
C(13)-C(14)	1.391(3)	C(1)-C(2)-H(2A)	121.2
C(13)-H(13A)	0.9500	C(4)-C(3)-C(2)	119.7(2)
C(14)-C(15)	1.384(4)	C(4)-C(3)-H(3A)	120.2
C(14)-H(14A)	0.9500	C(2)-C(3)-H(3A)	120.2
C(15)-C(16)	1.381(4)	C(3)-C(4)-C(5)	118.4(2)
C(15)-H(15A)	0.9500	C(3)-C(4)-H(4A)	120.8
C(16)-C(17)	1.393(3)	C(5)-C(4)-H(4A)	120.8
C(16)-H(16A)	0.9500	N(1)-C(5)-C(4)	122.74(19)
C(17)-H(17A)	0.9500	N(1)-C(5)-C(5)#1	116.2(2)
O(1S)-C(1S)	1.415(9)	C(4)-C(5)-C(5)#1	121.1(2)
O(1S)-C(4S)	1.428(9)	C(11)-C(6)-C(7)	119.7(2)
O(2S)-C(2S)	1.419(6)	C(11)-C(6)-P(1)	117.46(16)
O(2S)-C(3S)	1.462(8)	C(7)-C(6)-P(1)	122.78(16)
C(1S)-C(2S)	1.484(7)	C(8)-C(7)-C(6)	119.7(2)
C(1S)-H(1SA)	0.9900	C(8)-C(7)-H(7A)	120.1
C(1S)-H(1SB)	0.9900	C(6)-C(7)-H(7A)	120.1
C(2S)-H(2SA)	0.9900	C(9)-C(8)-C(7)	120.3(2)
C(2S)-H(2SB)	0.9900	C(9)-C(8)-H(8A)	119.9
C(3S)-C(4S)	1.480(9)	C(7)-C(8)-H(8A)	119.9
C(3S)-H(3SA)	0.9900	C(10)-C(9)-C(8)	120.2(2)
C(3S)-H(3SB)	0.9900	C(10)-C(9)-H(9A)	119.9
C(4S)-H(4SA)	0.9900	C(8)-C(9)-H(9A)	119.9
C(4S)-H(4SD)	0.9900	C(9)-C(10)-C(11)	120.1(2)

C(9)-C(10)-H(10A)	119.9	O(2S)-C(3S)-H(3SA)	112.4
C(11)-C(10)-H(10A)	119.9	C(4S)-C(3S)-H(3SA)	112.4
C(6)-C(11)-C(10)	119.9(2)	O(2S)-C(3S)-H(3SB)	112.4
C(6)-C(11)-H(11A)	120.0	C(4S)-C(3S)-H(3SB)	112.4
C(10)-C(11)-H(11A)	120.0	H(3SA)-C(3S)-H(3SB)	110.0
C(13)-C(12)-C(17)	119.6(2)	O(1S)-C(4S)-C(3S)	117(2)
C(13)-C(12)-P(1)	123.90(17)	O(1S)-C(4S)-H(4SA)	108.0
C(17)-C(12)-P(1)	116.44(17)	C(3S)-C(4S)-H(4SA)	108.0
C(14)-C(13)-C(12)	119.8(2)	O(1S)-C(4S)-H(4SD)	108.0
C(14)-C(13)-H(13A)	120.1	C(3S)-C(4S)-H(4SD)	108.0
C(12)-C(13)-H(13A)	120.1	H(4SA)-C(4S)-H(4SD)	107.2
C(15)-C(14)-C(13)	120.4(2)	C(1S')-O(1S')-C(4S')	129(3)
C(15)-C(14)-H(14A)	119.8	C(2S')-O(2S')-C(3S')	118.4(10)
C(13)-C(14)-H(14A)	119.8	O(1S')-C(1S')-C(2S')	113.4(16)
C(16)-C(15)-C(14)	120.0(2)	O(1S')-C(1S')-H(1SC)	108.9
C(16)-C(15)-H(15A)	120.0	C(2S')-C(1S')-H(1SC)	108.9
C(14)-C(15)-H(15A)	120.0	O(1S')-C(1S')-H(1SD)	108.9
C(15)-C(16)-C(17)	120.4(2)	C(2S')-C(1S')-H(1SD)	108.9
C(15)-C(16)-H(16A)	119.8	H(1SC)-C(1S')-H(1SD)	107.7
C(17)-C(16)-H(16A)	119.8	O(2S')-C(2S')-C(1S')	114.0(8)
C(16)-C(17)-C(12)	119.8(2)	O(2S')-C(2S')-H(2SC)	108.7
C(16)-C(17)-H(17A)	120.1	C(1S')-C(2S')-H(2SC)	108.7
C(12)-C(17)-H(17A)	120.1	O(2S')-C(2S')-H(2SD)	108.7
C(1S)-O(1S)-C(4S)	95.0(13)	C(1S')-C(2S')-H(2SD)	108.7
C(2S)-O(2S)-C(3S)	111.1(7)	H(2SC)-C(2S')-H(2SD)	107.6
O(1S)-C(1S)-C(2S)	116.5(12)	O(2S')-C(3S')-C(4S')	121(2)
O(1S)-C(1S)-H(1SA)	108.2	O(2S')-C(3S')-H(3SC)	107.0
C(2S)-C(1S)-H(1SA)	108.2	C(4S')-C(3S')-H(3SC)	107.0
O(1S)-C(1S)-H(1SB)	108.2	O(2S')-C(3S')-H(3SD)	107.0
C(2S)-C(1S)-H(1SB)	108.2	C(4S')-C(3S')-H(3SD)	107.0
H(1SA)-C(1S)-H(1SB)	107.3	H(3SC)-C(3S')-H(3SD)	106.7
O(2S)-C(2S)-C(1S)	111.0(5)	O(1S')-C(4S')-C(3S')	102(3)
O(2S)-C(2S)-H(2SA)	109.4	O(1S')-C(4S')-H(4SB)	111.3
C(1S)-C(2S)-H(2SA)	109.4	C(3S')-C(4S')-H(4SB)	111.3
O(2S)-C(2S)-H(2SB)	109.4	O(1S')-C(4S')-H(4SC)	111.3
C(1S)-C(2S)-H(2SB)	109.4	C(3S')-C(4S')-H(4SC)	111.3
H(2SA)-C(2S)-H(2SB)	108.0	H(4SB)-C(4S')-H(4SC)	109.2
O(2S)-C(3S)-C(4S)	96.6(10)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

Table 11 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for DPPO. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	16(1)	15(1)	14(1)	0(1)	5(1)	0(1)
O(1)	21(1)	20(1)	17(1)	1(1)	8(1)	-1(1)
N(1)	18(1)	15(1)	16(1)	0(1)	6(1)	0(1)
C(1)	15(1)	16(1)	16(1)	2(1)	4(1)	2(1)
C(2)	22(1)	18(1)	17(1)	2(1)	8(1)	1(1)
C(3)	28(1)	20(1)	24(1)	2(1)	11(1)	-8(1)
C(4)	28(1)	20(1)	18(1)	-3(1)	8(1)	-7(1)
C(5)	18(1)	15(1)	17(1)	1(1)	6(1)	1(1)
C(6)	18(1)	16(1)	15(1)	0(1)	3(1)	-1(1)
C(7)	25(1)	22(1)	24(1)	3(1)	11(1)	2(1)
C(8)	31(1)	25(1)	24(1)	6(1)	10(1)	-1(1)
C(9)	36(1)	20(1)	28(1)	6(1)	8(1)	5(1)
C(10)	35(1)	27(1)	35(1)	5(1)	15(1)	14(1)
C(11)	26(1)	23(1)	23(1)	3(1)	12(1)	4(1)
C(12)	17(1)	14(1)	20(1)	2(1)	6(1)	0(1)
C(13)	21(1)	26(1)	21(1)	0(1)	6(1)	3(1)
C(14)	22(1)	31(1)	31(1)	2(1)	13(1)	4(1)
C(15)	16(1)	25(1)	37(1)	2(1)	6(1)	0(1)
C(16)	22(1)	29(1)	26(1)	0(1)	1(1)	-3(1)
C(17)	22(1)	22(1)	20(1)	0(1)	5(1)	-2(1)
O(1S)	57(3)	53(5)	89(9)	4(4)	32(3)	20(3)
O(2S)	46(2)	77(3)	68(3)	-30(2)	31(2)	-9(2)
C(1S)	61(4)	65(5)	72(5)	-26(4)	16(3)	2(3)
C(2S)	54(3)	71(4)	86(4)	-31(3)	36(3)	-31(3)
C(3S)	36(6)	93(4)	119(8)	-69(5)	24(5)	-40(4)
C(4S)	100(10)	58(3)	113(8)	-11(5)	69(7)	-18(6)
O(1S')	57(3)	53(5)	89(9)	4(4)	32(3)	20(3)
O(2S')	46(2)	77(3)	68(3)	-30(2)	31(2)	-9(2)
C(1S')	61(4)	65(5)	72(5)	-26(4)	16(3)	2(3)
C(2S')	54(3)	71(4)	86(4)	-31(3)	36(3)	-31(3)
C(3S')	36(6)	93(4)	119(8)	-69(5)	24(5)	-40(4)
C(4S')	100(10)	58(3)	113(8)	-11(5)	69(7)	-18(6)

Table 12 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for DPPO.

	x	y	z	U(eq)
H(2A)	-552	4831	3725	22
H(3A)	-1930	4070	2208	27
H(4A)	-1652	4156	229	26
H(7A)	2535	6718	1836	28
H(8A)	1666	7705	761	31
H(9A)	-444	8318	1119	34
H(10A)	-1676	7958	2566	38
H(11A)	-822	6971	3654	27
H(13A)	3754	5656	2269	27
H(14A)	6576	5587	2790	32
H(15A)	8137	5753	4804	32
H(16A)	6889	5977	6313	32
H(17A)	4068	6056	5812	26
H(1SA)	6679	8494	6200	80
H(1SB)	6504	9221	5612	80
H(2SA)	6979	8818	3870	80
H(2SB)	8407	8576	5029	80
H(3SA)	4896	7280	3460	99
H(3SB)	4712	8044	2972	99
H(4SA)	3582	7765	4684	99
H(4SD)	5425	7755	5498	99
H(1SC)	6756	9070	5711	80
H(1SD)	5161	9488	5066	80
H(2SC)	5196	9217	3238	80
H(2SD)	7084	9275	3935	80
H(3SC)	6430	7588	4622	99
H(3SD)	5155	7503	3315	99
H(4SB)	3192	8029	3898	99
H(4SC)	4087	7571	5057	99

Table 13 Torsion angles [°] for DPPO.

C(5)-N(1)-C(1)-C(2)	0.4(3)	P(1)-C(6)-C(11)-C(10)	-177.79(19)
C(5)-N(1)-C(1)-P(1)	-176.57(15)	C(9)-C(10)-C(11)-C(6)	0.1(4)
O(1)-P(1)-C(1)-N(1)	169.28(14)	O(1)-P(1)-C(12)-C(13)	164.79(18)
C(12)-P(1)-C(1)-N(1)	-66.40(17)	C(6)-P(1)-C(12)-C(13)	-70.2(2)
C(6)-P(1)-C(1)-N(1)	47.22(17)	C(1)-P(1)-C(12)-C(13)	41.0(2)
O(1)-P(1)-C(1)-C(2)	-7.8(2)	O(1)-P(1)-C(12)-C(17)	-16.8(2)
C(12)-P(1)-C(1)-C(2)	116.48(18)	C(6)-P(1)-C(12)-C(17)	108.20(18)
C(6)-P(1)-C(1)-C(2)	-129.90(17)	C(1)-P(1)-C(12)-C(17)	-140.57(17)
N(1)-C(1)-C(2)-C(3)	-0.6(3)	C(17)-C(12)-C(13)-C(14)	-1.2(3)
P(1)-C(1)-C(2)-C(3)	176.27(17)	P(1)-C(12)-C(13)-C(14)	177.17(18)
C(1)-C(2)-C(3)-C(4)	0.2(3)	C(12)-C(13)-C(14)-C(15)	0.5(4)
C(2)-C(3)-C(4)-C(5)	0.3(3)	C(13)-C(14)-C(15)-C(16)	0.5(4)
C(1)-N(1)-C(5)-C(4)	0.2(3)	C(14)-C(15)-C(16)-C(17)	-0.7(4)
C(1)-N(1)-C(5)-C(5)#1	179.5(2)	C(15)-C(16)-C(17)-C(12)	0.0(4)
C(3)-C(4)-C(5)-N(1)	-0.5(3)	C(13)-C(12)-C(17)-C(16)	1.0(3)
C(3)-C(4)-C(5)-C(5)#1	-179.9(2)	P(1)-C(12)-C(17)-C(16)	-177.52(18)
O(1)-P(1)-C(6)-C(11)	-21.3(2)	C(4S)-O(1S)-C(1S)-C(2S)	56.2(14)
C(12)-P(1)-C(6)-C(11)	-146.05(18)	C(3S)-O(2S)-C(2S)-C(1S)	54.5(10)
C(1)-P(1)-C(6)-C(11)	99.95(18)	O(1S)-C(1S)-C(2S)-O(2S)	-54.4(11)
O(1)-P(1)-C(6)-C(7)	160.93(18)	C(2S)-O(2S)-C(3S)-C(4S)	-59.7(12)
C(12)-P(1)-C(6)-C(7)	36.2(2)	C(1S)-O(1S)-C(4S)-C(3S)	-74.9(15)
C(1)-P(1)-C(6)-C(7)	-77.8(2)	O(2S)-C(3S)-C(4S)-O(1S)	78.8(14)
C(11)-C(6)-C(7)-C(8)	0.0(3)	C(4S')-O(1S')-C(1S')-C(2S')	5(2)
P(1)-C(6)-C(7)-C(8)	177.70(18)	C(3S')-O(2S')-C(2S')-C(1S')	25.7(13)
C(6)-C(7)-C(8)-C(9)	-0.2(4)	O(1S')-C(1S')-C(2S')-O(2S')	-35.9(15)
C(7)-C(8)-C(9)-C(10)	0.4(4)	C(2S')-O(2S')-C(3S')-C(4S')	16(2)
C(8)-C(9)-C(10)-C(11)	-0.4(4)	C(1S')-O(1S')-C(4S')-C(3S')	31(3)
C(7)-C(6)-C(11)-C(10)	0.1(4)	O(2S')-C(3S')-C(4S')-O(1S')	-42(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

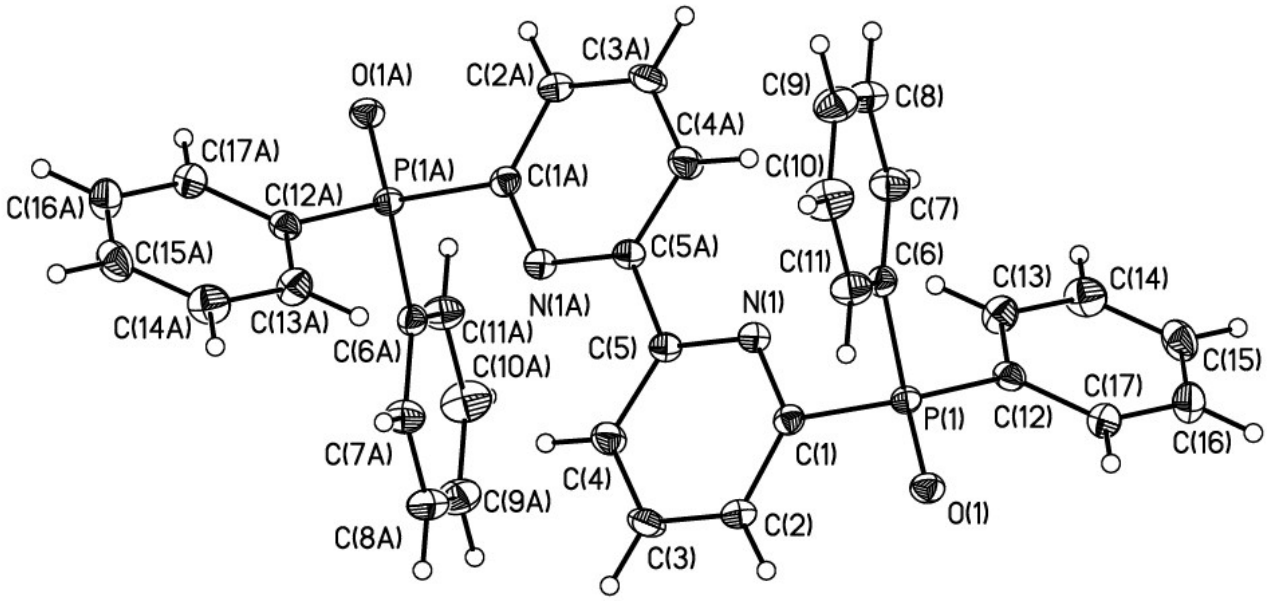

Figure 3 General view of the DPPO structure in crystal. Non-hydrogen atoms are represented as probability ellipsoids of atomic vibrations (p=0.5).

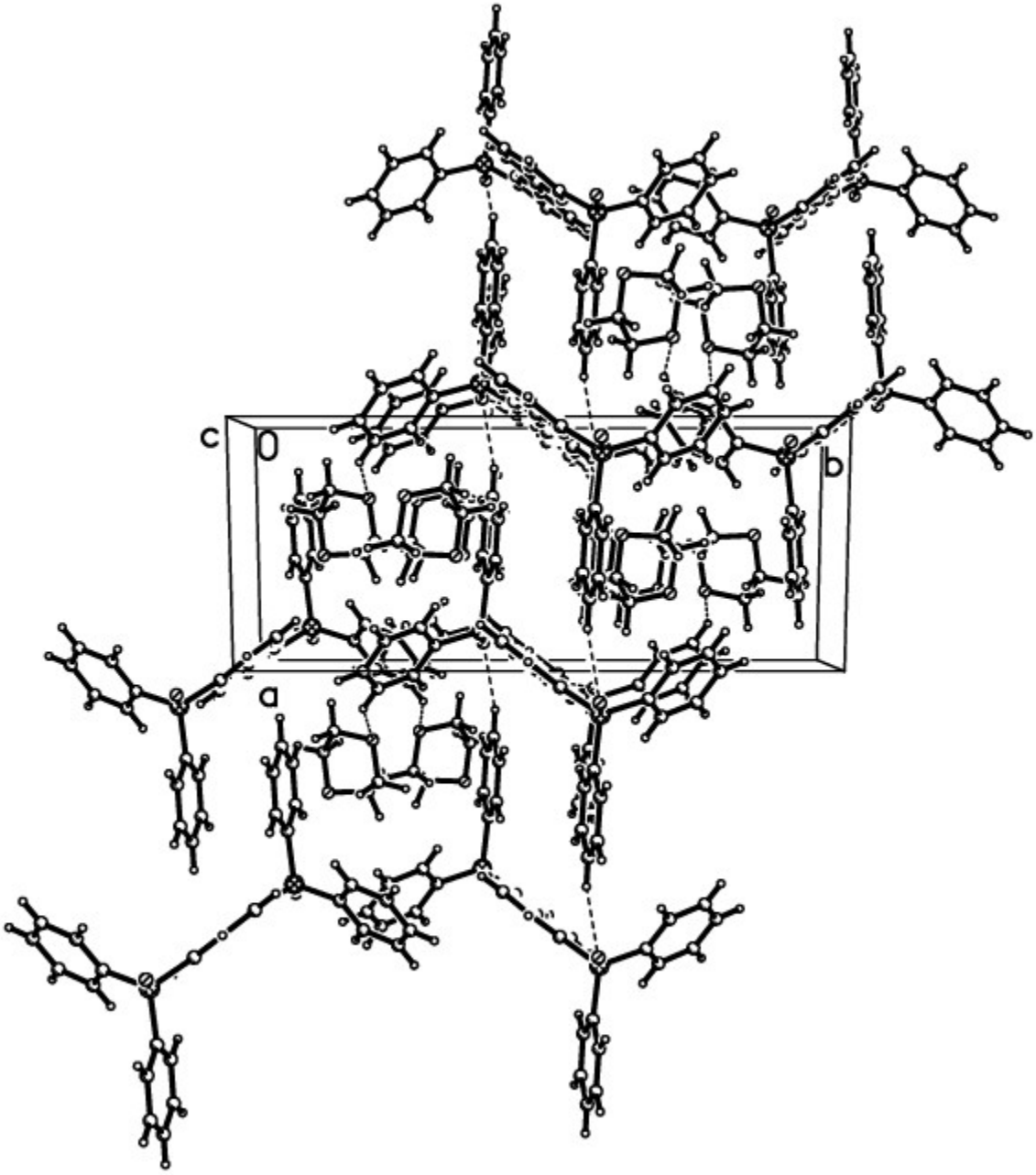

Figure 4 A fragment of DPPO crystal packing along the *ab* plane of the unit cell.

Structure of 9-diphnylphosphinoylphenanthrolinona-2

Table 14 Crystal data and structure refinement for PO-1.

Identification code	a	
Empirical formula	C24 H17 N2 O2 P	
Formula weight	396.36	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.100(3) Å	α= 90.29(3)°.
	b = 10.175(3) Å	β= 104.27(3)°.
	c = 11.792(2) Å	γ = 91.442(19)°.
Volume	941.5(5) $Å^3$	
Z	2	
Density (calculated)	1.398 Mg/m^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	412	
Crystal size	0.160 x 0.130 x 0.080 mm^3	
Theta range for data collection	2.002 to 28.997°.	
Index ranges	-11<=h<=11, -13<=k<=13, -16<=l<=16	
Reflections collected	10451	
Independent reflections	4941 [R(int) = 0.0710]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.995 and 0.961	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4941 / 0 / 330	
Goodness-of-fit on F^2	0.971	
Final R indices [I>2sigma(I)]	R1 = 0.0639, wR2 = 0.1116	
R indices (all data)	R1 = 0.1302, wR2 = 0.1390	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.472 and -0.513 e. $Å^{-3}$	

Table 15 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PO-1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	155(1)	1989(1)	1846(1)	15(1)
O(1)	-1243(2)	1199(2)	1068(2)	21(1)
O(2)	6643(2)	4886(2)	6051(2)	26(1)
N(1)	2269(3)	1787(2)	4004(2)	16(1)
C(2)	1065(3)	1133(3)	3210(2)	15(1)
C(3)	551(3)	-181(3)	3342(2)	18(1)
C(4A)	2602(3)	-195(3)	5208(2)	17(1)
C(4B)	3033(3)	1127(3)	4991(2)	16(1)
C(4)	1335(4)	-836(3)	4337(2)	21(1)
C(5)	3456(4)	-797(3)	6278(2)	22(1)
C(6B)	4351(3)	1817(3)	5835(2)	17(1)
C(6A)	5150(3)	1203(3)	6882(2)	19(1)
C(6)	4666(4)	-113(3)	7087(2)	22(1)
C(7)	6474(4)	1939(3)	7696(2)	24(1)
C(8)	6961(4)	3154(3)	7445(2)	23(1)
C(9)	6181(3)	3791(3)	6341(2)	20(1)
N(10)	4866(3)	3074(2)	5611(2)	18(1)
C(10)	1960(3)	2248(2)	1227(2)	15(1)
C(11)	3246(3)	3193(3)	1685(2)	18(1)
C(12)	4699(4)	3267(3)	1256(2)	22(1)
C(13)	4882(4)	2404(3)	377(2)	23(1)
C(14)	3608(4)	1475(3)	-88(2)	22(1)
C(15)	2147(4)	1395(3)	334(2)	18(1)
C(16)	-503(3)	3580(3)	2230(2)	14(1)
C(17)	-756(3)	3907(3)	3324(2)	19(1)
C(18)	-1451(4)	5109(3)	3509(3)	24(1)
C(19)	-1853(4)	6003(3)	2605(3)	24(1)
C(20)	-1594(4)	5695(3)	1508(3)	24(1)
C(21)	-932(3)	4489(3)	1322(2)	20(1)

Table 16 Bond lengths [Å] and angles [°] for PO-1.

P(1)-O(1)	1.4848(19)	C(21)-H(21)	0.99(3)
P(1)-C(10)	1.803(3)		
P(1)-C(16)	1.806(3)	O(1)-P(1)-C(10)	112.72(11)
P(1)-C(2)	1.830(3)	O(1)-P(1)-C(16)	113.33(11)
O(2)-C(9)	1.243(3)	C(10)-P(1)-C(16)	107.71(12)
N(1)-C(2)	1.335(3)	O(1)-P(1)-C(2)	111.66(12)
N(1)-C(4B)	1.365(3)	C(10)-P(1)-C(2)	103.18(12)
C(2)-C(3)	1.411(4)	C(16)-P(1)-C(2)	107.61(12)
C(3)-C(4)	1.374(4)	C(2)-N(1)-C(4B)	117.1(2)
C(3)-H(3)	0.93(2)	N(1)-C(2)-C(3)	123.7(2)
C(4A)-C(4)	1.404(4)	N(1)-C(2)-P(1)	116.66(19)
C(4A)-C(4B)	1.422(4)	C(3)-C(2)-P(1)	119.5(2)
C(4A)-C(5)	1.430(4)	C(4)-C(3)-C(2)	118.6(3)
C(4B)-C(6B)	1.433(4)	C(4)-C(3)-H(3)	122.6(15)
C(4)-H(4)	0.96(3)	C(2)-C(3)-H(3)	118.8(15)
C(5)-C(6)	1.361(4)	C(4)-C(4A)-C(4B)	116.9(2)
C(5)-H(5)	0.92(3)	C(4)-C(4A)-C(5)	123.7(3)
C(6B)-N(10)	1.382(3)	C(4B)-C(4A)-C(5)	119.4(2)
C(6B)-C(6A)	1.402(3)	N(1)-C(4B)-C(4A)	123.5(2)
C(6A)-C(6)	1.425(4)	N(1)-C(4B)-C(6B)	117.3(2)
C(6A)-C(7)	1.441(4)	C(4A)-C(4B)-C(6B)	119.2(2)
C(6)-H(6)	0.95(3)	C(3)-C(4)-C(4A)	120.2(3)
C(7)-C(8)	1.344(4)	C(3)-C(4)-H(4)	120.4(16)
C(7)-H(7)	1.01(3)	C(4A)-C(4)-H(4)	119.4(15)
C(8)-C(9)	1.462(4)	C(6)-C(5)-C(4A)	120.5(3)
C(8)-H(8)	0.92(3)	C(6)-C(5)-H(5)	121.8(17)
C(9)-N(10)	1.383(3)	C(4A)-C(5)-H(5)	117.7(17)
N(10)-H(10N)	0.86(3)	N(10)-C(6B)-C(6A)	119.8(2)
C(10)-C(15)	1.401(3)	N(10)-C(6B)-C(4B)	120.3(2)
C(10)-C(11)	1.403(4)	C(6A)-C(6B)-C(4B)	119.9(2)
C(11)-C(12)	1.391(4)	C(6B)-C(6A)-C(6)	119.6(2)
C(11)-H(11)	0.98(3)	C(6B)-C(6A)-C(7)	117.6(3)
C(12)-C(13)	1.393(4)	C(6)-C(6A)-C(7)	122.9(2)
C(12)-H(12)	0.95(3)	C(5)-C(6)-C(6A)	121.3(3)
C(13)-C(14)	1.387(4)	C(5)-C(6)-H(6)	121.0(17)
C(13)-H(13)	0.96(3)	C(6A)-C(6)-H(6)	117.7(17)
C(14)-C(15)	1.393(4)	C(8)-C(7)-C(6A)	121.2(3)
C(14)-H(14)	0.91(3)	C(8)-C(7)-H(7)	124.7(16)
C(15)-H(15)	0.96(3)	C(6A)-C(7)-H(7)	114.1(16)
C(16)-C(17)	1.395(3)	C(7)-C(8)-C(9)	122.0(3)
C(16)-C(21)	1.402(4)	C(7)-C(8)-H(8)	119.9(18)
C(17)-C(18)	1.397(4)	C(9)-C(8)-H(8)	118.0(18)
C(17)-H(17)	0.97(3)	O(2)-C(9)-N(10)	121.1(2)
C(18)-C(19)	1.386(4)	O(2)-C(9)-C(8)	124.1(2)
C(18)-H(18)	0.99(3)	N(10)-C(9)-C(8)	114.8(3)
C(19)-C(20)	1.396(4)	C(6B)-N(10)-C(9)	124.6(2)
C(19)-H(19)	0.99(3)	C(6B)-N(10)-H(10N)	119.7(19)
C(20)-C(21)	1.389(4)	C(9)-N(10)-H(10N)	115.8(19)
C(20)-H(20)	0.96(3)	C(15)-C(10)-C(11)	119.5(2)

C(15)-C(10)-P(1)	118.3(2)	C(17)-C(16)-P(1)	124.4(2)
C(11)-C(10)-P(1)	121.9(2)	C(21)-C(16)-P(1)	116.5(2)
C(12)-C(11)-C(10)	119.8(3)	C(16)-C(17)-C(18)	120.7(3)
C(12)-C(11)-H(11)	119.1(16)	C(16)-C(17)-H(17)	121.5(16)
C(10)-C(11)-H(11)	121.1(16)	C(18)-C(17)-H(17)	117.7(16)
C(11)-C(12)-C(13)	120.2(3)	C(19)-C(18)-C(17)	119.8(3)
C(11)-C(12)-H(12)	118.9(17)	C(19)-C(18)-H(18)	117.7(16)
C(13)-C(12)-H(12)	120.8(17)	C(17)-C(18)-H(18)	122.5(16)
C(14)-C(13)-C(12)	120.3(3)	C(18)-C(19)-C(20)	120.2(3)
C(14)-C(13)-H(13)	118.7(17)	C(18)-C(19)-H(19)	119.0(17)
C(12)-C(13)-H(13)	120.9(17)	C(20)-C(19)-H(19)	120.9(17)
C(13)-C(14)-C(15)	119.9(3)	C(21)-C(20)-C(19)	119.9(3)
C(13)-C(14)-H(14)	123.0(16)	C(21)-C(20)-H(20)	121.0(17)
C(15)-C(14)-H(14)	117.1(16)	C(19)-C(20)-H(20)	119.1(17)
C(14)-C(15)-C(10)	120.3(3)	C(20)-C(21)-C(16)	120.7(3)
C(14)-C(15)-H(15)	119.2(17)	C(20)-C(21)-H(21)	120.9(16)
C(10)-C(15)-H(15)	120.5(17)	C(16)-C(21)-H(21)	118.4(16)
C(17)-C(16)-C(21)	118.8(3)		

Symmetry transformations used to generate equivalent atoms:

Table 17 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for PO-1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	14(1)	14(1)	18(1)	0(1)	4(1)	1(1)
O(1)	16(1)	18(1)	26(1)	-6(1)	2(1)	-1(1)
O(2)	27(1)	21(1)	26(1)	1(1)	1(1)	-1(1)
N(1)	13(1)	17(1)	19(1)	2(1)	6(1)	4(1)
C(2)	12(1)	16(1)	20(1)	2(1)	10(1)	3(1)
C(3)	14(1)	17(1)	24(1)	-2(1)	9(1)	0(1)
C(4A)	15(1)	17(1)	23(1)	4(1)	12(1)	6(1)
C(4B)	16(1)	16(1)	19(1)	1(1)	9(1)	4(1)
C(4)	23(2)	14(1)	31(2)	2(1)	16(1)	2(1)
C(5)	23(2)	17(2)	30(2)	9(1)	16(1)	6(1)
C(6B)	18(2)	16(1)	19(1)	2(1)	10(1)	5(1)
C(6A)	18(2)	21(2)	20(1)	1(1)	10(1)	8(1)
C(6)	21(2)	25(2)	22(1)	10(1)	10(1)	12(1)
C(7)	24(2)	29(2)	18(1)	3(1)	4(1)	11(1)
C(8)	21(2)	27(2)	20(1)	-3(1)	2(1)	5(1)
C(9)	19(2)	20(2)	22(1)	-3(1)	6(1)	4(1)
N(10)	21(1)	17(1)	17(1)	2(1)	3(1)	4(1)
C(10)	13(1)	14(1)	17(1)	4(1)	3(1)	5(1)
C(11)	17(2)	18(1)	19(1)	-1(1)	5(1)	1(1)
C(12)	17(2)	26(2)	24(1)	1(1)	5(1)	-3(1)
C(13)	15(2)	32(2)	24(1)	6(1)	7(1)	5(1)
C(14)	26(2)	24(2)	16(1)	0(1)	5(1)	10(1)
C(15)	19(2)	16(1)	18(1)	-1(1)	2(1)	3(1)
C(16)	7(1)	17(1)	19(1)	-2(1)	2(1)	0(1)
C(17)	20(2)	20(2)	18(1)	3(1)	3(1)	2(1)
C(18)	22(2)	25(2)	24(1)	-7(1)	5(1)	4(1)
C(19)	18(2)	18(2)	38(2)	-2(1)	10(1)	7(1)
C(20)	22(2)	19(2)	31(2)	10(1)	8(1)	5(1)
C(21)	17(2)	23(2)	21(1)	2(1)	7(1)	1(1)

Table 18 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for PO-1.

	x	y	z	U(eq)
H(3)	-310(30)	-570(20)	2760(20)	12(7)
H(4)	1010(30)	-1730(30)	4450(20)	19(7)
H(5)	3160(30)	-1650(30)	6400(20)	23(8)
H(6)	5240(30)	-510(30)	7800(20)	20(7)
H(7)	6990(30)	1450(30)	8440(20)	24(8)
H(8)	7850(40)	3590(30)	7960(20)	28(8)
H(10N)	4340(40)	3460(30)	4980(20)	22(8)
H(11)	3150(30)	3800(30)	2310(20)	24(8)
H(12)	5550(40)	3920(30)	1570(20)	22(8)
H(13)	5910(40)	2400(30)	110(20)	27(8)
H(14)	3680(30)	890(20)	-660(20)	13(7)
H(15)	1270(30)	760(30)	0(20)	25(8)
H(17)	-450(30)	3320(30)	3980(20)	17(7)
H(18)	-1640(30)	5370(30)	4280(20)	20(7)
H(19)	-2330(40)	6860(30)	2750(20)	31(8)
H(20)	-1880(30)	6320(30)	890(20)	24(8)
H(21)	-770(30)	4250(30)	540(20)	26(8)

Table 19 Torsion angles [°] for PO-1.

C(4B)-N(1)-C(2)-C(3)	0.2(4)	C(7)-C(8)-C(9)-O(2)	-176.6(3)
C(4B)-N(1)-C(2)-P(1)	-175.86(18)	C(7)-C(8)-C(9)-N(10)	2.7(4)
O(1)-P(1)-C(2)-N(1)	-176.32(18)	C(6A)-C(6B)-N(10)-C(9)	1.9(4)
C(10)-P(1)-C(2)-N(1)	62.4(2)	C(4B)-C(6B)-N(10)-C(9)	-176.6(2)
C(16)-P(1)-C(2)-N(1)	-51.4(2)	O(2)-C(9)-N(10)-C(6B)	175.6(2)
O(1)-P(1)-C(2)-C(3)	7.4(2)	C(8)-C(9)-N(10)-C(6B)	-3.8(4)
C(10)-P(1)-C(2)-C(3)	-113.9(2)	O(1)-P(1)-C(10)-C(15)	-20.2(2)
C(16)-P(1)-C(2)-C(3)	132.4(2)	C(16)-P(1)-C(10)-C(15)	-146.0(2)
N(1)-C(2)-C(3)-C(4)	-0.5(4)	C(2)-P(1)-C(10)-C(15)	100.4(2)
P(1)-C(2)-C(3)-C(4)	175.5(2)	O(1)-P(1)-C(10)-C(11)	165.8(2)
C(2)-N(1)-C(4B)-C(4A)	-0.5(4)	C(16)-P(1)-C(10)-C(11)	40.0(2)
C(2)-N(1)-C(4B)-C(6B)	178.7(2)	C(2)-P(1)-C(10)-C(11)	-73.6(2)
C(4)-C(4A)-C(4B)-N(1)	0.9(4)	C(15)-C(10)-C(11)-C(12)	-0.5(4)
C(5)-C(4A)-C(4B)-N(1)	-179.0(2)	P(1)-C(10)-C(11)-C(12)	173.4(2)
C(4)-C(4A)-C(4B)-C(6B)	-178.3(2)	C(10)-C(11)-C(12)-C(13)	-0.2(4)
C(5)-C(4A)-C(4B)-C(6B)	1.8(4)	C(11)-C(12)-C(13)-C(14)	0.8(4)
C(2)-C(3)-C(4)-C(4A)	1.0(4)	C(12)-C(13)-C(14)-C(15)	-0.6(4)
C(4B)-C(4A)-C(4)-C(3)	-1.2(4)	C(13)-C(14)-C(15)-C(10)	-0.1(4)
C(5)-C(4A)-C(4)-C(3)	178.8(3)	C(11)-C(10)-C(15)-C(14)	0.7(4)
C(4)-C(4A)-C(5)-C(6)	-179.6(3)	P(1)-C(10)-C(15)-C(14)	-173.5(2)
C(4B)-C(4A)-C(5)-C(6)	0.3(4)	O(1)-P(1)-C(16)-C(17)	105.9(2)
N(1)-C(4B)-C(6B)-N(10)	-3.3(4)	C(10)-P(1)-C(16)-C(17)	-128.7(2)
C(4A)-C(4B)-C(6B)-N(10)	175.9(2)	C(2)-P(1)-C(16)-C(17)	-18.0(3)
N(1)-C(4B)-C(6B)-C(6A)	178.2(2)	O(1)-P(1)-C(16)-C(21)	-67.9(2)
C(4A)-C(4B)-C(6B)-C(6A)	-2.6(4)	C(10)-P(1)-C(16)-C(21)	57.5(2)
N(10)-C(6B)-C(6A)-C(6)	-177.3(2)	C(2)-P(1)-C(16)-C(21)	168.12(19)
C(4B)-C(6B)-C(6A)-C(6)	1.3(4)	C(21)-C(16)-C(17)-C(18)	1.1(4)
N(10)-C(6B)-C(6A)-C(7)	1.1(4)	P(1)-C(16)-C(17)-C(18)	-172.6(2)
C(4B)-C(6B)-C(6A)-C(7)	179.6(2)	C(16)-C(17)-C(18)-C(19)	-1.7(4)
C(4A)-C(5)-C(6)-C(6A)	-1.7(4)	C(17)-C(18)-C(19)-C(20)	1.2(4)
C(6B)-C(6A)-C(6)-C(5)	0.9(4)	C(18)-C(19)-C(20)-C(21)	0.0(4)
C(7)-C(6A)-C(6)-C(5)	-177.4(3)	C(19)-C(20)-C(21)-C(16)	-0.6(4)
C(6B)-C(6A)-C(7)-C(8)	-2.0(4)	C(17)-C(16)-C(21)-C(20)	0.1(4)
C(6)-C(6A)-C(7)-C(8)	176.3(3)	P(1)-C(16)-C(21)-C(20)	174.3(2)
C(6A)-C(7)-C(8)-C(9)	0.0(4)		

Symmetry transformations used to generate equivalent atoms:

Table 20 Hydrogen bonds for PO-1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(10)-H(10N)...O(2)#1	0.86(3)	2.13(3)	2.937(3)	155(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

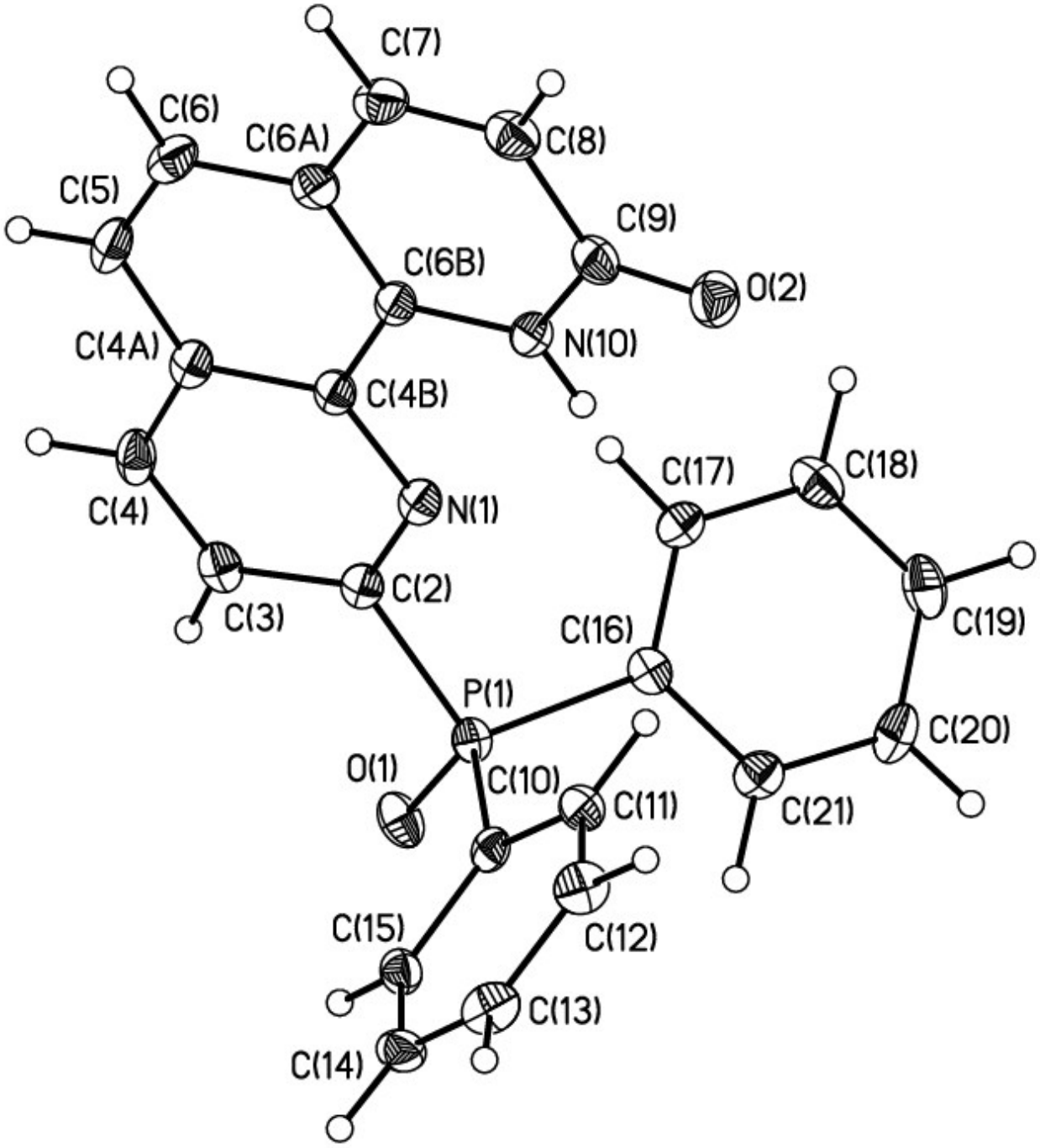

Figure 5 A general view of the PO-1 **structure in representation of non-hydrogen atoms by probability ellipsoids of atomic displacements (p=0.5).**

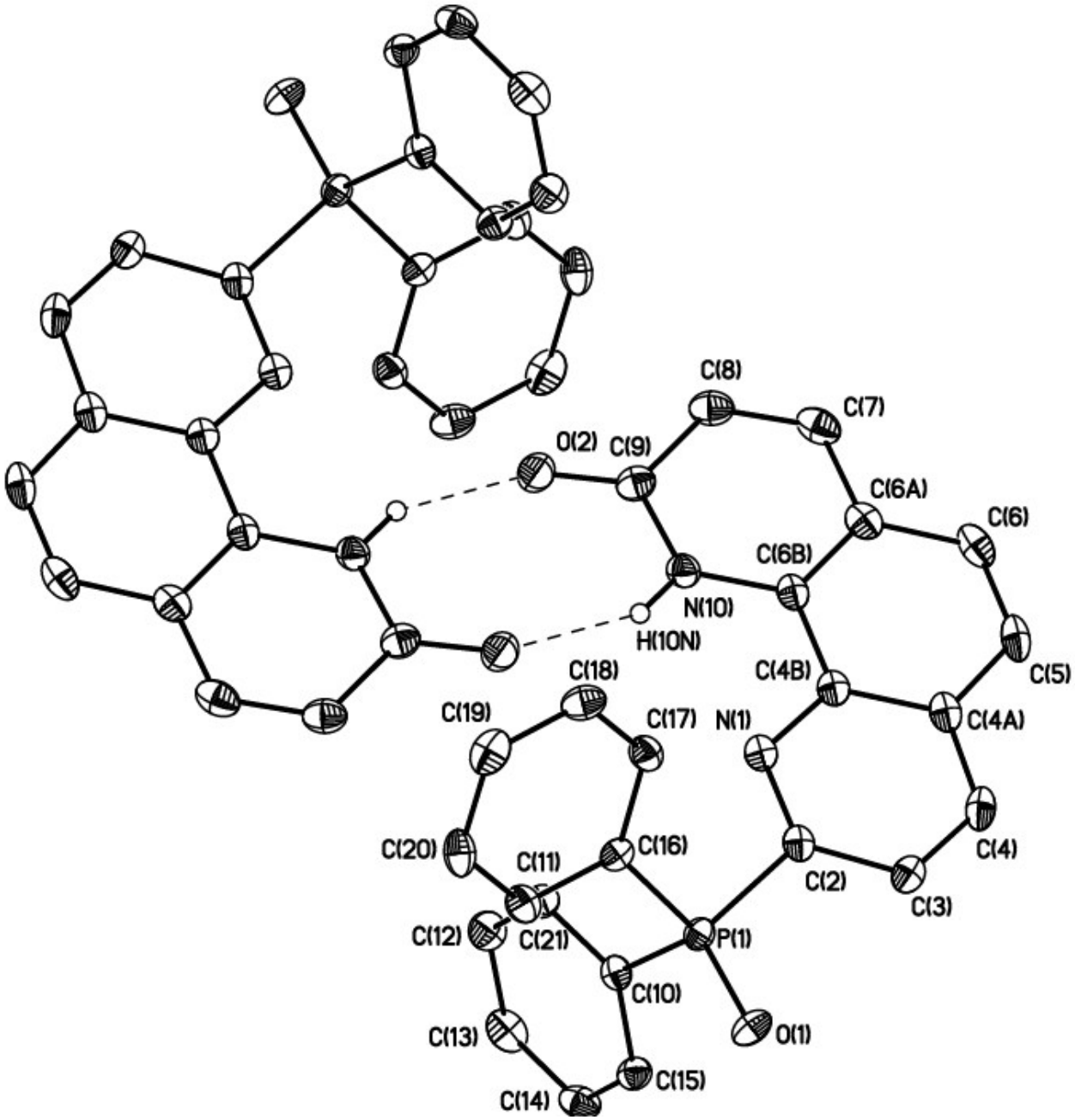

Figure 6 The centrosymmetric hydrogen-bonded dimer of PO-1 **in crystal in representation of non-hydrogen atoms by probability ellipsoids of atomic displacements (p=0.5). All hydrogen atoms are omitted for clarity with the only exception of the H(10N) atom involved in the H-bond. Atom labels are presented only for the independent part.**

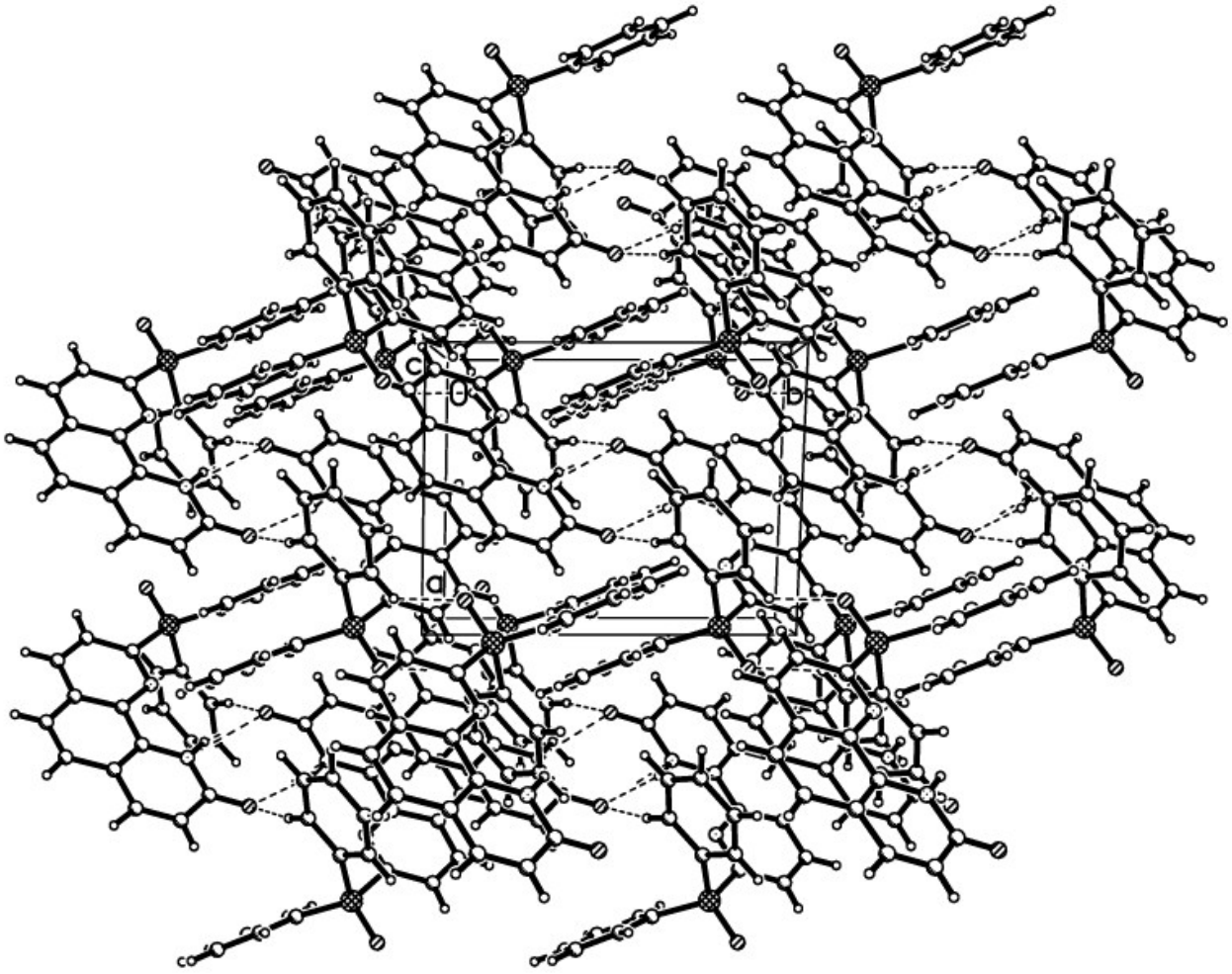

Figure 7 A fragment of the PO-1 **crystal packing along the *ab* plane.**

PnPPO Structure

Table 21 Crystal data and structure refinement for PnPPO.

Identification code	a_sq	
Empirical formula	C36 H26 N2 O2 P2	
Formula weight	580.53	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5375(11) Å	α= 69.800(3)°.
	b = 12.2811(16) Å	β= 84.355(3)°.
	c = 15.439(2) Å	γ = 84.962(3)°.
Volume	1509.3(3) $Å^3$	
Z	2	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.179 mm^{-1}	
F(000)	604	
Crystal size	0.380 x 0.320 x 0.190 mm^3	
Theta range for data collection	2.401 to 27.999°.	
Index ranges	-11<=h<=11, -16<=k<=16, -20<=l<=20	
Reflections collected	16937	
Independent reflections	7281 [R(int) = 0.1196]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.975 and 0.922	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7281 / 0 / 379	
Goodness-of-fit on F^2	0.872	
Final R indices [I>2sigma(I)]	R1 = 0.0738, wR2 = 0.1568	
R indices (all data)	R1 = 0.1998, wR2 = 0.2189	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.469 and -0.541 e. $Å^{-3}$	

Table 22 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PnPPO. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	7401(1)	5221(1)	3190(1)	30(1)
P(2)	11374(2)	370(1)	2170(1)	36(1)
O(1)	6342(3)	6097(2)	3465(2)	36(1)
O(2)	12347(4)	-698(3)	2168(2)	46(1)
N(1)	7699(4)	2864(3)	3714(2)	27(1)
N(2)	9231(4)	974(3)	3343(2)	30(1)
C(1)	7281(5)	5352(4)	2000(3)	32(1)
C(2)	8238(6)	4680(5)	1596(3)	44(1)
C(3)	8052(7)	4744(5)	703(4)	57(2)
C(4)	6898(7)	5490(5)	201(4)	58(2)
C(5)	5955(8)	6178(5)	594(4)	61(2)
C(6)	6115(6)	6117(4)	1497(4)	45(1)
C(7)	9431(5)	5330(3)	3338(3)	25(1)
C(8)	10253(6)	4529(4)	4041(3)	36(1)
C(9)	11781(6)	4706(4)	4158(3)	41(1)
C(10)	12495(6)	5692(4)	3586(3)	38(1)
C(11)	11684(6)	6507(4)	2899(4)	42(1)
C(12)	10163(6)	6326(4)	2778(3)	40(1)
C(13)	6914(5)	3745(4)	3905(3)	27(1)
C(14)	5763(5)	3625(4)	4636(3)	32(1)
C(15)	5460(5)	2520(4)	5226(3)	33(1)
C(16)	6289(5)	1570(4)	5074(3)	28(1)
C(17)	7385(5)	1772(3)	4292(3)	27(1)
C(18)	6085(6)	408(4)	5701(3)	35(1)
C(19)	6897(5)	-500(4)	5557(3)	35(1)
C(20)	8010(5)	-339(4)	4758(3)	31(1)
C(21)	8232(5)	787(4)	4112(3)	28(1)
C(22)	8889(6)	-1275(4)	4593(3)	38(1)
C(23)	9927(6)	-1085(4)	3833(3)	37(1)
C(24)	10055(5)	67(4)	3216(3)	32(1)
C(25)	10082(6)	910(4)	1250(3)	39(1)
C(26)	10344(8)	1904(5)	491(4)	64(2)
C(27)	9359(9)	2246(6)	-229(4)	82(2)
C(28)	8145(9)	1574(6)	-203(4)	73(2)
C(29)	7867(7)	601(5)	537(4)	62(2)
C(30)	8811(7)	256(5)	1266(4)	53(2)
C(31)	12560(6)	1533(4)	2134(3)	32(1)
C(32)	14162(6)	1394(4)	1977(3)	39(1)
C(33)	15137(6)	2233(4)	2010(3)	46(1)
C(34)	14484(7)	3207(4)	2188(3)	43(1)
C(35)	12880(6)	3372(4)	2320(3)	39(1)
C(36)	11898(6)	2525(4)	2304(3)	36(1)

Table 23 Bond lengths [Å] and angles [°] for PnPPO.

P(1)-O(1)	1.491(3)	C(22)-H(22A)	0.9500
P(1)-C(1)	1.799(5)	C(23)-C(24)	1.413(6)
P(1)-C(7)	1.793(4)	C(23)-H(23A)	0.9500
P(1)-C(13)	1.827(4)	C(25)-C(30)	1.399(7)
P(2)-O(2)	1.490(3)	C(25)-C(26)	1.386(7)
P(2)-C(31)	1.805(4)	C(26)-C(27)	1.386(8)
P(2)-C(25)	1.790(5)	C(26)-H(26A)	0.9500
P(2)-C(24)	1.820(5)	C(27)-C(28)	1.370(9)
N(1)-C(13)	1.327(5)	C(27)-H(27A)	0.9500
N(1)-C(17)	1.362(5)	C(28)-C(29)	1.357(8)
N(2)-C(24)	1.327(5)	C(28)-H(28A)	0.9500
N(2)-C(21)	1.356(5)	C(29)-C(30)	1.372(8)
C(1)-C(2)	1.369(7)	C(29)-H(29A)	0.9500
C(1)-C(6)	1.401(6)	C(30)-H(30A)	0.9500
C(2)-C(3)	1.379(7)	C(31)-C(32)	1.372(6)
C(2)-H(2A)	0.9500	C(31)-C(36)	1.394(6)
C(3)-C(4)	1.382(8)	C(32)-C(33)	1.397(6)
C(3)-H(3A)	0.9500	C(32)-H(32A)	0.9500
C(4)-C(5)	1.366(8)	C(33)-C(34)	1.378(7)
C(4)-H(4A)	0.9500	C(33)-H(33A)	0.9500
C(5)-C(6)	1.390(7)	C(34)-C(35)	1.372(7)
C(5)-H(5A)	0.9500	C(34)-H(34A)	0.9500
C(6)-H(6A)	0.9500	C(35)-C(36)	1.400(6)
C(7)-C(12)	1.390(6)	C(35)-H(35A)	0.9500
C(7)-C(8)	1.390(6)	C(36)-H(36A)	0.9500
C(8)-C(9)	1.380(6)		
C(8)-H(8A)	0.9500	O(1)-P(1)-C(1)	112.7(2)
C(9)-C(10)	1.379(6)	O(1)-P(1)-C(7)	112.31(19)
C(9)-H(9A)	0.9500	C(1)-P(1)-C(7)	107.0(2)
C(10)-C(11)	1.377(6)	O(1)-P(1)-C(13)	110.9(2)
C(10)-H(10A)	0.9500	C(1)-P(1)-C(13)	107.6(2)
C(11)-C(12)	1.377(6)	C(7)-P(1)-C(13)	106.04(19)
C(11)-H(11A)	0.9500	O(2)-P(2)-C(31)	112.4(2)
C(12)-H(12A)	0.9500	O(2)-P(2)-C(25)	113.9(2)
C(13)-C(14)	1.398(6)	C(31)-P(2)-C(25)	108.4(2)
C(14)-C(15)	1.378(6)	O(2)-P(2)-C(24)	110.5(2)
C(14)-H(14A)	0.9500	C(31)-P(2)-C(24)	107.1(2)
C(15)-C(16)	1.389(6)	C(25)-P(2)-C(24)	104.1(2)
C(15)-H(15A)	0.9500	C(13)-N(1)-C(17)	117.1(4)
C(16)-C(18)	1.435(6)	C(24)-N(2)-C(21)	118.2(4)
C(16)-C(17)	1.417(6)	C(2)-C(1)-C(6)	119.6(5)
C(17)-C(21)	1.450(6)	C(2)-C(1)-P(1)	121.7(4)
C(18)-C(19)	1.333(6)	C(6)-C(1)-P(1)	118.6(4)
C(18)-H(18A)	0.9500	C(1)-C(2)-C(3)	120.5(5)
C(19)-C(20)	1.448(6)	C(1)-C(2)-H(2A)	119.7
C(19)-H(19A)	0.9500	C(3)-C(2)-H(2A)	119.7
C(20)-C(22)	1.401(6)	C(4)-C(3)-C(2)	120.4(6)
C(20)-C(21)	1.414(6)	C(4)-C(3)-H(3A)	119.8
C(22)-C(23)	1.363(6)	C(2)-C(3)-H(3A)	119.8

C(3)-C(4)-C(5)	119.5(6)	C(19)-C(20)-C(21)	120.1(4)
C(3)-C(4)-H(4A)	120.3	N(2)-C(21)-C(17)	119.1(4)
C(5)-C(4)-H(4A)	120.3	N(2)-C(21)-C(20)	122.1(4)
C(6)-C(5)-C(4)	120.9(6)	C(17)-C(21)-C(20)	118.7(4)
C(6)-C(5)-H(5A)	119.5	C(23)-C(22)-C(20)	120.1(4)
C(4)-C(5)-H(5A)	119.5	C(23)-C(22)-H(22A)	119.9
C(5)-C(6)-C(1)	119.1(5)	C(20)-C(22)-H(22A)	119.9
C(5)-C(6)-H(6A)	120.5	C(22)-C(23)-C(24)	118.3(4)
C(1)-C(6)-H(6A)	120.5	C(22)-C(23)-H(23A)	120.9
C(12)-C(7)-C(8)	118.5(4)	C(24)-C(23)-H(23A)	120.9
C(12)-C(7)-P(1)	117.9(3)	N(2)-C(24)-C(23)	123.4(4)
C(8)-C(7)-P(1)	123.2(3)	N(2)-C(24)-P(2)	116.3(3)
C(9)-C(8)-C(7)	120.4(4)	C(23)-C(24)-P(2)	120.3(4)
C(9)-C(8)-H(8A)	119.8	C(30)-C(25)-C(26)	118.4(5)
C(7)-C(8)-H(8A)	119.8	C(30)-C(25)-P(2)	118.4(4)
C(10)-C(9)-C(8)	120.1(5)	C(26)-C(25)-P(2)	123.0(4)
C(10)-C(9)-H(9A)	119.9	C(27)-C(26)-C(25)	120.7(6)
C(8)-C(9)-H(9A)	119.9	C(27)-C(26)-H(26A)	119.7
C(9)-C(10)-C(11)	120.2(5)	C(25)-C(26)-H(26A)	119.7
C(9)-C(10)-H(10A)	119.9	C(28)-C(27)-C(26)	119.6(6)
C(11)-C(10)-H(10A)	119.9	C(28)-C(27)-H(27A)	120.2
C(10)-C(11)-C(12)	119.7(4)	C(26)-C(27)-H(27A)	120.2
C(10)-C(11)-H(11A)	120.2	C(27)-C(28)-C(29)	120.5(6)
C(12)-C(11)-H(11A)	120.2	C(27)-C(28)-H(28A)	119.8
C(7)-C(12)-C(11)	121.1(4)	C(29)-C(28)-H(28A)	119.8
C(7)-C(12)-H(12A)	119.5	C(30)-C(29)-C(28)	121.0(6)
C(11)-C(12)-H(12A)	119.5	C(30)-C(29)-H(29A)	119.5
N(1)-C(13)-C(14)	124.5(4)	C(28)-C(29)-H(29A)	119.5
N(1)-C(13)-P(1)	118.2(3)	C(29)-C(30)-C(25)	119.9(5)
C(14)-C(13)-P(1)	117.3(3)	C(29)-C(30)-H(30A)	120.1
C(15)-C(14)-C(13)	118.2(4)	C(25)-C(30)-H(30A)	120.1
C(15)-C(14)-H(14A)	120.9	C(32)-C(31)-C(36)	120.1(4)
C(13)-C(14)-H(14A)	120.9	C(32)-C(31)-P(2)	118.0(4)
C(14)-C(15)-C(16)	119.5(4)	C(36)-C(31)-P(2)	121.9(4)
C(14)-C(15)-H(15A)	120.2	C(31)-C(32)-C(33)	120.0(5)
C(16)-C(15)-H(15A)	120.3	C(31)-C(32)-H(32A)	120.0
C(15)-C(16)-C(18)	121.5(4)	C(33)-C(32)-H(32A)	120.0
C(15)-C(16)-C(17)	118.4(4)	C(32)-C(33)-C(34)	119.9(5)
C(18)-C(16)-C(17)	120.1(4)	C(32)-C(33)-H(33A)	120.1
N(1)-C(17)-C(21)	118.8(4)	C(34)-C(33)-H(33A)	120.1
N(1)-C(17)-C(16)	122.2(4)	C(35)-C(34)-C(33)	120.6(5)
C(21)-C(17)-C(16)	119.0(4)	C(35)-C(34)-H(34A)	119.7
C(19)-C(18)-C(16)	121.3(4)	C(33)-C(34)-H(34A)	119.7
C(19)-C(18)-H(18A)	119.4	C(34)-C(35)-C(36)	119.8(5)
C(16)-C(18)-H(18A)	119.4	C(34)-C(35)-H(35A)	120.1
C(18)-C(19)-C(20)	120.7(4)	C(36)-C(35)-H(35A)	120.1
C(18)-C(19)-H(19A)	119.6	C(31)-C(36)-C(35)	119.6(5)
C(20)-C(19)-H(19A)	119.6	C(31)-C(36)-H(36A)	120.2
C(22)-C(20)-C(19)	122.0(4)	C(35)-C(36)-H(36A)	120.2
C(22)-C(20)-C(21)	117.8(4)		

Symmetry transformations used to generate equivalent atoms:

Table 24 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for PnPPO. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	28(1)	25(1)	34(1)	-6(1)	-5(1)	-4(1)
P(2)	42(1)	27(1)	43(1)	-17(1)	9(1)	-12(1)
O(1)	32(2)	26(2)	48(2)	-10(2)	-3(2)	-1(1)
O(2)	56(2)	29(2)	56(2)	-21(2)	13(2)	-8(2)
N(1)	31(2)	25(2)	25(2)	-8(2)	-6(2)	-4(2)
N(2)	31(2)	30(2)	30(2)	-12(2)	-1(2)	-9(2)
C(1)	34(3)	32(3)	27(2)	0(2)	-10(2)	-12(2)
C(2)	43(3)	59(3)	28(3)	-11(2)	-2(2)	-3(3)
C(3)	53(4)	79(4)	39(3)	-21(3)	11(3)	-15(3)
C(4)	67(4)	73(4)	31(3)	-4(3)	-10(3)	-35(3)
C(5)	75(5)	50(4)	47(4)	8(3)	-27(3)	-19(3)
C(6)	48(3)	34(3)	46(3)	-2(2)	-15(3)	-8(2)
C(7)	27(2)	21(2)	26(2)	-8(2)	-4(2)	-2(2)
C(8)	38(3)	30(3)	37(3)	-5(2)	-5(2)	-6(2)
C(9)	36(3)	43(3)	43(3)	-10(2)	-11(2)	-7(2)
C(10)	33(3)	39(3)	46(3)	-19(2)	-4(2)	-8(2)
C(11)	42(3)	32(3)	50(3)	-9(2)	-5(3)	-13(2)
C(12)	42(3)	32(3)	42(3)	-5(2)	-7(3)	-8(2)
C(13)	25(2)	33(2)	24(2)	-8(2)	-5(2)	-4(2)
C(14)	28(3)	34(3)	34(3)	-13(2)	1(2)	-1(2)
C(15)	32(3)	37(3)	28(3)	-11(2)	2(2)	-5(2)
C(16)	27(3)	31(2)	24(2)	-7(2)	-2(2)	-7(2)
C(17)	25(2)	27(2)	26(2)	-4(2)	-6(2)	-4(2)
C(18)	36(3)	36(3)	30(3)	-7(2)	0(2)	-9(2)
C(19)	36(3)	30(3)	33(3)	-2(2)	-5(2)	-8(2)
C(20)	32(3)	26(2)	35(3)	-6(2)	-5(2)	-8(2)
C(21)	33(3)	26(2)	25(2)	-6(2)	0(2)	-10(2)
C(22)	42(3)	26(2)	37(3)	-2(2)	1(2)	-11(2)
C(23)	39(3)	25(2)	46(3)	-10(2)	2(3)	-5(2)
C(24)	33(3)	27(2)	40(3)	-14(2)	2(2)	-9(2)
C(25)	56(3)	33(3)	29(3)	-12(2)	3(2)	-6(2)
C(26)	97(5)	58(4)	43(4)	-18(3)	-4(4)	-32(4)
C(27)	136(7)	67(4)	40(4)	-7(3)	-21(4)	-30(5)
C(28)	105(6)	76(5)	47(4)	-29(4)	-17(4)	-5(4)
C(29)	57(4)	76(4)	59(4)	-32(4)	3(3)	-12(3)
C(30)	53(4)	57(4)	51(4)	-21(3)	5(3)	-14(3)
C(31)	38(3)	26(2)	29(3)	-5(2)	4(2)	-13(2)
C(32)	46(3)	33(3)	34(3)	-6(2)	3(2)	-7(2)
C(33)	43(3)	44(3)	43(3)	3(2)	-9(3)	-17(3)
C(34)	60(4)	35(3)	30(3)	-2(2)	-9(3)	-21(3)
C(35)	55(4)	29(3)	37(3)	-12(2)	-4(3)	-13(2)
C(36)	44(3)	29(2)	32(3)	-6(2)	1(2)	-11(2)

Table 25 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for PnPPO.

	x	y	z	U(eq)
H(2A)	9036	4166	1934	53
H(3A)	8721	4272	430	69
H(4A)	6762	5524	-411	70
H(5A)	5179	6705	244	73
H(6A)	5443	6589	1769	54
H(8A)	9761	3855	4444	44
H(9A)	12342	4148	4634	49
H(10A)	13549	5808	3666	45
H(11A)	12171	7191	2510	50
H(12A)	9606	6892	2305	48
H(14A)	5205	4287	4725	38
H(15A)	4690	2410	5732	39
H(18A)	5358	283	6228	42
H(19A)	6743	-1260	5983	42
H(22A)	8760	-2044	5010	45
H(23A)	10549	-1710	3722	44
H(26A)	11207	2355	464	77
H(27A)	9524	2941	-738	98
H(28A)	7492	1790	-707	88
H(29A)	7007	153	551	74
H(30A)	8601	-425	1780	63
H(32A)	14609	727	1846	47
H(33A)	16248	2131	1909	56
H(34A)	15151	3770	2219	51
H(35A)	12438	4058	2422	47
H(36A)	10788	2626	2408	43

Table 26 Torsion angles [°] for PnPPO.

O(1)-P(1)-C(1)-C(2)	175.5(4)	C(16)-C(18)-C(19)-C(20)	-0.2(7)
C(7)-P(1)-C(1)-C(2)	51.6(4)	C(18)-C(19)-C(20)-C(22)	179.5(4)
C(13)-P(1)-C(1)-C(2)	-62.0(4)	C(18)-C(19)-C(20)-C(21)	-0.9(7)
O(1)-P(1)-C(1)-C(6)	-8.1(4)	C(24)-N(2)-C(21)-C(17)	176.6(4)
C(7)-P(1)-C(1)-C(6)	-132.0(4)	C(24)-N(2)-C(21)-C(20)	-2.1(6)
C(13)-P(1)-C(1)-C(6)	114.4(4)	N(1)-C(17)-C(21)-N(2)	-4.4(6)
C(6)-C(1)-C(2)-C(3)	-0.6(7)	C(16)-C(17)-C(21)-N(2)	177.2(4)
P(1)-C(1)-C(2)-C(3)	175.7(4)	N(1)-C(17)-C(21)-C(20)	174.4(4)
C(1)-C(2)-C(3)-C(4)	0.2(8)	C(16)-C(17)-C(21)-C(20)	-4.0(6)
C(2)-C(3)-C(4)-C(5)	0.9(8)	C(22)-C(20)-C(21)-N(2)	1.3(7)
C(3)-C(4)-C(5)-C(6)	-1.6(8)	C(19)-C(20)-C(21)-N(2)	-178.3(4)
C(4)-C(5)-C(6)-C(1)	1.1(8)	C(22)-C(20)-C(21)-C(17)	-177.4(4)
C(2)-C(1)-C(6)-C(5)	0.0(7)	C(19)-C(20)-C(21)-C(17)	3.0(6)
P(1)-C(1)-C(6)-C(5)	-176.5(4)	C(19)-C(20)-C(22)-C(23)	-179.8(4)
O(1)-P(1)-C(7)-C(12)	-66.5(4)	C(21)-C(20)-C(22)-C(23)	0.6(7)
C(1)-P(1)-C(7)-C(12)	57.7(4)	C(20)-C(22)-C(23)-C(24)	-1.6(7)
C(13)-P(1)-C(7)-C(12)	172.3(4)	C(21)-N(2)-C(24)-C(23)	1.0(7)
O(1)-P(1)-C(7)-C(8)	106.8(4)	C(21)-N(2)-C(24)-P(2)	179.9(3)
C(1)-P(1)-C(7)-C(8)	-129.0(4)	C(22)-C(23)-C(24)-N(2)	0.9(7)
C(13)-P(1)-C(7)-C(8)	-14.4(4)	C(22)-C(23)-C(24)-P(2)	-178.0(4)
C(12)-C(7)-C(8)-C(9)	-2.0(7)	O(2)-P(2)-C(24)-N(2)	173.8(3)
P(1)-C(7)-C(8)-C(9)	-175.3(4)	C(31)-P(2)-C(24)-N(2)	51.1(4)
C(7)-C(8)-C(9)-C(10)	1.0(8)	C(25)-P(2)-C(24)-N(2)	-63.6(4)
C(8)-C(9)-C(10)-C(11)	0.4(8)	O(2)-P(2)-C(24)-C(23)	-7.3(5)
C(9)-C(10)-C(11)-C(12)	-0.8(8)	C(31)-P(2)-C(24)-C(23)	-130.0(4)
C(8)-C(7)-C(12)-C(11)	1.6(7)	C(25)-P(2)-C(24)-C(23)	115.4(4)
P(1)-C(7)-C(12)-C(11)	175.3(4)	O(2)-P(2)-C(25)-C(30)	68.6(5)
C(10)-C(11)-C(12)-C(7)	-0.2(8)	C(31)-P(2)-C(25)-C(30)	-165.5(4)
C(17)-N(1)-C(13)-C(14)	-2.1(6)	C(24)-P(2)-C(25)-C(30)	-51.7(4)
C(17)-N(1)-C(13)-P(1)	176.0(3)	O(2)-P(2)-C(25)-C(26)	-106.8(5)
O(1)-P(1)-C(13)-N(1)	176.5(3)	C(31)-P(2)-C(25)-C(26)	19.1(5)
C(1)-P(1)-C(13)-N(1)	52.9(4)	C(24)-P(2)-C(25)-C(26)	132.8(5)
C(7)-P(1)-C(13)-N(1)	-61.3(4)	C(30)-C(25)-C(26)-C(27)	0.6(9)
O(1)-P(1)-C(13)-C(14)	-5.2(4)	P(2)-C(25)-C(26)-C(27)	176.1(5)
C(1)-P(1)-C(13)-C(14)	-128.9(4)	C(25)-C(26)-C(27)-C(28)	-2.1(10)
C(7)-P(1)-C(13)-C(14)	117.0(3)	C(26)-C(27)-C(28)-C(29)	2.4(11)
N(1)-C(13)-C(14)-C(15)	2.8(7)	C(27)-C(28)-C(29)-C(30)	-1.3(10)
P(1)-C(13)-C(14)-C(15)	-175.3(3)	C(28)-C(29)-C(30)-C(25)	-0.1(9)
C(13)-C(14)-C(15)-C(16)	-0.4(7)	C(26)-C(25)-C(30)-C(29)	0.5(8)
C(14)-C(15)-C(16)-C(18)	176.1(4)	P(2)-C(25)-C(30)-C(29)	-175.2(4)
C(14)-C(15)-C(16)-C(17)	-2.3(7)	O(2)-P(2)-C(31)-C(32)	9.1(4)
C(13)-N(1)-C(17)-C(21)	-179.3(4)	C(25)-P(2)-C(31)-C(32)	-117.6(4)
C(13)-N(1)-C(17)-C(16)	-0.9(6)	C(24)-P(2)-C(31)-C(32)	130.6(4)
C(15)-C(16)-C(17)-N(1)	3.1(6)	O(2)-P(2)-C(31)-C(36)	-167.8(4)
C(18)-C(16)-C(17)-N(1)	-175.4(4)	C(25)-P(2)-C(31)-C(36)	65.5(4)
C(15)-C(16)-C(17)-C(21)	-178.6(4)	C(24)-P(2)-C(31)-C(36)	-46.3(4)
C(18)-C(16)-C(17)-C(21)	3.0(6)	C(36)-C(31)-C(32)-C(33)	1.6(7)
C(15)-C(16)-C(18)-C(19)	-179.3(4)	P(2)-C(31)-C(32)-C(33)	-175.4(4)
C(17)-C(16)-C(18)-C(19)	-0.9(7)	C(31)-C(32)-C(33)-C(34)	-0.9(7)

C(32)-C(33)-C(34)-C(35)	-1.0(7)	P(2)-C(31)-C(36)-C(35)	176.3(3)
C(33)-C(34)-C(35)-C(36)	2.1(7)	C(34)-C(35)-C(36)-C(31)	-1.3(7)
C(32)-C(31)-C(36)-C(35)	-0.5(7)		

Symmetry transformations used to generate equivalent atoms:

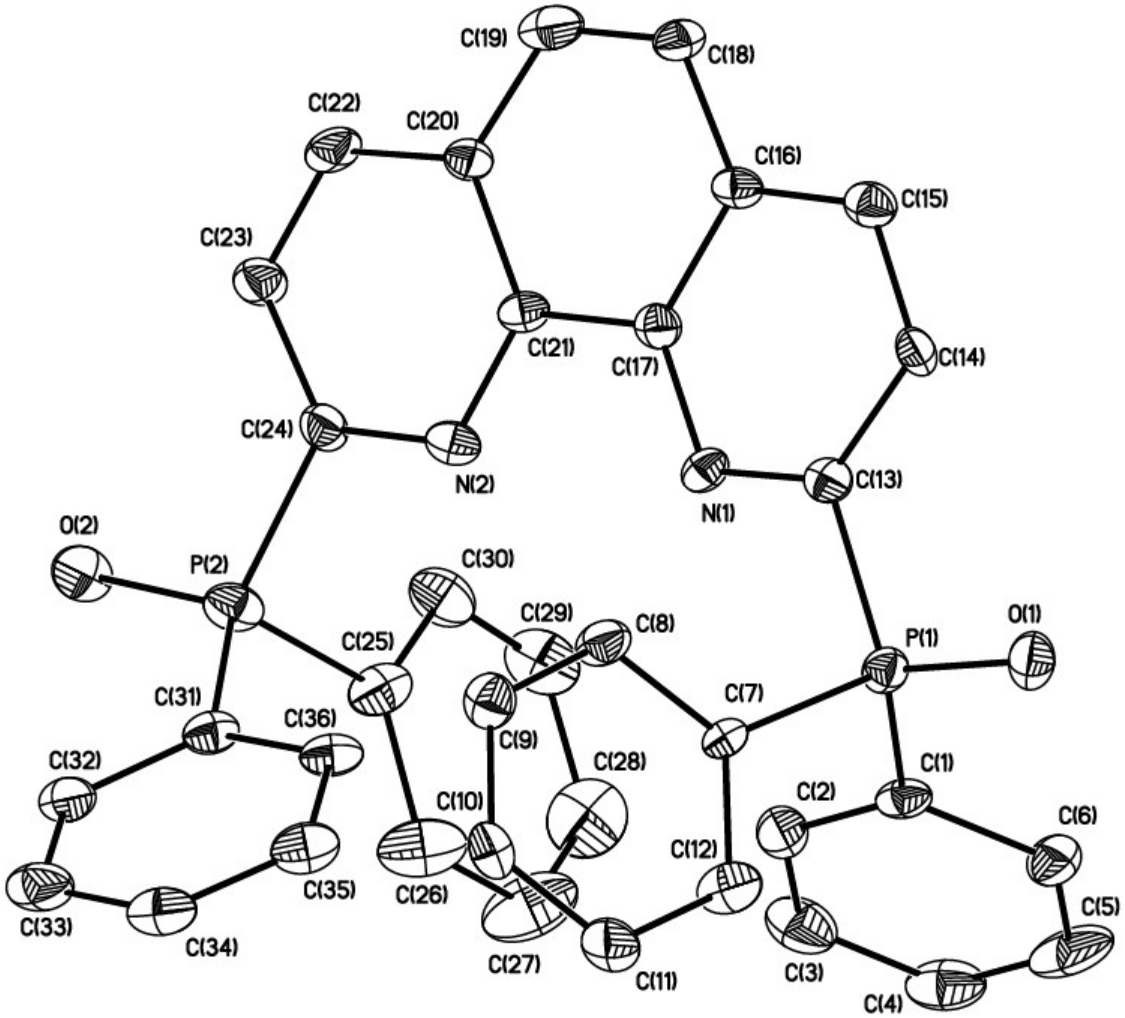

Figure 8 The general view of PnPPO in the representation of non-hydrogen atoms as probability ellipsoids of atomic displacements (p=0.5). Hydrogen atoms are omitted for clarity.

Structure of DPPO**Gd(NO3)3**

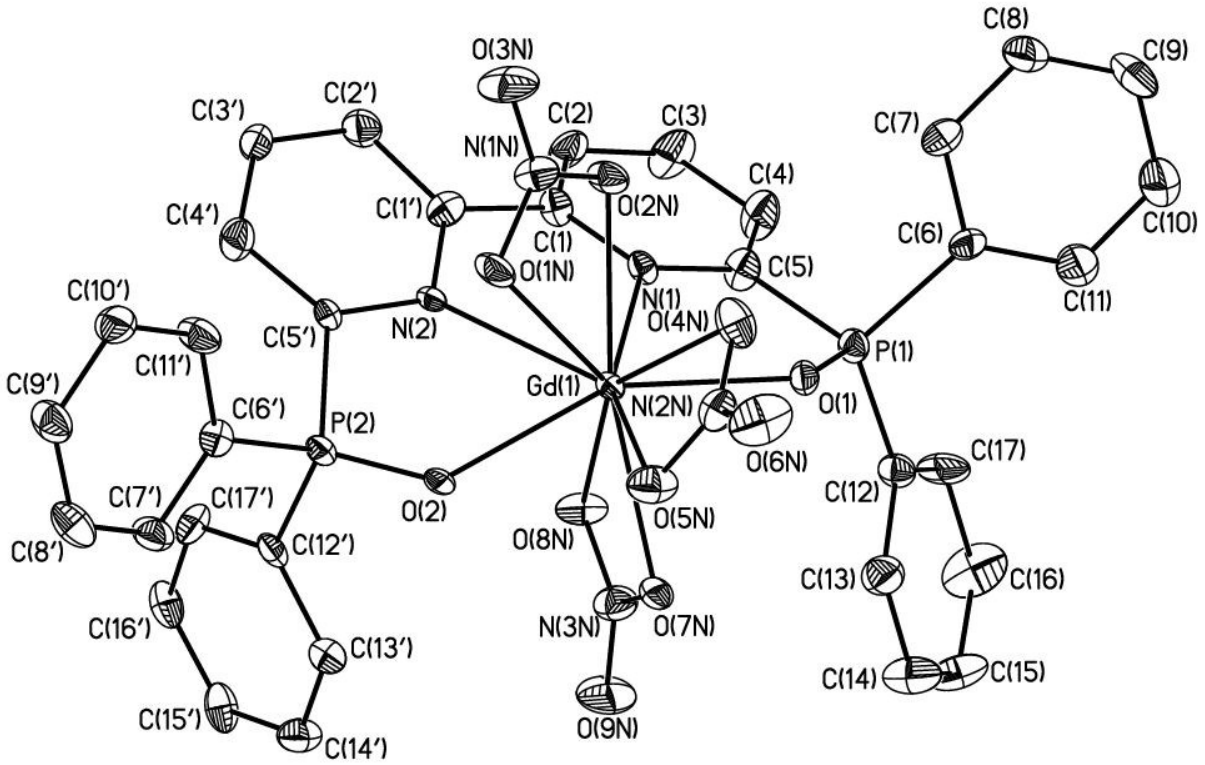

Figure 9 General view of one of the two independent molecules in DPPOGd(NO3)3 with atoms given as thermal ellipsoids (p=50%). Hydrogen atoms are omitted for clarity.

Table 27 Crystal data and structure refinement for DPPOGd(NO3)3.

Identification code	DPPOGd(NO3)3	
Empirical formula	C34 H26 Gd N5 O11 P2	
Formula weight	899.79	
Temperature	120(2) K	
Wavelength	0.71073 E	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 20.593(2) Å	α= 90°.
	b = 17.456(2) Å	β= 90.195(3)°.
	c = 19.150(2) Å	γ = 90°.
Volume	6883.7(14) $Å^3$	
Z	8	
Density (calculated)	1.736 Mg/m^3	
Absorption coefficient	2.090 mm^{-1}	
F(000)	3576	
Crystal size	0.350 x 0.050 x 0.050 mm^3	
Theta range for data collection	0.989 to 27.000°.	
Index ranges	-26<=h<=26, -22<=k<=22, -24<=l<=24	
Reflections collected	71003	
Independent reflections	15030 [R(int) = 0.1374]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15030 / 0 / 955	
Goodness-of-fit on F^2	1.020	
Final R indices [for 10163 rfln with I>2sigma(I)]		R1 = 0.0575, wR2 = 0.1198
R indices (all data)	R1 = 0.0992, wR2 = 0.1401	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.305 and -2.709 e. $Å^{-3}$	

Table 28 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for DPPOGd(NO3)3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Gd(1)	3487(1)	9262(1)	2885(1)	12(1)
Gd(2)	-1538(1)	9137(1)	2180(1)	12(1)
P(1)	2730(1)	9801(1)	1292(1)	15(1)
O(1)	2955(2)	10015(3)	2013(2)	16(1)
P(2)	4586(1)	8040(1)	3693(1)	15(1)
O(2)	4394(2)	8857(3)	3543(3)	17(1)
N(1)	2927(3)	8435(3)	1849(3)	14(1)
N(2)	3606(3)	7741(3)	2871(3)	12(1)
C(1')	3163(4)	7310(4)	2533(4)	17(2)
C(1)	2891(3)	7662(4)	1894(4)	16(2)
C(2')	3000(4)	6585(4)	2758(4)	22(2)
C(2)	2633(4)	7218(4)	1361(4)	23(2)
C(3')	3327(4)	6265(4)	3323(4)	23(2)
C(3)	2408(4)	7568(4)	755(4)	29(2)
C(4')	3820(4)	6675(4)	3638(4)	22(2)
C(4)	2443(4)	8352(4)	703(4)	27(2)
C(5)	2700(4)	8757(4)	1258(4)	19(2)
C(5')	3936(3)	7418(4)	3403(4)	18(2)
C(6')	4743(3)	7830(4)	4595(4)	16(2)
C(6)	1913(4)	10081(4)	1100(4)	20(2)
C(7')	5371(4)	7911(4)	4861(4)	23(2)
C(7)	1425(4)	9760(5)	1505(4)	26(2)
C(8')	5490(4)	7757(5)	5558(4)	28(2)
C(8)	782(4)	9943(5)	1384(5)	35(2)
C(9')	5009(4)	7489(5)	5984(4)	25(2)
C(9)	617(4)	10434(5)	851(5)	37(2)
C(10)	1102(4)	10751(5)	442(5)	38(2)
C(10')	4373(4)	7413(5)	5728(4)	26(2)
C(11')	4249(4)	7600(5)	5035(4)	24(2)
C(11)	1741(4)	10578(5)	571(4)	29(2)
C(12')	5273(3)	7774(4)	3179(4)	16(2)
C(12)	3277(3)	10161(4)	644(4)	17(2)
C(13)	3801(4)	10590(4)	881(4)	26(2)
C(13')	5649(4)	8374(4)	2921(4)	21(2)
C(14')	6168(4)	8216(5)	2482(4)	26(2)
C(14)	4249(4)	10877(5)	418(5)	33(2)
C(15)	4174(4)	10756(5)	-281(5)	33(2)
C(15')	6291(4)	7476(4)	2284(4)	22(2)
C(16')	5929(4)	6881(5)	2534(4)	22(2)
C(16)	3655(5)	10352(5)	-528(4)	40(2)
C(17')	5410(4)	7027(4)	2977(4)	20(2)
C(17)	3204(4)	10046(5)	-69(4)	27(2)
P(1A)	-336(1)	7912(1)	1591(1)	17(1)
O(1A)	-540(2)	8718(3)	1734(3)	19(1)
P(2A)	-2398(1)	9769(1)	3650(1)	15(1)
O(2A)	-2172(2)	9953(3)	2920(2)	16(1)
N(1A)	-1393(3)	7626(3)	2313(3)	17(1)

N(2A)	-2173(3)	8365(3)	3191(3)	16(1)
C(1A)	-1841(3)	7196(4)	2643(4)	18(2)
C(1")	-2237(3)	7600(4)	3170(4)	14(1)
C(2A)	-1914(4)	6426(4)	2507(4)	23(2)
C(2")	-2608(4)	7195(4)	3645(4)	20(2)
C(3")	-2918(4)	7588(5)	4179(4)	25(2)
C(3A)	-1464(4)	6061(4)	2095(4)	27(2)
C(4A)	-964(4)	6475(5)	1803(4)	27(2)
C(4")	-2861(4)	8375(4)	4209(4)	21(2)
C(5")	-2488(4)	8733(4)	3707(4)	17(2)
C(5A)	-955(3)	7267(4)	1908(4)	18(2)
C(6")	-3195(4)	10140(4)	3840(4)	18(2)
C(6A)	-203(4)	7707(4)	692(4)	20(2)
C(7")	-3389(4)	10280(4)	4524(4)	22(2)
C(7A)	-658(4)	7303(5)	295(4)	33(2)
C(8A)	-559(5)	7205(5)	-418(5)	39(2)
C(8")	-4028(4)	10463(5)	4663(5)	29(2)
C(9")	-4464(4)	10506(5)	4119(5)	30(2)
C(9A)	-17(4)	7516(6)	-730(5)	38(2)
C(10")	-4275(4)	10410(5)	3445(4)	27(2)
C(10A)	434(5)	7923(5)	-340(5)	38(2)
C(11A)	339(4)	8027(5)	374(4)	27(2)
C(11")	-3641(4)	10208(4)	3296(4)	26(2)
C(12A)	371(4)	7696(4)	2095(4)	21(2)
C(12")	-1832(3)	10092(4)	4296(4)	17(2)
C(13")	-1463(4)	10722(4)	4127(4)	25(2)
C(13A)	644(4)	6957(4)	2112(4)	26(2)
C(14A)	1147(4)	6804(5)	2580(4)	28(2)
C(14")	-1000(4)	11002(5)	4598(4)	33(2)
C(15")	-900(4)	10630(5)	5212(4)	31(2)
C(15A)	1384(4)	7350(4)	3019(4)	23(2)
C(16A)	1102(4)	8083(5)	3012(4)	27(2)
C(16")	-1268(5)	10003(6)	5388(5)	43(3)
C(17A)	600(4)	8243(5)	2558(4)	26(2)
C(17")	-1744(5)	9729(5)	4934(4)	36(2)
N(3N)	4620(3)	9577(4)	2020(3)	23(2)
O(2N)	2444(2)	8684(3)	3216(3)	21(1)
O(7N)	4402(2)	10065(3)	2445(3)	18(1)
O(8NA)	-869(2)	9022(3)	3247(3)	23(1)
O(5NA)	-1145(3)	10120(3)	1288(3)	27(1)
O(4NA)	-2178(3)	10066(3)	1460(3)	26(1)
O(8N)	4272(2)	8963(3)	1947(3)	22(1)
O(7NA)	-720(2)	10060(3)	2663(3)	20(1)
N(1N)	2573(3)	8566(4)	3846(3)	21(1)
O(4N)	2737(3)	10217(3)	3467(3)	27(1)
N(2NA)	-1702(4)	10377(4)	1136(3)	26(2)
O(1NA)	-2544(2)	8527(3)	1747(3)	20(1)
O(5N)	3753(3)	10360(3)	3658(3)	28(1)
O(2NA)	-1750(2)	8545(3)	1011(3)	22(1)
N(2N)	3182(3)	10593(4)	3772(3)	21(1)
O(1N)	3144(2)	8759(3)	4050(3)	22(1)
O(6NA)	-1782(3)	10885(3)	711(3)	38(2)
N(1NA)	-2344(3)	8367(4)	1143(3)	22(2)
O(9NA)	-76(3)	9794(4)	3532(3)	38(2)

N(3NA)	-534(3)	9626(4)	3155(3)	26(2)
O(9N)	5129(3)	9666(4)	1711(3)	36(2)
O(3N)	2180(3)	8292(4)	4253(3)	35(2)
O(6N)	3058(3)	11142(3)	4151(3)	38(2)
O(3NA)	-2691(3)	8066(4)	702(3)	38(2)

Table 29 Bond lengths [Å] and angles [°] for DPPOGd(NO3)3.

Gd(1)-O(2)	2.359(5)	C(4)-C(5)	1.381(10)
Gd(1)-O(1)	2.388(5)	C(4)-H(4A)	0.9500
Gd(1)-O(2N)	2.457(5)	C(6')-C(11')	1.383(10)
Gd(1)-O(8N)	2.477(5)	C(6')-C(7')	1.394(10)
Gd(1)-O(5N)	2.482(5)	C(6)-C(11)	1.379(11)
Gd(1)-O(7N)	2.498(5)	C(6)-C(7)	1.389(10)
Gd(1)-O(1N)	2.501(5)	C(7')-C(8')	1.383(11)
Gd(1)-O(4N)	2.533(5)	C(7')-H(7'A)	0.9500
Gd(1)-N(2)	2.665(5)	C(7)-C(8)	1.382(11)
Gd(1)-N(1)	2.708(6)	C(7)-H(7A)	0.9500
Gd(1)-N(1N)	2.903(6)	C(8')-C(9')	1.367(11)
Gd(1)-N(3N)	2.920(6)	C(8')-H(8'A)	0.9500
Gd(2)-O(1A)	2.346(5)	C(8)-C(9)	1.374(12)
Gd(2)-O(2A)	2.399(5)	C(8)-H(8A)	0.9500
Gd(2)-O(8NA)	2.469(5)	C(9')-C(10')	1.403(11)
Gd(2)-O(1NA)	2.469(5)	C(9')-H(9'A)	0.9500
Gd(2)-O(4NA)	2.501(5)	C(9)-C(10)	1.386(12)
Gd(2)-O(2NA)	2.502(5)	C(9)-H(9A)	0.9500
Gd(2)-O(7NA)	2.507(5)	C(10)-C(11)	1.370(11)
Gd(2)-O(5NA)	2.555(5)	C(10)-H(10A)	0.9500
Gd(2)-N(1A)	2.666(6)	C(10')-C(11')	1.391(10)
Gd(2)-N(2A)	2.700(6)	C(10')-H(10B)	0.9500
Gd(2)-N(3NA)	2.909(6)	C(11')-H(11A)	0.9500
Gd(2)-N(1NA)	2.911(6)	C(11)-H(11B)	0.9500
P(1)-O(1)	1.503(5)	C(12')-C(17')	1.390(9)
P(1)-C(6)	1.789(8)	C(12')-C(13')	1.395(10)
P(1)-C(12)	1.792(8)	C(12)-C(17)	1.387(10)
P(1)-C(5)	1.824(7)	C(12)-C(13)	1.389(10)
P(2)-O(2)	1.507(5)	C(13)-C(14)	1.376(11)
P(2)-C(12')	1.789(7)	C(13)-H(13A)	0.9500
P(2)-C(6')	1.795(7)	C(13')-C(14')	1.390(11)
P(2)-C(5')	1.809(7)	C(13')-H(13B)	0.9500
N(1)-C(5)	1.346(9)	C(14')-C(15')	1.369(11)
N(1)-C(1)	1.353(9)	C(14')-H(14A)	0.9500
N(2)-C(1')	1.347(9)	C(14)-C(15)	1.363(12)
N(2)-C(5')	1.347(9)	C(14)-H(14B)	0.9500
C(1')-C(2')	1.379(10)	C(15)-C(16)	1.364(12)
C(1')-C(1)	1.479(10)	C(15)-H(15A)	0.9500
C(1)-C(2)	1.385(10)	C(15')-C(16')	1.367(11)
C(2')-C(3')	1.390(10)	C(15')-H(15B)	0.9500
C(2')-H(2'A)	0.9500	C(16')-C(17')	1.390(10)
C(2)-C(3)	1.391(10)	C(16')-H(16A)	0.9500
C(2)-H(2A)	0.9500	C(16)-C(17)	1.387(11)
C(3')-C(4')	1.380(10)	C(16)-H(16B)	0.9500
C(3')-H(3'A)	0.9500	C(17')-H(17A)	0.9500
C(3)-C(4)	1.375(10)	C(17)-H(17B)	0.9500
C(3)-H(3A)	0.9500	P(1A)-O(1A)	1.494(5)
C(4')-C(5')	1.395(10)	P(1A)-C(6A)	1.780(8)
C(4')-H(4'A)	0.9500	P(1A)-C(12A)	1.783(8)

P(1A)-C(5A)	1.807(7)	C(14A)-C(15A)	1.360(11)
P(2A)-O(2A)	1.509(5)	C(14A)-H(14C)	0.9500
P(2A)-C(12")	1.788(7)	C(14")-C(15")	1.359(12)
P(2A)-C(6")	1.802(7)	C(14")-H(14D)	0.9500
P(2A)-C(5")	1.820(7)	C(15")-C(16")	1.373(12)
N(1A)-C(5A)	1.348(9)	C(15")-H(15C)	0.9500
N(1A)-C(1A)	1.348(9)	C(15A)-C(16A)	1.406(11)
N(2A)-C(1")	1.342(9)	C(15A)-H(15D)	0.9500
N(2A)-C(5")	1.348(9)	C(16A)-C(17A)	1.375(11)
C(1A)-C(2A)	1.376(10)	C(16A)-H(16C)	0.9500
C(1A)-C(1")	1.480(10)	C(16")-C(17")	1.393(12)
C(1")-C(2")	1.384(10)	C(16")-H(16D)	0.9500
C(2A)-C(3A)	1.375(11)	C(17A)-H(17C)	0.9500
C(2A)-H(2AA)	0.9500	C(17")-H(17D)	0.9500
C(2")-C(3")	1.388(10)	N(3N)-O(9N)	1.213(8)
C(2")-H(2"A)	0.9500	N(3N)-O(7N)	1.262(8)
C(3")-C(4")	1.380(11)	N(3N)-O(8N)	1.296(8)
C(3")-H(3"A)	0.9500	O(2N)-N(1N)	1.251(7)
C(3A)-C(4A)	1.378(11)	O(8NA)-N(3NA)	1.272(8)
C(3A)-H(3AA)	0.9500	O(5NA)-N(2NA)	1.265(8)
C(4A)-C(5A)	1.397(10)	O(4NA)-N(2NA)	1.284(8)
C(4A)-H(4AA)	0.9500	O(7NA)-N(3NA)	1.268(8)
C(4")-C(5")	1.383(10)	N(1N)-O(3N)	1.223(8)
C(4")-H(4"A)	0.9500	N(1N)-O(1N)	1.282(8)
C(6")-C(11")	1.392(10)	O(4N)-N(2N)	1.267(8)
C(6")-C(7")	1.393(10)	N(2NA)-O(6NA)	1.214(8)
C(6A)-C(11A)	1.391(11)	O(1NA)-N(1NA)	1.262(8)
C(6A)-C(7A)	1.395(11)	O(5N)-N(2N)	1.264(8)
C(7")-C(8")	1.382(11)	O(2NA)-N(1NA)	1.286(8)
C(7")-H(7"A)	0.9500	N(2N)-O(6N)	1.229(8)
C(7A)-C(8A)	1.392(11)	N(1NA)-O(3NA)	1.223(8)
C(7A)-H(7AA)	0.9500	O(9NA)-N(3NA)	1.223(8)
C(8A)-C(9A)	1.379(13)	O(2)-Gd(1)-O(1)	154.03(16)
C(8A)-H(8AA)	0.9500	O(2)-Gd(1)-O(2N)	115.48(16)
C(8")-C(9")	1.375(12)	O(1)-Gd(1)-O(2N)	90.45(16)
C(8")-H(8"A)	0.9500	O(2)-Gd(1)-O(8N)	78.84(18)
C(9")-C(10")	1.360(12)	O(1)-Gd(1)-O(8N)	84.71(17)
C(9")-H(9"A)	0.9500	O(2N)-Gd(1)-O(8N)	132.41(17)
C(9A)-C(10A)	1.387(12)	O(2)-Gd(1)-O(5N)	74.90(18)
C(9A)-H(9AA)	0.9500	O(1)-Gd(1)-O(5N)	95.24(18)
C(10")-C(11")	1.383(11)	O(2N)-Gd(1)-O(5N)	110.76(17)
C(10")-H(10C)	0.9500	O(8N)-Gd(1)-O(5N)	116.82(17)
C(10A)-C(11A)	1.394(11)	O(2)-Gd(1)-O(7N)	75.54(16)
C(10A)-H(10D)	0.9500	O(1)-Gd(1)-O(7N)	78.49(16)
C(11A)-H(11C)	0.9500	O(2N)-Gd(1)-O(7N)	168.12(16)
C(11")-H(11D)	0.9500	O(8N)-Gd(1)-O(7N)	51.54(16)
C(12A)-C(17A)	1.386(11)	O(5N)-Gd(1)-O(7N)	66.54(17)
C(12A)-C(13A)	1.408(10)	O(2)-Gd(1)-O(1N)	69.13(16)
C(12")-C(13")	1.377(10)	O(1)-Gd(1)-O(1N)	133.37(16)
C(12")-C(17")	1.388(11)	O(2N)-Gd(1)-O(1N)	51.38(16)
C(13")-C(14")	1.397(11)	O(8N)-Gd(1)-O(1N)	139.47(17)
C(13")-H(13C)	0.9500	O(5N)-Gd(1)-O(1N)	78.57(18)
C(13A)-C(14A)	1.394(11)	O(7N)-Gd(1)-O(1N)	135.48(16)
C(13A)-H(13D)	0.9500	O(2)-Gd(1)-O(4N)	116.38(17)

O(1)-Gd(1)-O(4N)	70.55(16)	O(1A)-Gd(2)-O(2NA)	72.33(17)
O(2N)-Gd(1)-O(4N)	67.81(18)	O(2A)-Gd(2)-O(2NA)	132.86(16)
O(8N)-Gd(1)-O(4N)	149.11(18)	O(8NA)-Gd(2)-O(2NA)	143.33(17)
O(5N)-Gd(1)-O(4N)	50.42(18)	O(1NA)-Gd(2)-O(2NA)	51.57(17)
O(7N)-Gd(1)-O(4N)	103.94(17)	O(4NA)-Gd(2)-O(2NA)	71.62(17)
O(1N)-Gd(1)-O(4N)	70.37(17)	O(1A)-Gd(2)-O(7NA)	75.27(17)
O(2)-Gd(1)-N(2)	68.55(16)	O(2A)-Gd(2)-O(7NA)	76.47(16)
O(1)-Gd(1)-N(2)	125.70(16)	O(8NA)-Gd(2)-O(7NA)	51.26(16)
O(2N)-Gd(1)-N(2)	70.99(17)	O(1NA)-Gd(2)-O(7NA)	164.38(17)
O(8N)-Gd(1)-N(2)	73.94(17)	O(4NA)-Gd(2)-O(7NA)	97.99(18)
O(5N)-Gd(1)-N(2)	138.99(18)	O(2NA)-Gd(2)-O(7NA)	135.32(17)
O(7N)-Gd(1)-N(2)	119.07(16)	O(1A)-Gd(2)-O(5NA)	71.67(18)
O(1N)-Gd(1)-N(2)	71.66(17)	O(2A)-Gd(2)-O(5NA)	99.81(17)
O(4N)-Gd(1)-N(2)	135.70(18)	O(8NA)-Gd(2)-O(5NA)	115.49(17)
O(2)-Gd(1)-N(1)	124.50(17)	O(1NA)-Gd(2)-O(5NA)	109.48(17)
O(1)-Gd(1)-N(1)	65.70(17)	O(4NA)-Gd(2)-O(5NA)	50.50(17)
O(2N)-Gd(1)-N(1)	66.45(17)	O(2NA)-Gd(2)-O(5NA)	74.62(17)
O(8N)-Gd(1)-N(1)	68.53(17)	O(7NA)-Gd(2)-O(5NA)	66.44(17)
O(5N)-Gd(1)-N(1)	160.27(18)	O(1A)-Gd(2)-N(1A)	68.19(17)
O(7N)-Gd(1)-N(1)	111.86(17)	O(2A)-Gd(2)-N(1A)	126.28(17)
O(1N)-Gd(1)-N(1)	110.21(17)	O(8NA)-Gd(2)-N(1A)	77.16(17)
O(4N)-Gd(1)-N(1)	114.53(17)	O(1NA)-Gd(2)-N(1A)	72.53(17)
N(2)-Gd(1)-N(1)	60.06(17)	O(4NA)-Gd(2)-N(1A)	138.86(18)
O(2)-Gd(1)-N(1N)	92.86(17)	O(2NA)-Gd(2)-N(1A)	72.35(17)
O(1)-Gd(1)-N(1N)	112.15(17)	O(7NA)-Gd(2)-N(1A)	121.69(17)
O(2N)-Gd(1)-N(1N)	25.28(16)	O(5NA)-Gd(2)-N(1A)	133.86(18)
O(8N)-Gd(1)-N(1N)	142.99(17)	O(1A)-Gd(2)-N(2A)	122.19(17)
O(5N)-Gd(1)-N(1N)	95.00(18)	O(2A)-Gd(2)-N(2A)	66.85(17)
O(7N)-Gd(1)-N(1N)	160.04(17)	O(8NA)-Gd(2)-N(2A)	68.63(17)
O(1N)-Gd(1)-N(1N)	26.11(16)	O(1NA)-Gd(2)-N(2A)	67.52(17)
O(4N)-Gd(1)-N(1N)	66.33(18)	O(4NA)-Gd(2)-N(2A)	117.60(17)
N(2)-Gd(1)-N(1N)	69.49(17)	O(2NA)-Gd(2)-N(2A)	110.60(17)
N(1)-Gd(1)-N(1N)	88.08(17)	O(7NA)-Gd(2)-N(2A)	112.48(17)
O(2)-Gd(1)-N(3N)	74.10(17)	O(5NA)-Gd(2)-N(2A)	165.91(18)
O(1)-Gd(1)-N(3N)	82.25(17)	N(1A)-Gd(2)-N(2A)	59.47(18)
O(2N)-Gd(1)-N(3N)	157.67(18)	O(1A)-Gd(2)-N(3NA)	72.75(18)
O(8N)-Gd(1)-N(3N)	26.18(16)	O(2A)-Gd(2)-N(3NA)	80.37(18)
O(5N)-Gd(1)-N(3N)	90.98(18)	O(8NA)-Gd(2)-N(3NA)	25.74(17)
O(7N)-Gd(1)-N(3N)	25.45(16)	O(1NA)-Gd(2)-N(3NA)	159.23(18)
O(1N)-Gd(1)-N(3N)	143.21(17)	O(4NA)-Gd(2)-N(3NA)	122.39(19)
O(4N)-Gd(1)-N(3N)	127.98(18)	O(2NA)-Gd(2)-N(3NA)	144.79(18)
N(2)-Gd(1)-N(3N)	96.22(18)	O(7NA)-Gd(2)-N(3NA)	25.72(16)
N(1)-Gd(1)-N(3N)	91.38(18)	O(5NA)-Gd(2)-N(3NA)	90.32(18)
N(1N)-Gd(1)-N(3N)	163.73(18)	N(1A)-Gd(2)-N(3NA)	98.57(18)
O(1A)-Gd(2)-O(2A)	151.55(17)	N(2A)-Gd(2)-N(3NA)	91.74(18)
O(1A)-Gd(2)-O(8NA)	77.81(17)	O(1A)-Gd(2)-N(1NA)	96.09(18)
O(2A)-Gd(2)-O(8NA)	82.06(17)	O(2A)-Gd(2)-N(1NA)	111.56(18)
O(1A)-Gd(2)-O(1NA)	118.63(17)	O(8NA)-Gd(2)-N(1NA)	147.35(17)
O(2A)-Gd(2)-O(1NA)	89.82(17)	O(1NA)-Gd(2)-N(1NA)	25.47(17)
O(8NA)-Gd(2)-O(1NA)	135.02(17)	O(4NA)-Gd(2)-N(1NA)	67.99(18)
O(1A)-Gd(2)-O(4NA)	117.54(17)	O(2NA)-Gd(2)-N(1NA)	26.11(17)
O(2A)-Gd(2)-O(4NA)	69.76(17)	O(7NA)-Gd(2)-N(1NA)	158.31(17)
O(8NA)-Gd(2)-O(4NA)	143.18(18)	O(5NA)-Gd(2)-N(1NA)	92.04(17)
O(1NA)-Gd(2)-O(4NA)	69.81(18)	N(1A)-Gd(2)-N(1NA)	70.91(18)

N(2A)-Gd(2)-N(1NA)	89.02(17)	C(7')-C(6')-P(2)	119.7(6)
N(3NA)-Gd(2)-N(1NA)	167.21(19)	C(11)-C(6)-C(7)	118.6(8)
O(1)-P(1)-C(6)	114.1(3)	C(11)-C(6)-P(1)	124.2(6)
O(1)-P(1)-C(12)	110.9(3)	C(7)-C(6)-P(1)	117.2(6)
C(6)-P(1)-C(12)	110.7(3)	C(8')-C(7')-C(6')	119.6(7)
O(1)-P(1)-C(5)	106.9(3)	C(8')-C(7')-H(7'A)	120.2
C(6)-P(1)-C(5)	103.5(3)	C(6')-C(7')-H(7'A)	120.2
C(12)-P(1)-C(5)	110.3(3)	C(8)-C(7)-C(6)	120.5(8)
P(1)-O(1)-Gd(1)	130.2(3)	C(8)-C(7)-H(7A)	119.7
O(2)-P(2)-C(12')	110.4(3)	C(6)-C(7)-H(7A)	119.7
O(2)-P(2)-C(6')	115.1(3)	C(9')-C(8')-C(7')	121.0(7)
C(12')-P(2)-C(6')	109.6(3)	C(9')-C(8')-H(8'A)	119.5
O(2)-P(2)-C(5')	108.4(3)	C(7')-C(8')-H(8'A)	119.5
C(12')-P(2)-C(5')	105.1(3)	C(9)-C(8)-C(7)	120.2(8)
C(6')-P(2)-C(5')	107.7(3)	C(9)-C(8)-H(8A)	119.9
P(2)-O(2)-Gd(1)	126.3(3)	C(7)-C(8)-H(8A)	119.9
C(5)-N(1)-C(1)	116.8(6)	C(8')-C(9')-C(10')	120.1(7)
C(5)-N(1)-Gd(1)	122.5(4)	C(8')-C(9')-H(9'A)	119.9
C(1)-N(1)-Gd(1)	120.6(4)	C(10')-C(9')-H(9'A)	119.9
C(1')-N(2)-C(5')	118.0(6)	C(8)-C(9)-C(10)	119.4(8)
C(1')-N(2)-Gd(1)	120.0(4)	C(8)-C(9)-H(9A)	120.3
C(5')-N(2)-Gd(1)	117.1(4)	C(10)-C(9)-H(9A)	120.3
N(2)-C(1')-C(2')	121.9(7)	C(11)-C(10)-C(9)	120.3(8)
N(2)-C(1')-C(1)	114.8(6)	C(11)-C(10)-H(10A)	119.9
C(2')-C(1')-C(1)	123.3(7)	C(9)-C(10)-H(10A)	119.9
N(1)-C(1)-C(2)	122.2(7)	C(11')-C(10')-C(9')	118.6(7)
N(1)-C(1)-C(1')	116.5(6)	C(11')-C(10')-H(10B)	120.7
C(2)-C(1)-C(1')	121.3(6)	C(9')-C(10')-H(10B)	120.7
C(1')-C(2')-C(3')	119.7(7)	C(6')-C(11')-C(10')	121.0(7)
C(1')-C(2')-H(2'A)	120.2	C(6')-C(11')-H(11A)	119.5
C(3')-C(2')-H(2'A)	120.2	C(10')-C(11')-H(11A)	119.5
C(1)-C(2)-C(3)	119.7(7)	C(10)-C(11)-C(6)	121.0(8)
C(1)-C(2)-H(2A)	120.2	C(10)-C(11)-H(11B)	119.5
C(3)-C(2)-H(2A)	120.2	C(6)-C(11)-H(11B)	119.5
C(4')-C(3')-C(2')	119.1(7)	C(17')-C(12')-C(13')	119.6(7)
C(4')-C(3')-H(3'A)	120.5	C(17')-C(12')-P(2)	124.0(6)
C(2')-C(3')-H(3'A)	120.5	C(13')-C(12')-P(2)	116.2(5)
C(4)-C(3)-C(2)	118.6(7)	C(17)-C(12)-C(13)	118.7(7)
C(4)-C(3)-H(3A)	120.7	C(17)-C(12)-P(1)	124.4(6)
C(2)-C(3)-H(3A)	120.7	C(13)-C(12)-P(1)	116.9(6)
C(3')-C(4')-C(5')	117.9(7)	C(14)-C(13)-C(12)	120.5(8)
C(3')-C(4')-H(4'A)	121.0	C(14)-C(13)-H(13A)	119.7
C(5')-C(4')-H(4'A)	121.0	C(12)-C(13)-H(13A)	119.7
C(3)-C(4)-C(5)	118.4(7)	C(14')-C(13')-C(12')	119.6(7)
C(3)-C(4)-H(4A)	120.8	C(14')-C(13')-H(13B)	120.2
C(5)-C(4)-H(4A)	120.8	C(12')-C(13')-H(13B)	120.2
N(1)-C(5)-C(4)	124.3(7)	C(15')-C(14')-C(13')	119.9(7)
N(1)-C(5)-P(1)	112.1(5)	C(15')-C(14')-H(14A)	120.0
C(4)-C(5)-P(1)	123.5(6)	C(13')-C(14')-H(14A)	120.0
N(2)-C(5')-C(4')	123.2(7)	C(15)-C(14)-C(13)	120.1(8)
N(2)-C(5')-P(2)	110.6(5)	C(15)-C(14)-H(14B)	120.0
C(4')-C(5')-P(2)	125.9(6)	C(13)-C(14)-H(14B)	120.0
C(11')-C(6')-C(7')	119.4(7)	C(14)-C(15)-C(16)	120.5(8)
C(11')-C(6')-P(2)	120.9(6)	C(14)-C(15)-H(15A)	119.8

C(16)-C(15)-H(15A)	119.8	C(3A)-C(4A)-C(5A)	118.1(7)
C(16')-C(15')-C(14')	121.2(7)	C(3A)-C(4A)-H(4AA)	121.0
C(16')-C(15')-H(15B)	119.4	C(5A)-C(4A)-H(4AA)	121.0
C(14')-C(15')-H(15B)	119.4	C(3")-C(4")-C(5")	117.9(7)
C(15')-C(16')-C(17')	119.7(7)	C(3")-C(4")-H(4"A)	121.0
C(15')-C(16')-H(16A)	120.1	C(5")-C(4")-H(4"A)	121.0
C(17')-C(16')-H(16A)	120.1	N(2A)-C(5")-C(4")	124.3(7)
C(15)-C(16)-C(17)	120.3(8)	N(2A)-C(5")-P(2A)	112.4(5)
C(15)-C(16)-H(16B)	119.9	C(4")-C(5")-P(2A)	123.2(6)
C(17)-C(16)-H(16B)	119.9	N(1A)-C(5A)-C(4A)	122.3(7)
C(12')-C(17')-C(16')	119.9(7)	N(1A)-C(5A)-P(1A)	112.2(5)
C(12')-C(17')-H(17A)	120.0	C(4A)-C(5A)-P(1A)	125.3(6)
C(16')-C(17')-H(17A)	120.0	C(11")-C(6")-C(7")	119.9(7)
C(12)-C(17)-C(16)	119.9(7)	C(11")-C(6")-P(2A)	118.6(6)
C(12)-C(17)-H(17B)	120.1	C(7")-C(6")-P(2A)	121.2(6)
C(16)-C(17)-H(17B)	120.1	C(11A)-C(6A)-C(7A)	120.2(7)
O(1A)-P(1A)-C(6A)	114.2(3)	C(11A)-C(6A)-P(1A)	117.9(6)
O(1A)-P(1A)-C(12A)	109.2(3)	C(7A)-C(6A)-P(1A)	121.6(6)
C(6A)-P(1A)-C(12A)	110.7(3)	C(8")-C(7")-C(6")	119.9(8)
O(1A)-P(1A)-C(5A)	109.1(3)	C(8")-C(7")-H(7"A)	120.1
C(6A)-P(1A)-C(5A)	108.0(4)	C(6")-C(7")-H(7"A)	120.1
C(12A)-P(1A)-C(5A)	105.2(4)	C(8A)-C(7A)-C(6A)	119.8(8)
P(1A)-O(1A)-Gd(2)	127.4(3)	C(8A)-C(7A)-H(7AA)	120.1
O(2A)-P(2A)-C(12")	111.8(3)	C(6A)-C(7A)-H(7AA)	120.1
O(2A)-P(2A)-C(6")	113.3(3)	C(9A)-C(8A)-C(7A)	119.9(9)
C(12")-P(2A)-C(6")	109.7(3)	C(9A)-C(8A)-H(8AA)	120.1
O(2A)-P(2A)-C(5")	107.4(3)	C(7A)-C(8A)-H(8AA)	120.1
C(12")-P(2A)-C(5")	109.8(3)	C(9")-C(8")-C(7")	119.2(8)
C(6")-P(2A)-C(5")	104.6(3)	C(9")-C(8")-H(8"A)	120.4
P(2A)-O(2A)-Gd(2)	126.2(3)	C(7")-C(8")-H(8"A)	120.4
C(5A)-N(1A)-C(1A)	118.1(6)	C(10")-C(9")-C(8")	121.6(8)
C(5A)-N(1A)-Gd(2)	118.7(5)	C(10")-C(9")-H(9"A)	119.2
C(1A)-N(1A)-Gd(2)	121.3(5)	C(8")-C(9")-H(9"A)	119.2
C(1")-N(2A)-C(5")	116.7(6)	C(8A)-C(9A)-C(10A)	120.6(8)
C(1")-N(2A)-Gd(2)	121.5(5)	C(8A)-C(9A)-H(9AA)	119.7
C(5")-N(2A)-Gd(2)	121.5(5)	C(10A)-C(9A)-H(9AA)	119.7
N(1A)-C(1A)-C(2A)	122.0(7)	C(9")-C(10")-C(11")	120.0(8)
N(1A)-C(1A)-C(1")	115.7(6)	C(9")-C(10")-H(10C)	120.0
C(2A)-C(1A)-C(1")	122.3(7)	C(11")-C(10")-H(10C)	120.0
N(2A)-C(1")-C(2")	122.9(6)	C(9A)-C(10A)-C(11A)	120.0(8)
N(2A)-C(1")-C(1A)	116.1(6)	C(9A)-C(10A)-H(10D)	120.0
C(2")-C(1")-C(1A)	120.8(6)	C(11A)-C(10A)-H(10D)	120.0
C(3A)-C(2A)-C(1A)	119.2(7)	C(6A)-C(11A)-C(10A)	119.5(8)
C(3A)-C(2A)-H(2AA)	120.4	C(6A)-C(11A)-H(11C)	120.2
C(1A)-C(2A)-H(2AA)	120.4	C(10A)-C(11A)-H(11C)	120.2
C(1")-C(2")-C(3")	119.3(7)	C(10")-C(11")-C(6")	119.3(7)
C(1")-C(2")-H(2"A)	120.4	C(10")-C(11")-H(11D)	120.3
C(3")-C(2")-H(2"A)	120.4	C(6")-C(11")-H(11D)	120.3
C(4")-C(3")-C(2")	118.9(7)	C(17A)-C(12A)-C(13A)	118.7(7)
C(4")-C(3")-H(3"A)	120.6	C(17A)-C(12A)-P(1A)	118.5(6)
C(2")-C(3")-H(3"A)	120.6	C(13A)-C(12A)-P(1A)	122.1(6)
C(2A)-C(3A)-C(4A)	119.7(7)	C(13")-C(12")-C(17")	120.0(7)
C(2A)-C(3A)-H(3AA)	120.2	C(13")-C(12")-P(2A)	116.7(6)
C(4A)-C(3A)-H(3AA)	120.2	C(17")-C(12")-P(2A)	123.3(6)

C(12")-C(13")-C(14")	120.3(7)	N(2NA)-O(5NA)-Gd(2)	95.9(4)
C(12")-C(13")-H(13C)	119.8	N(2NA)-O(4NA)-Gd(2)	98.0(4)
C(14")-C(13")-H(13C)	119.8	N(3N)-O(8N)-Gd(1)	96.3(4)
C(14A)-C(13A)-C(12A)	119.2(8)	N(3NA)-O(7NA)-Gd(2)	95.2(4)
C(14A)-C(13A)-H(13D)	120.4	O(3N)-N(1N)-O(2N)	122.7(6)
C(12A)-C(13A)-H(13D)	120.4	O(3N)-N(1N)-O(1N)	121.1(6)
C(15A)-C(14A)-C(13A)	121.8(8)	O(2N)-N(1N)-O(1N)	116.2(6)
C(15A)-C(14A)-H(14C)	119.1	O(3N)-N(1N)-Gd(1)	178.3(6)
C(13A)-C(14A)-H(14C)	119.1	O(2N)-N(1N)-Gd(1)	57.0(3)
C(15")-C(14")-C(13")	119.4(8)	O(1N)-N(1N)-Gd(1)	59.2(3)
C(15")-C(14")-H(14D)	120.3	N(2N)-O(4N)-Gd(1)	95.9(4)
C(13")-C(14")-H(14D)	120.3	O(6NA)-N(2NA)-O(5NA)	122.4(7)
C(14")-C(15")-C(16")	120.8(8)	O(6NA)-N(2NA)-O(4NA)	122.0(7)
C(14")-C(15")-H(15C)	119.6	O(5NA)-N(2NA)-O(4NA)	115.6(6)
C(16")-C(15")-H(15C)	119.6	O(6NA)-N(2NA)-Gd(2)	178.6(6)
C(14A)-C(15A)-C(16A)	119.0(7)	O(5NA)-N(2NA)-Gd(2)	59.0(3)
C(14A)-C(15A)-H(15D)	120.5	O(4NA)-N(2NA)-Gd(2)	56.6(3)
C(16A)-C(15A)-H(15D)	120.5	N(1NA)-O(1NA)-Gd(2)	97.2(4)
C(17A)-C(16A)-C(15A)	120.0(8)	N(2N)-O(5N)-Gd(1)	98.5(4)
C(17A)-C(16A)-H(16C)	120.0	N(1NA)-O(2NA)-Gd(2)	95.0(4)
C(15A)-C(16A)-H(16C)	120.0	O(6N)-N(2N)-O(5N)	123.2(7)
C(15")-C(16")-C(17")	120.5(8)	O(6N)-N(2N)-O(4N)	121.6(7)
C(15")-C(16")-H(16D)	119.8	O(5N)-N(2N)-O(4N)	115.1(6)
C(17")-C(16")-H(16D)	119.8	O(6N)-N(2N)-Gd(1)	179.0(5)
C(16A)-C(17A)-C(12A)	121.3(8)	O(5N)-N(2N)-Gd(1)	56.4(4)
C(16A)-C(17A)-H(17C)	119.4	O(4N)-N(2N)-Gd(1)	58.8(3)
C(12A)-C(17A)-H(17C)	119.4	N(1N)-O(1N)-Gd(1)	94.7(4)
C(12")-C(17")-C(16")	118.9(8)	O(3NA)-N(1NA)-O(1NA)	122.4(7)
C(12")-C(17")-H(17D)	120.6	O(3NA)-N(1NA)-O(2NA)	121.4(7)
C(16")-C(17")-H(17D)	120.6	O(1NA)-N(1NA)-O(2NA)	116.1(6)
O(9N)-N(3N)-O(7N)	122.5(7)	O(3NA)-N(1NA)-Gd(2)	178.0(5)
O(9N)-N(3N)-O(8N)	122.1(7)	O(1NA)-N(1NA)-Gd(2)	57.3(3)
O(7N)-N(3N)-O(8N)	115.4(6)	O(2NA)-N(1NA)-Gd(2)	58.9(3)
O(9N)-N(3N)-Gd(1)	173.2(5)	O(9NA)-N(3NA)-O(7NA)	121.7(7)
O(7N)-N(3N)-Gd(1)	58.3(3)	O(9NA)-N(3NA)-O(8NA)	122.4(7)
O(8N)-N(3N)-Gd(1)	57.5(3)	O(7NA)-N(3NA)-O(8NA)	115.9(6)
N(1N)-O(2N)-Gd(1)	97.7(4)	O(9NA)-N(3NA)-Gd(2)	174.5(6)
N(3N)-O(7N)-Gd(1)	96.3(4)	O(7NA)-N(3NA)-Gd(2)	59.1(3)
N(3NA)-O(8NA)-Gd(2)	96.8(4)	O(8NA)-N(3NA)-Gd(2)	57.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 30 Anisotropic displacement parameters (Å ^{2}x 10^3) for DPPOGd(NO3)3. The anisotropic displacement factor exponent takes the form: -2π^2[h^2 a*^{2}U^{11} + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Gd(1)	9(1)	15(1)	11(1)	0(1)	-1(1)	1(1)
Gd(2)	9(1)	16(1)	11(1)	0(1)	-1(1)	1(1)
P(1)	16(1)	16(1)	14(1)	1(1)	-3(1)	0(1)
O(1)	15(3)	16(2)	17(3)	3(2)	1(2)	3(2)
P(2)	11(1)	19(1)	17(1)	2(1)	-3(1)	0(1)
O(2)	10(2)	20(3)	20(3)	6(2)	-8(2)	-5(2)
N(1)	13(3)	13(3)	15(3)	-4(2)	-3(2)	2(2)
N(2)	8(3)	13(3)	16(3)	0(2)	-2(2)	-1(2)
C(1')	21(4)	17(4)	14(4)	-1(3)	4(3)	-2(3)
C(1)	18(4)	17(4)	13(4)	-3(3)	-3(3)	2(3)
C(2')	20(4)	20(4)	26(4)	-2(3)	-5(3)	-2(3)
C(2)	29(5)	14(4)	25(4)	1(3)	-7(4)	-8(3)
C(3')	22(4)	18(4)	30(5)	7(3)	-8(4)	-4(3)
C(3)	46(5)	17(4)	24(5)	-5(3)	-9(4)	-10(4)
C(4')	26(4)	23(4)	18(4)	5(3)	-2(3)	1(3)
C(4)	40(5)	24(4)	16(4)	3(3)	-12(4)	-3(4)
C(5)	27(4)	20(4)	10(4)	-1(3)	-5(3)	-1(3)
C(5')	11(4)	20(4)	22(4)	8(3)	-5(3)	0(3)
C(6')	19(4)	16(4)	14(4)	-1(3)	2(3)	2(3)
C(6)	19(4)	15(4)	25(4)	2(3)	-4(3)	-6(3)
C(7')	14(4)	30(4)	24(4)	2(3)	3(3)	0(3)
C(7)	24(4)	28(4)	25(5)	11(4)	5(4)	-4(3)
C(8')	21(4)	39(5)	24(5)	-5(4)	-11(4)	2(4)
C(8)	18(4)	45(5)	41(6)	16(4)	1(4)	-4(4)
C(9')	21(4)	35(5)	20(4)	2(4)	-5(3)	1(4)
C(9)	16(4)	44(6)	50(6)	2(5)	-6(4)	5(4)
C(10)	29(5)	42(6)	42(6)	16(5)	-4(4)	3(4)
C(10')	23(4)	33(5)	22(4)	10(4)	-1(3)	-5(4)
C(11')	16(4)	35(5)	20(4)	1(3)	-3(3)	-3(3)
C(11)	24(4)	33(5)	29(5)	8(4)	2(4)	1(4)
C(12')	11(4)	16(4)	21(4)	-2(3)	-4(3)	4(3)
C(12)	16(4)	20(4)	16(4)	-2(3)	-2(3)	-2(3)
C(13)	26(4)	28(4)	24(4)	4(3)	-4(4)	-6(3)
C(13')	16(4)	22(4)	25(4)	1(3)	-2(3)	0(3)
C(14')	19(4)	29(4)	29(5)	4(4)	3(4)	-5(3)
C(14)	28(5)	43(5)	29(5)	-2(4)	5(4)	-14(4)
C(15)	35(5)	32(5)	32(5)	-3(4)	15(4)	-15(4)
C(15')	26(4)	23(4)	17(4)	-4(3)	-1(3)	12(3)
C(16')	22(4)	25(4)	20(4)	-1(3)	-1(3)	10(3)
C(16)	58(7)	46(6)	15(4)	-8(4)	10(4)	-13(5)
C(17')	28(4)	14(4)	19(4)	5(3)	4(3)	0(3)
C(17)	21(4)	35(5)	24(5)	-3(4)	-5(3)	-15(4)
P(1A)	11(1)	19(1)	21(1)	-2(1)	3(1)	1(1)
O(1A)	10(3)	22(3)	26(3)	-4(2)	4(2)	0(2)
P(2A)	15(1)	17(1)	13(1)	0(1)	0(1)	1(1)
O(2A)	17(3)	17(3)	14(3)	0(2)	3(2)	0(2)
N(1A)	13(3)	19(3)	18(3)	0(3)	-2(3)	-1(2)

N(2A)	14(3)	17(3)	17(3)	0(2)	-5(3)	0(2)
C(1A)	14(4)	20(4)	19(4)	3(3)	2(3)	-1(3)
C(1")	8(3)	16(3)	17(4)	0(3)	0(3)	2(3)
C(2A)	20(4)	23(4)	27(5)	-4(3)	3(3)	-9(3)
C(2")	24(4)	18(4)	18(4)	5(3)	-2(3)	1(3)
C(3")	25(4)	29(4)	21(4)	4(3)	5(3)	-8(4)
C(3A)	39(5)	14(4)	27(5)	-8(3)	13(4)	-8(3)
C(4A)	30(5)	24(4)	27(5)	-4(3)	6(4)	1(3)
C(4")	28(4)	23(4)	11(4)	3(3)	-2(3)	1(3)
C(5")	20(4)	20(4)	11(4)	-1(3)	-3(3)	4(3)
C(5A)	12(4)	17(4)	25(4)	-4(3)	6(3)	-3(3)
C(6")	19(4)	15(4)	21(4)	1(3)	1(3)	3(3)
C(6A)	20(4)	17(4)	23(4)	-5(3)	0(3)	10(3)
C(7")	28(4)	26(4)	10(4)	-3(3)	7(3)	2(3)
C(7A)	34(5)	41(5)	24(5)	-3(4)	3(4)	3(4)
C(8A)	41(6)	46(6)	29(5)	-15(4)	-3(4)	-2(5)
C(8")	25(5)	33(5)	29(5)	-4(4)	9(4)	3(4)
C(9")	20(4)	27(4)	43(6)	-8(4)	5(4)	2(3)
C(9A)	36(5)	54(6)	24(5)	-8(4)	1(4)	13(5)
C(10")	18(4)	28(4)	34(5)	-5(4)	-13(4)	4(3)
C(10A)	37(5)	48(6)	31(5)	1(4)	15(4)	-1(4)
C(11A)	27(5)	26(4)	27(5)	2(4)	3(4)	-1(4)
C(11")	26(5)	29(4)	24(5)	-10(4)	-3(4)	3(4)
C(12A)	15(4)	23(4)	24(4)	1(3)	10(3)	2(3)
C(12")	13(4)	21(4)	19(4)	1(3)	3(3)	2(3)
C(13")	35(5)	25(4)	16(4)	6(3)	-4(4)	-3(4)
C(13A)	36(5)	18(4)	23(4)	-4(3)	-1(4)	8(3)
C(14A)	18(4)	31(5)	36(5)	10(4)	-4(4)	8(4)
C(14")	35(5)	36(5)	27(5)	-8(4)	-2(4)	-13(4)
C(15")	24(5)	40(5)	28(5)	-1(4)	-10(4)	-4(4)
C(15A)	13(4)	27(4)	28(5)	9(4)	-1(3)	-9(3)
C(16A)	18(4)	35(5)	29(5)	-3(4)	1(4)	-8(4)
C(16")	55(7)	50(6)	24(5)	15(4)	-25(5)	-11(5)
C(17A)	20(4)	27(4)	31(5)	1(4)	-1(4)	1(3)
C(17")	45(6)	37(5)	26(5)	7(4)	-9(4)	-6(4)
N(3N)	21(4)	28(4)	19(4)	2(3)	2(3)	-6(3)
O(2N)	16(3)	33(3)	15(3)	4(2)	-5(2)	-6(2)
O(7N)	12(3)	17(3)	27(3)	0(2)	2(2)	2(2)
O(8NA)	22(3)	23(3)	23(3)	5(2)	-4(2)	0(2)
O(5NA)	21(3)	31(3)	28(3)	14(3)	-6(3)	-5(2)
O(4NA)	22(3)	34(3)	23(3)	7(3)	5(2)	6(2)
O(8N)	20(3)	24(3)	22(3)	-12(2)	9(2)	-7(2)
O(7NA)	21(3)	19(3)	20(3)	2(2)	-1(2)	-1(2)
N(1N)	23(4)	25(3)	14(3)	-1(3)	1(3)	-8(3)
O(4N)	26(3)	31(3)	23(3)	-5(2)	-2(3)	9(3)
N(2NA)	39(4)	22(4)	17(4)	-1(3)	-16(3)	-4(3)
O(1NA)	12(3)	33(3)	16(3)	2(2)	-2(2)	-9(2)
O(5N)	24(3)	29(3)	33(3)	-5(3)	7(3)	-4(2)
O(2NA)	21(3)	26(3)	19(3)	-1(2)	3(2)	-3(2)
N(2N)	28(4)	22(3)	12(3)	2(3)	1(3)	0(3)
O(1N)	13(3)	34(3)	19(3)	3(2)	-6(2)	-3(2)
O(6NA)	50(4)	32(3)	30(3)	19(3)	-22(3)	-10(3)
N(1NA)	28(4)	21(3)	17(4)	0(3)	-2(3)	-7(3)
O(9NA)	32(4)	48(4)	35(4)	-5(3)	-24(3)	-5(3)

N(3NA)	22(4)	31(4)	24(4)	1(3)	-7(3)	-5(3)
O(9N)	22(3)	48(4)	39(4)	0(3)	18(3)	-3(3)
O(3N)	31(3)	58(4)	17(3)	7(3)	5(3)	-19(3)
O(6N)	50(4)	27(3)	36(4)	-18(3)	15(3)	-6(3)
O(3NA)	37(4)	53(4)	25(3)	-15(3)	-11(3)	-14(3)

Table 31 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for DPPOGd(NO3)3.

	x	y	z	U(eq)
H(2'A)	2666	6305	2528	27
H(2A)	2611	6677	1410	28
H(3'A)	3212	5771	3491	28
H(3A)	2233	7270	383	35
H(4'A)	4072	6457	4004	27
H(4A)	2294	8609	296	32
H(7'A)	5714	8070	4565	27
H(7A)	1535	9411	1867	31
H(8'A)	5912	7839	5745	34
H(8A)	452	9730	1671	41
H(9'A)	5106	7354	6453	30
H(9A)	174	10555	762	44
H(10A)	992	11089	72	45
H(10B)	4034	7236	6023	31
H(11A)	3817	7571	4860	28
H(11B)	2070	10804	292	35
H(13A)	3852	10685	1366	31
H(13B)	5551	8889	3044	25
H(14A)	6437	8620	2319	31
H(14B)	4612	11159	586	40
H(15A)	4484	10956	-598	40
H(15B)	6635	7375	1968	26
H(16A)	6031	6369	2405	27
H(16B)	3602	10279	-1016	47
H(17A)	5150	6616	3142	24
H(17B)	2847	9759	-242	32
H(2AA)	-2270	6151	2696	28
H(2"A)	-2651	6655	3605	24
H(3"A)	-3164	7319	4519	30
H(3AA)	-1499	5526	2011	32
H(4AA)	-635	6229	1539	32
H(4"A)	-3072	8661	4564	25
H(7"A)	-3082	10250	4895	26
H(7AA)	-1034	7096	511	39
H(8AA)	-864	6923	-689	47
H(8"A)	-4165	10558	5128	35
H(9"A)	-4908	10606	4217	36
H(9AA)	47	7451	-1218	45
H(10C)	-4579	10481	3076	32
H(10D)	808	8131	-559	46
H(11C)	643	8314	642	32
H(11D)	-3512	10117	2828	32
H(13C)	-1523	10968	3689	30
H(13D)	488	6568	1808	31
H(14C)	1330	6304	2593	34
H(14D)	-757	11449	4489	39
H(15C)	-572	10805	5523	37
H(15D)	1734	7237	3327	27

H(16C)	1258	8469	3320	33
H(16D)	-1197	9754	5823	52
H(17C)	408	8738	2563	31
H(17D)	-2003	9301	5059	44

Table 32 Torsion angles [°] for DPPOGd(NO3)3.

C(6)-P(1)-O(1)-Gd(1)	131.2(4)	C(6')-P(2)-C(5')-C(4')	-32.7(8)
C(12)-P(1)-O(1)-Gd(1)	-102.9(4)	O(2)-P(2)-C(6')-C(11')	88.5(7)
C(5)-P(1)-O(1)-Gd(1)	17.4(5)	C(12')-P(2)-C(6')-C(11')	-146.4(6)
C(12')-P(2)-O(2)-Gd(1)	105.7(4)	C(5')-P(2)-C(6')-C(11')	-32.6(7)
C(6')-P(2)-O(2)-Gd(1)	-129.6(4)	O(2)-P(2)-C(6')-C(7')	-90.4(6)
C(5')-P(2)-O(2)-Gd(1)	-9.0(5)	C(12')-P(2)-C(6')-C(7')	34.7(7)
C(5')-N(2)-C(1')-C(2')	6.3(10)	C(5')-P(2)-C(6')-C(7')	148.5(6)
Gd(1)-N(2)-C(1')-C(2')	-148.1(6)	O(1)-P(1)-C(6)-C(11)	119.0(7)
C(5')-N(2)-C(1')-C(1)	-171.4(6)	C(12)-P(1)-C(6)-C(11)	-7.0(8)
Gd(1)-N(2)-C(1')-C(1)	34.2(8)	C(5)-P(1)-C(6)-C(11)	-125.2(7)
C(5)-N(1)-C(1)-C(2)	-0.1(11)	O(1)-P(1)-C(6)-C(7)	-62.2(7)
Gd(1)-N(1)-C(1)-C(2)	-177.2(6)	C(12)-P(1)-C(6)-C(7)	171.8(6)
C(5)-N(1)-C(1)-C(1')	177.8(6)	C(5)-P(1)-C(6)-C(7)	53.6(7)
Gd(1)-N(1)-C(1)-C(1')	0.7(8)	C(11')-C(6')-C(7')-C(8')	0.3(11)
N(2)-C(1')-C(1)-N(1)	-22.4(9)	P(2)-C(6')-C(7')-C(8')	179.2(6)
C(2')-C(1')-C(1)-N(1)	160.0(7)	C(11)-C(6)-C(7)-C(8)	-0.7(12)
N(2)-C(1')-C(1)-C(2)	155.5(7)	P(1)-C(6)-C(7)-C(8)	-179.5(7)
C(2')-C(1')-C(1)-C(2)	-22.1(11)	C(6')-C(7')-C(8')-C(9')	3.4(12)
N(2)-C(1')-C(2')-C(3')	-4.0(12)	C(6)-C(7)-C(8)-C(9)	1.4(14)
C(1)-C(1')-C(2')-C(3')	173.4(7)	C(7')-C(8')-C(9')-C(10')	-4.2(13)
N(1)-C(1)-C(2)-C(3)	0.6(12)	C(7)-C(8)-C(9)-C(10)	-1.0(15)
C(1')-C(1)-C(2)-C(3)	-177.2(7)	C(8)-C(9)-C(10)-C(11)	-0.2(15)
C(1')-C(2')-C(3')-C(4')	-1.6(12)	C(8')-C(9')-C(10')-C(11')	1.3(12)
C(1)-C(2)-C(3)-C(4)	-0.5(13)	C(7')-C(6')-C(11')-C(10')	-3.2(12)
C(2')-C(3')-C(4')-C(5')	4.5(12)	P(2)-C(6')-C(11')-C(10')	177.9(6)
C(2)-C(3)-C(4)-C(5)	0.0(13)	C(9')-C(10')-C(11')-C(6')	2.5(12)
C(1)-N(1)-C(5)-C(4)	-0.5(11)	C(9)-C(10)-C(11)-C(6)	0.9(14)
Gd(1)-N(1)-C(5)-C(4)	176.5(6)	C(7)-C(6)-C(11)-C(10)	-0.4(13)
C(1)-N(1)-C(5)-P(1)	176.2(5)	P(1)-C(6)-C(11)-C(10)	178.3(7)
Gd(1)-N(1)-C(5)-P(1)	-6.7(7)	O(2)-P(2)-C(12')-C(17')	-153.2(6)
C(3)-C(4)-C(5)-N(1)	0.6(13)	C(6')-P(2)-C(12')-C(17')	79.0(7)
C(3)-C(4)-C(5)-P(1)	-175.8(7)	C(5')-P(2)-C(12')-C(17')	-36.5(7)
O(1)-P(1)-C(5)-N(1)	-4.6(6)	O(2)-P(2)-C(12')-C(13')	20.7(7)
C(6)-P(1)-C(5)-N(1)	-125.4(6)	C(6')-P(2)-C(12')-C(13')	-107.0(6)
C(12)-P(1)-C(5)-N(1)	116.1(6)	C(5')-P(2)-C(12')-C(13')	137.5(6)
O(1)-P(1)-C(5)-C(4)	172.2(7)	O(1)-P(1)-C(12)-C(17)	178.9(6)
C(6)-P(1)-C(5)-C(4)	51.4(8)	C(6)-P(1)-C(12)-C(17)	-53.3(8)
C(12)-P(1)-C(5)-C(4)	-67.1(8)	C(5)-P(1)-C(12)-C(17)	60.7(8)
C(1')-N(2)-C(5')-C(4')	-3.1(11)	O(1)-P(1)-C(12)-C(13)	-1.7(7)
Gd(1)-N(2)-C(5')-C(4')	152.0(6)	C(6)-P(1)-C(12)-C(13)	126.0(6)
C(1')-N(2)-C(5')-P(2)	171.2(5)	C(5)-P(1)-C(12)-C(13)	-120.0(6)
Gd(1)-N(2)-C(5')-P(2)	-33.7(6)	C(17)-C(12)-C(13)-C(14)	-1.6(12)
C(3')-C(4')-C(5')-N(2)	-2.3(12)	P(1)-C(12)-C(13)-C(14)	179.0(7)
C(3')-C(4')-C(5')-P(2)	-175.7(6)	C(17')-C(12')-C(13')-C(14')	-1.9(11)
O(2)-P(2)-C(5')-N(2)	28.1(6)	P(2)-C(12')-C(13')-C(14')	-176.1(6)
C(12')-P(2)-C(5')-N(2)	-90.0(6)	C(12')-C(13')-C(14')-C(15')	2.6(12)
C(6')-P(2)-C(5')-N(2)	153.2(5)	C(12)-C(13)-C(14)-C(15)	1.4(13)
O(2)-P(2)-C(5')-C(4')	-157.8(7)	C(13)-C(14)-C(15)-C(16)	0.0(14)
C(12')-P(2)-C(5')-C(4')	84.1(7)	C(13')-C(14')-C(15')-C(16')	-2.8(12)

C(14')-C(15')-C(16')-C(17')	2.4(12)	C(12A)-P(1A)-C(5A)-N(1A)	105.2(6)
C(14)-C(15)-C(16)-C(17)	-1.2(15)	O(1A)-P(1A)-C(5A)-C(4A)	173.1(7)
C(13')-C(12')-C(17')-C(16')	1.5(11)	C(6A)-P(1A)-C(5A)-C(4A)	48.4(8)
P(2)-C(12')-C(17')-C(16')	175.2(6)	C(12A)-P(1A)-C(5A)-C(4A)	-69.8(8)
C(15')-C(16')-C(17')-C(12')	-1.7(11)	O(2A)-P(2A)-C(6")-C(11")	30.6(7)
C(13)-C(12)-C(17)-C(16)	0.5(12)	C(12")-P(2A)-C(6")-C(11")	156.3(6)
P(1)-C(12)-C(17)-C(16)	179.9(7)	C(5")-P(2A)-C(6")-C(11")	-86.1(7)
C(15)-C(16)-C(17)-C(12)	0.9(14)	O(2A)-P(2A)-C(6")-C(7")	-156.3(6)
C(6A)-P(1A)-O(1A)-Gd(2)	114.7(4)	C(12")-P(2A)-C(6")-C(7")	-30.6(7)
C(12A)-P(1A)-O(1A)-Gd(2)	-120.7(4)	C(5")-P(2A)-C(6")-C(7")	87.0(7)
C(5A)-P(1A)-O(1A)-Gd(2)	-6.3(5)	O(1A)-P(1A)-C(6A)-C(11A)	70.9(7)
C(12")-P(2A)-O(2A)-Gd(2)	91.7(4)	C(12A)-P(1A)-C(6A)-C(11A)	-52.9(7)
C(6")-P(2A)-O(2A)-Gd(2)	-143.7(3)	C(5A)-P(1A)-C(6A)-C(11A)	-167.5(6)
C(5")-P(2A)-O(2A)-Gd(2)	-28.7(4)	O(1A)-P(1A)-C(6A)-C(7A)	-102.8(7)
C(5A)-N(1A)-C(1A)-C(2A)	-8.4(11)	C(12A)-P(1A)-C(6A)-C(7A)	133.4(7)
Gd(2)-N(1A)-C(1A)-C(2A)	155.6(6)	C(5A)-P(1A)-C(6A)-C(7A)	18.8(7)
C(5A)-N(1A)-C(1A)-C(1")	170.2(6)	C(11")-C(6")-C(7")-C(8")	1.9(12)
Gd(2)-N(1A)-C(1A)-C(1")	-25.8(8)	P(2A)-C(6")-C(7")-C(8")	-171.1(6)
C(5")-N(2A)-C(1")-C(2")	0.4(10)	C(11A)-C(6A)-C(7A)-C(8A)	1.6(12)
Gd(2)-N(2A)-C(1")-C(2")	-174.0(5)	P(1A)-C(6A)-C(7A)-C(8A)	175.2(7)
C(5")-N(2A)-C(1")-C(1A)	-174.5(6)	C(6A)-C(7A)-C(8A)-C(9A)	-0.9(14)
Gd(2)-N(2A)-C(1")-C(1A)	11.1(8)	C(6")-C(7")-C(8")-C(9")	-0.2(12)
N(1A)-C(1A)-C(1")-N(2A)	9.2(9)	C(7")-C(8")-C(9")-C(10")	-3.2(13)
C(2A)-C(1A)-C(1")-N(2A)	-172.2(7)	C(7A)-C(8A)-C(9A)-C(10A)	0.5(15)
N(1A)-C(1A)-C(1")-C(2")	-165.8(7)	C(8")-C(9")-C(10")-C(11")	4.8(13)
C(2A)-C(1A)-C(1")-C(2")	12.8(11)	C(8A)-C(9A)-C(10A)-C(11A)	-0.6(14)
N(1A)-C(1A)-C(2A)-C(3A)	8.7(12)	C(7A)-C(6A)-C(11A)-C(10A)	-1.7(12)
C(1")-C(1A)-C(2A)-C(3A)	-169.8(7)	P(1A)-C(6A)-C(11A)-C(10A)	-175.5(6)
N(2A)-C(1")-C(2")-C(3")	-1.7(11)	C(9A)-C(10A)-C(11A)-C(6A)	1.2(13)
C(1A)-C(1")-C(2")-C(3")	173.0(7)	C(9")-C(10")-C(11")-C(6")	-2.9(12)
C(1")-C(2")-C(3")-C(4")	1.9(11)	C(7")-C(6")-C(11")-C(10")	-0.4(12)
C(1A)-C(2A)-C(3A)-C(4A)	-2.4(13)	P(2A)-C(6")-C(11")-C(10")	172.8(6)
C(2A)-C(3A)-C(4A)-C(5A)	-3.7(13)	O(1A)-P(1A)-C(12A)-C(17A)	4.1(7)
C(2")-C(3")-C(4")-C(5")	-0.9(11)	C(6A)-P(1A)-C(12A)-C(17A)	130.8(6)
C(1")-N(2A)-C(5")-C(4")	0.7(11)	C(5A)-P(1A)-C(12A)-C(17A)	-112.8(6)
Gd(2)-N(2A)-C(5")-C(4")	175.1(5)	O(1A)-P(1A)-C(12A)-C(13A)	174.7(6)
C(1")-N(2A)-C(5")-P(2A)	-176.9(5)	C(6A)-P(1A)-C(12A)-C(13A)	-58.7(7)
Gd(2)-N(2A)-C(5")-P(2A)	-2.5(7)	C(5A)-P(1A)-C(12A)-C(13A)	57.8(7)
C(3")-C(4")-C(5")-N(2A)	-0.4(12)	O(2A)-P(2A)-C(12")-C(13")	28.9(7)
C(3")-C(4")-C(5")-P(2A)	176.9(6)	C(6")-P(2A)-C(12")-C(13")	-97.6(6)
O(2A)-P(2A)-C(5")-N(2A)	17.4(6)	C(5")-P(2A)-C(12")-C(13")	147.9(6)
C(12")-P(2A)-C(5")-N(2A)	-104.3(5)	O(2A)-P(2A)-C(12")-C(17")	-149.5(7)
C(6")-P(2A)-C(5")-N(2A)	138.1(5)	C(6")-P(2A)-C(12")-C(17")	84.0(7)
O(2A)-P(2A)-C(5")-C(4")	-160.2(6)	C(5")-P(2A)-C(12")-C(17")	-30.5(8)
C(12")-P(2A)-C(5")-C(4")	78.1(7)	C(17")-C(12")-C(13")-C(14")	-0.3(12)
C(6")-P(2A)-C(5")-C(4")	-39.6(7)	P(2A)-C(12")-C(13")-C(14")	-178.7(6)
C(1A)-N(1A)-C(5A)-C(4A)	2.0(11)	C(17A)-C(12A)-C(13A)-C(14A)	-1.7(12)
Gd(2)-N(1A)-C(5A)-C(4A)	-162.4(6)	P(1A)-C(12A)-C(13A)-C(14A)	-172.2(6)
C(1A)-N(1A)-C(5A)-P(1A)	-173.2(5)	C(12A)-C(13A)-C(14A)-C(15A)	-0.3(13)
Gd(2)-N(1A)-C(5A)-P(1A)	22.4(7)	C(12")-C(13")-C(14")-C(15")	2.5(13)
C(3A)-C(4A)-C(5A)-N(1A)	4.0(12)	C(13")-C(14")-C(15")-C(16")	-2.9(14)
C(3A)-C(4A)-C(5A)-P(1A)	178.5(6)	C(13A)-C(14A)-C(15A)-C(16A)	1.6(12)
O(1A)-P(1A)-C(5A)-N(1A)	-11.9(6)	C(14A)-C(15A)-C(16A)-C(17A)	-0.8(12)
C(6A)-P(1A)-C(5A)-N(1A)	-136.6(5)	C(14")-C(15")-C(16")-C(17")	1.1(15)

C(15A)-C(16A)-C(17A)-C(12A)	-1.2(12)	Gd(2)-O(4NA)-N(2NA)-O(5NA)	0.0(6)
C(13A)-C(12A)-C(17A)-C(16A)	2.4(12)	Gd(1)-O(5N)-N(2N)-O(6N)	178.9(6)
P(1A)-C(12A)-C(17A)-C(16A)	173.3(6)	Gd(1)-O(5N)-N(2N)-O(4N)	-0.8(6)
C(13")-C(12")-C(17")-C(16")	-1.5(13)	Gd(1)-O(4N)-N(2N)-O(6N)	-178.9(6)
P(2A)-C(12")-C(17")-C(16")	176.9(7)	Gd(1)-O(4N)-N(2N)-O(5N)	0.8(6)
C(15")-C(16")-C(17")-C(12")	1.1(15)	O(3N)-N(1N)-O(1N)-Gd(1)	-178.0(6)
O(9N)-N(3N)-O(7N)-Gd(1)	-172.0(6)	O(2N)-N(1N)-O(1N)-Gd(1)	1.2(6)
O(8N)-N(3N)-O(7N)-Gd(1)	6.3(6)	Gd(2)-O(1NA)-N(1NA)-O(3NA)	-177.6(6)
O(9N)-N(3N)-O(8N)-Gd(1)	172.0(6)	Gd(2)-O(1NA)-N(1NA)-O(2NA)	1.9(6)
O(7N)-N(3N)-O(8N)-Gd(1)	-6.4(6)	Gd(2)-O(2NA)-N(1NA)-O(3NA)	177.6(6)
Gd(1)-O(2N)-N(1N)-O(3N)	178.0(6)	Gd(2)-O(2NA)-N(1NA)-O(1NA)	-1.9(6)
Gd(1)-O(2N)-N(1N)-O(1N)	-1.3(6)	Gd(2)-O(7NA)-N(3NA)-O(9NA)	173.6(7)
Gd(2)-O(5NA)-N(2NA)-O(6NA)	179.9(6)	Gd(2)-O(7NA)-N(3NA)-O(8NA)	-8.9(7)
Gd(2)-O(5NA)-N(2NA)-O(4NA)	0.0(6)	Gd(2)-O(8NA)-N(3NA)-O(9NA)	-173.5(7)
Gd(2)-O(4NA)-N(2NA)-O(6NA)	-179.9(6)	Gd(2)-O(8NA)-N(3NA)-O(7NA)	9.1(7)

Symmetry transformations used to generate equivalent atoms:

Structure of PnPPOEu(TFA)3H2O

Table 33 Crystal data and structure refinement for PnPPOEu(TFA)3H2O.

Identification code	a	
Empirical formula	C42 H30 Eu F9 N2 O10 P2	
Formula weight	1107.58	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Pna2_1$	
Unit cell dimensions	a = 19.8440(13) Å	α= 90°.
	b = 13.4298(9) Å	β= 90°.
	c = 16.6234(12) Å	γ = 90°.
Volume	4430.2(5) $Å^3$	
Z	4	
Density (calculated)	1.661 Mg/m^3	
Absorption coefficient	1.585 mm^{-1}	
F(000)	2200	
Crystal size	0.210 x 0.160 x 0.110 mm^3	
Theta range for data collection	1.831 to 28.997°.	
Index ranges	-27<=h<=25, -16<=k<=18, -22<=l<=22	
Reflections collected	35051	
Independent reflections	11776 [R(int) = 0.0807]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.849 and 0.723	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11776 / 61 / 622	
Goodness-of-fit on F^2	1.012	
Final R indices [I>2sigma(I)]	R1 = 0.0458, wR2 = 0.0816	
R indices (all data)	R1 = 0.0770, wR2 = 0.0934	
Absolute structure parameter	0.013(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.073 and -0.650 e. $Å^{-3}$	

Table 34 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for PnPPOEu(TFA)3H2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Eu(1)	6644(1)	2343(1)	356(1)	17(1)
P(1)	7308(1)	3835(2)	1880(1)	22(1)
P(2)	5450(1)	1438(2)	-976(1)	25(1)
O(1)	7418(3)	3090(5)	1221(4)	25(2)
O(2)	6167(3)	1423(5)	-699(4)	22(2)
N(1)	6054(3)	3348(5)	1543(4)	19(1)
N(2)	5316(3)	2395(4)	412(7)	19(1)
C(1)	5372(4)	3334(6)	1631(5)	20(2)
C(2)	6408(4)	3860(6)	2089(5)	24(2)
C(3)	6116(4)	4340(6)	2740(5)	26(2)
C(4)	5439(4)	4322(6)	2821(5)	27(2)
C(5)	5039(4)	3818(6)	2262(5)	24(2)
C(6)	4329(5)	3777(7)	2313(5)	34(2)
C(7)	3956(4)	3312(7)	1744(6)	33(2)
C(8)	4276(4)	2834(6)	1082(6)	27(2)
C(9)	3914(4)	2357(6)	458(10)	31(3)
C(10)	4234(4)	1939(7)	-163(5)	27(2)
C(11)	4948(4)	1967(6)	-164(5)	22(2)
C(12)	4980(4)	2833(6)	1019(5)	21(2)
C(13)	7716(4)	3495(6)	2794(5)	26(2)
C(14)	7609(5)	2543(6)	3064(5)	37(2)
C(15)	7900(5)	2221(7)	3766(6)	40(2)
C(16)	8290(5)	2862(7)	4208(6)	41(2)
C(17)	8390(5)	3814(9)	3954(8)	48(3)
C(18)	8108(5)	4140(7)	3244(6)	37(2)
C(19)	7540(4)	5055(6)	1566(5)	28(2)
C(20)	7428(5)	5898(7)	2031(6)	38(2)
C(21)	7595(6)	6825(8)	1728(8)	54(3)
C(22)	7867(6)	6903(9)	964(8)	66(4)
C(23)	7971(5)	6084(8)	510(7)	58(3)
C(24)	7813(5)	5144(8)	801(6)	42(2)
C(25)	5355(4)	2213(7)	-1835(5)	30(2)
C(26)	4737(5)	2406(8)	-2194(6)	44(3)
C(27)	4694(5)	3040(8)	-2842(6)	45(3)
C(28)	5260(6)	3492(8)	-3133(7)	53(3)
C(29)	5864(6)	3325(9)	-2785(7)	56(3)
C(30)	5924(5)	2679(8)	-2135(6)	45(3)
C(31)	5098(4)	235(6)	-1158(6)	33(2)
C(32)	4917(5)	-353(6)	-518(6)	36(2)
C(33)	4683(6)	-1305(8)	-645(9)	62(4)
C(34)	4633(6)	-1679(8)	-1391(10)	68(4)
C(35)	4823(7)	-1098(9)	-2036(9)	68(4)
C(36)	5060(6)	-134(8)	-1950(7)	49(3)
O(1W)	7478(3)	2754(5)	-663(4)	28(2)
F(1A)	7895(6)	-697(10)	741(7)	52(3)
F(1B)	5410(30)	6050(30)	-410(40)	42(6)

F(2B)	6150(30)	5820(40)	520(17)	75(8)
F(2A)	8837(5)	-47(9)	460(9)	58(2)
F(3B)	5279(19)	4900(50)	460(20)	68(7)
F(3A)	8327(17)	-970(20)	-417(18)	51(5)
F(3B')	5168(19)	4890(50)	210(20)	68(7)
F(2A')	8919(5)	-50(11)	-16(8)	58(2)
F(2B')	6040(30)	5590(40)	706(17)	75(8)
F(1A')	8193(7)	-433(11)	881(6)	52(3)
F(1B')	5550(30)	6200(30)	-350(40)	42(6)
F(3A')	8131(17)	-1060(20)	-314(18)	51(5)
F(1C)	6406(6)	-666(10)	665(5)	57(3)
F(2C)	5618(4)	-570(30)	1514(13)	46(4)
F(3C)	6532(7)	-1337(9)	1836(8)	46(3)
F(1C')	6659(6)	-952(9)	871(6)	57(3)
F(2C')	5633(4)	-610(30)	1288(13)	46(4)
F(3C')	6376(7)	-1171(9)	2089(6)	46(3)
O(1A)	7478(2)	1062(3)	309(5)	27(1)
O(1C)	6317(3)	1169(5)	1289(4)	34(2)
O(1B)	6341(3)	3876(4)	-175(3)	28(1)
O(2A)	8009(3)	913(4)	-884(4)	39(2)
O(2B)	6289(4)	4952(5)	-1189(4)	62(2)
O(2C)	6917(4)	503(5)	2289(4)	52(2)
C(1C)	6536(4)	468(6)	1713(5)	28(2)
C(1A)	7867(4)	673(6)	-191(5)	26(2)
C(1B)	6163(5)	4660(6)	-516(5)	29(2)
C(2B)	5732(4)	5358(6)	12(5)	33(2)
C(2C)	6285(3)	-566(6)	1452(4)	38(2)
C(2A)	8260(4)	-258(6)	118(5)	36(2)
O(1S)	7369(4)	4010(5)	8113(5)	63(2)

Table 35 Bond lengths [Å] and angles [°] for PnPPOEu(TFA)3H2O.

Eu(1)-O(1C)	2.306(7)	C(17)-H(17A)	0.9500
Eu(1)-O(1B)	2.318(5)	C(18)-H(18A)	0.9500
Eu(1)-O(1)	2.330(6)	C(19)-C(20)	1.387(12)
Eu(1)-O(2)	2.345(6)	C(19)-C(24)	1.388(12)
Eu(1)-O(1A)	2.389(5)	C(20)-C(21)	1.383(13)
Eu(1)-O(1W)	2.431(6)	C(20)-H(20A)	0.9500
Eu(1)-N(2)	2.638(5)	C(21)-C(22)	1.384(17)
Eu(1)-N(1)	2.663(7)	C(21)-H(21A)	0.9500
Eu(1)-P(2)	3.464(2)	C(22)-C(23)	1.350(16)
Eu(1)-P(1)	3.489(2)	C(22)-H(22A)	0.9500
Eu(1)-H(1WB)	2.6695	C(23)-C(24)	1.388(13)
P(1)-O(1)	1.500(7)	C(23)-H(23A)	0.9500
P(1)-C(19)	1.780(9)	C(24)-H(24A)	0.9500
P(1)-C(13)	1.780(8)	C(25)-C(30)	1.384(13)
P(1)-C(2)	1.820(8)	C(25)-C(26)	1.387(12)
P(2)-O(2)	1.495(7)	C(26)-C(27)	1.376(13)
P(2)-C(25)	1.777(9)	C(26)-H(26A)	0.9500
P(2)-C(31)	1.785(9)	C(27)-C(28)	1.364(15)
P(2)-C(11)	1.822(8)	C(27)-H(27A)	0.9500
N(1)-C(2)	1.339(10)	C(28)-C(29)	1.350(14)
N(1)-C(1)	1.361(9)	C(28)-H(28A)	0.9500
N(2)-C(11)	1.334(12)	C(29)-C(30)	1.391(14)
N(2)-C(12)	1.344(12)	C(29)-H(29A)	0.9500
C(1)-C(5)	1.400(11)	C(30)-H(30A)	0.9500
C(1)-C(12)	1.447(11)	C(31)-C(32)	1.374(12)
C(2)-C(3)	1.387(11)	C(31)-C(36)	1.408(14)
C(3)-C(4)	1.351(12)	C(32)-C(33)	1.376(13)
C(3)-H(3A)	0.9500	C(32)-H(32A)	0.9500
C(4)-C(5)	1.396(11)	C(33)-C(34)	1.342(17)
C(4)-H(4A)	0.9500	C(33)-H(33A)	0.9500
C(5)-C(6)	1.413(12)	C(34)-C(35)	1.378(18)
C(6)-C(7)	1.354(12)	C(34)-H(34A)	0.9500
C(6)-H(6A)	0.9500	C(35)-C(36)	1.386(16)
C(7)-C(8)	1.424(12)	C(35)-H(35A)	0.9500
C(7)-H(7A)	0.9500	C(36)-H(36A)	0.9500
C(8)-C(12)	1.402(11)	O(1W)-H(1WA)	0.8000
C(8)-C(9)	1.414(16)	O(1W)-H(1WB)	0.8000
C(9)-C(10)	1.335(15)	F(1A)-C(2A)	1.394(10)
C(9)-H(9A)	0.9500	F(1B)-C(2B)	1.322(13)
C(10)-C(11)	1.419(11)	F(2B)-C(2B)	1.341(13)
C(10)-H(10A)	0.9500	F(2A)-C(2A)	1.311(10)
C(13)-C(14)	1.372(12)	F(3B)-C(2B)	1.324(13)
C(13)-C(18)	1.384(12)	F(3A)-C(2A)	1.315(13)
C(14)-C(15)	1.371(13)	F(3B')-C(2B)	1.328(13)
C(14)-H(14A)	0.9500	F(2A')-C(2A)	1.355(11)
C(15)-C(16)	1.370(13)	F(2B')-C(2B)	1.341(13)
C(15)-H(15A)	0.9500	F(1A')-C(2A)	1.297(11)
C(16)-C(17)	1.361(15)	F(1B')-C(2B)	1.322(13)
C(16)-H(16A)	0.9500	F(3A')-C(2A)	1.318(12)
C(17)-C(18)	1.378(15)	F(1C)-C(2C)	1.337(7)

F(2C)-C(2C)	1.327(7)
F(3C)-C(2C)	1.311(7)
F(1C')-C(2C)	1.325(7)
F(2C')-C(2C)	1.323(7)
F(3C')-C(2C)	1.346(7)
O(1A)-C(1A)	1.249(10)
O(1C)-C(1C)	1.254(10)
O(1B)-C(1B)	1.248(9)
O(2A)-C(1A)	1.228(10)
O(2B)-C(1B)	1.211(10)
O(2C)-C(1C)	1.221(10)
C(1C)-C(2C)	1.538(11)
C(1A)-C(2A)	1.560(12)
C(1B)-C(2B)	1.543(12)
O(1S)-H(1SA)	0.8000
O(1S)-H(1SB)	0.8000

O(1C)-Eu(1)-O(1B)	142.2(2)
O(1C)-Eu(1)-O(1)	93.7(2)
O(1B)-Eu(1)-O(1)	91.3(2)
O(1C)-Eu(1)-O(2)	91.6(2)
O(1B)-Eu(1)-O(2)	94.5(2)
O(1)-Eu(1)-O(2)	162.6(2)
O(1C)-Eu(1)-O(1A)	74.0(2)
O(1B)-Eu(1)-O(1A)	143.8(2)
O(1)-Eu(1)-O(1A)	82.7(2)
O(2)-Eu(1)-O(1A)	82.9(2)
O(1C)-Eu(1)-O(1W)	144.7(2)
O(1B)-Eu(1)-O(1W)	73.1(2)
O(1)-Eu(1)-O(1W)	83.32(18)
O(2)-Eu(1)-O(1W)	82.8(2)
O(1A)-Eu(1)-O(1W)	70.7(2)
O(1C)-Eu(1)-N(2)	73.3(3)
O(1B)-Eu(1)-N(2)	74.4(2)
O(1)-Eu(1)-N(2)	128.7(3)
O(2)-Eu(1)-N(2)	68.7(3)
O(1A)-Eu(1)-N(2)	135.41(16)
O(1W)-Eu(1)-N(2)	134.3(3)
O(1C)-Eu(1)-N(1)	74.0(2)
O(1B)-Eu(1)-N(1)	73.6(2)
O(1)-Eu(1)-N(1)	67.3(2)
O(2)-Eu(1)-N(1)	130.05(19)
O(1A)-Eu(1)-N(1)	134.0(2)
O(1W)-Eu(1)-N(1)	134.5(2)
N(2)-Eu(1)-N(1)	61.4(3)
O(1C)-Eu(1)-P(2)	89.81(19)
O(1B)-Eu(1)-P(2)	83.76(15)
O(1)-Eu(1)-P(2)	175.08(16)
O(2)-Eu(1)-P(2)	20.05(15)
O(1A)-Eu(1)-P(2)	101.54(16)
O(1W)-Eu(1)-P(2)	95.75(16)
N(2)-Eu(1)-P(2)	49.3(2)
N(1)-Eu(1)-P(2)	110.52(14)
O(1C)-Eu(1)-P(1)	90.61(19)
O(1B)-Eu(1)-P(1)	82.21(15)
O(1)-Eu(1)-P(1)	19.25(15)
O(2)-Eu(1)-P(1)	176.68(15)
O(1A)-Eu(1)-P(1)	100.13(17)
O(1W)-Eu(1)-P(1)	96.81(16)
N(2)-Eu(1)-P(1)	109.7(2)
N(1)-Eu(1)-P(1)	48.46(14)
P(2)-Eu(1)-P(1)	157.57(5)
O(1C)-Eu(1)-H(1WB)	127.9
O(1B)-Eu(1)-H(1WB)	89.6
O(1)-Eu(1)-H(1WB)	87.7
O(2)-Eu(1)-H(1WB)	76.0
O(1A)-Eu(1)-H(1WB)	54.5
O(1W)-Eu(1)-H(1WB)	17.2
N(2)-Eu(1)-H(1WB)	139.6
N(1)-Eu(1)-H(1WB)	149.0
P(2)-Eu(1)-H(1WB)	92.9
P(1)-Eu(1)-H(1WB)	104.4
O(1)-P(1)-C(19)	111.3(4)
O(1)-P(1)-C(13)	112.7(4)
C(19)-P(1)-C(13)	111.6(4)
O(1)-P(1)-C(2)	107.1(4)
C(19)-P(1)-C(2)	107.0(4)
C(13)-P(1)-C(2)	106.8(4)
O(1)-P(1)-Eu(1)	30.8(2)
C(19)-P(1)-Eu(1)	114.4(3)
C(13)-P(1)-Eu(1)	130.1(3)
C(2)-P(1)-Eu(1)	77.2(3)
O(2)-P(2)-C(25)	110.9(4)
O(2)-P(2)-C(31)	114.4(4)
C(25)-P(2)-C(31)	110.6(4)
O(2)-P(2)-C(11)	107.2(4)
C(25)-P(2)-C(11)	108.0(4)
C(31)-P(2)-C(11)	105.3(4)
O(2)-P(2)-Eu(1)	32.5(2)
C(25)-P(2)-Eu(1)	112.3(3)
C(31)-P(2)-Eu(1)	133.9(3)
C(11)-P(2)-Eu(1)	76.3(3)
P(1)-O(1)-Eu(1)	130.0(3)
P(2)-O(2)-Eu(1)	127.4(4)
C(2)-N(1)-C(1)	117.2(7)
C(2)-N(1)-Eu(1)	122.1(5)
C(1)-N(1)-Eu(1)	120.7(5)
C(11)-N(2)-C(12)	117.1(6)
C(11)-N(2)-Eu(1)	120.7(6)
C(12)-N(2)-Eu(1)	122.2(6)
N(1)-C(1)-C(5)	122.8(7)
N(1)-C(1)-C(12)	117.7(7)
C(5)-C(1)-C(12)	119.4(7)
N(1)-C(2)-C(3)	123.2(7)
N(1)-C(2)-P(1)	112.2(6)
C(3)-C(2)-P(1)	124.6(6)

C(4)-C(3)-C(2)	119.0(8)	C(19)-C(20)-H(20A)	120.2
C(4)-C(3)-H(3A)	120.5	C(22)-C(21)-C(20)	119.7(11)
C(2)-C(3)-H(3A)	120.5	C(22)-C(21)-H(21A)	120.2
C(3)-C(4)-C(5)	120.5(8)	C(20)-C(21)-H(21A)	120.2
C(3)-C(4)-H(4A)	119.7	C(23)-C(22)-C(21)	120.7(11)
C(5)-C(4)-H(4A)	119.7	C(23)-C(22)-H(22A)	119.6
C(4)-C(5)-C(1)	117.2(7)	C(21)-C(22)-H(22A)	119.6
C(4)-C(5)-C(6)	123.0(8)	C(22)-C(23)-C(24)	120.8(11)
C(1)-C(5)-C(6)	119.8(8)	C(22)-C(23)-H(23A)	119.6
C(7)-C(6)-C(5)	121.4(8)	C(24)-C(23)-H(23A)	119.6
C(7)-C(6)-H(6A)	119.3	C(19)-C(24)-C(23)	119.1(10)
C(5)-C(6)-H(6A)	119.3	C(19)-C(24)-H(24A)	120.5
C(6)-C(7)-C(8)	120.3(8)	C(23)-C(24)-H(24A)	120.5
C(6)-C(7)-H(7A)	119.8	C(30)-C(25)-C(26)	118.8(9)
C(8)-C(7)-H(7A)	119.8	C(30)-C(25)-P(2)	117.9(7)
C(12)-C(8)-C(9)	116.8(8)	C(26)-C(25)-P(2)	123.3(8)
C(12)-C(8)-C(7)	120.2(8)	C(27)-C(26)-C(25)	120.5(10)
C(9)-C(8)-C(7)	123.1(8)	C(27)-C(26)-H(26A)	119.8
C(10)-C(9)-C(8)	121.1(7)	C(25)-C(26)-H(26A)	119.8
C(10)-C(9)-H(9A)	119.4	C(28)-C(27)-C(26)	120.1(10)
C(8)-C(9)-H(9A)	119.4	C(28)-C(27)-H(27A)	119.9
C(9)-C(10)-C(11)	117.6(8)	C(26)-C(27)-H(27A)	119.9
C(9)-C(10)-H(10A)	121.2	C(29)-C(28)-C(27)	120.3(10)
C(11)-C(10)-H(10A)	121.2	C(29)-C(28)-H(28A)	119.8
N(2)-C(11)-C(10)	123.9(8)	C(27)-C(28)-H(28A)	119.8
N(2)-C(11)-P(2)	113.6(6)	C(28)-C(29)-C(30)	120.8(11)
C(10)-C(11)-P(2)	122.4(6)	C(28)-C(29)-H(29A)	119.6
N(2)-C(12)-C(8)	123.4(7)	C(30)-C(29)-H(29A)	119.6
N(2)-C(12)-C(1)	117.7(7)	C(25)-C(30)-C(29)	119.5(9)
C(8)-C(12)-C(1)	118.8(7)	C(25)-C(30)-H(30A)	120.3
C(14)-C(13)-C(18)	119.5(8)	C(29)-C(30)-H(30A)	120.3
C(14)-C(13)-P(1)	116.6(7)	C(32)-C(31)-C(36)	120.5(9)
C(18)-C(13)-P(1)	123.8(7)	C(32)-C(31)-P(2)	119.4(7)
C(15)-C(14)-C(13)	120.5(9)	C(36)-C(31)-P(2)	119.8(8)
C(15)-C(14)-H(14A)	119.8	C(31)-C(32)-C(33)	120.3(10)
C(13)-C(14)-H(14A)	119.8	C(31)-C(32)-H(32A)	119.9
C(16)-C(15)-C(14)	119.7(9)	C(33)-C(32)-H(32A)	119.9
C(16)-C(15)-H(15A)	120.1	C(34)-C(33)-C(32)	120.9(12)
C(14)-C(15)-H(15A)	120.1	C(34)-C(33)-H(33A)	119.5
C(17)-C(16)-C(15)	120.4(9)	C(32)-C(33)-H(33A)	119.5
C(17)-C(16)-H(16A)	119.8	C(33)-C(34)-C(35)	119.2(11)
C(15)-C(16)-H(16A)	119.8	C(33)-C(34)-H(34A)	120.4
C(16)-C(17)-C(18)	120.4(10)	C(35)-C(34)-H(34A)	120.4
C(16)-C(17)-H(17A)	119.8	C(34)-C(35)-C(36)	122.8(12)
C(18)-C(17)-H(17A)	119.8	C(34)-C(35)-H(35A)	118.6
C(17)-C(18)-C(13)	119.5(9)	C(36)-C(35)-H(35A)	118.6
C(17)-C(18)-H(18A)	120.3	C(35)-C(36)-C(31)	116.3(12)
C(13)-C(18)-H(18A)	120.3	C(35)-C(36)-H(36A)	121.8
C(20)-C(19)-C(24)	120.2(9)	C(31)-C(36)-H(36A)	121.8
C(20)-C(19)-P(1)	123.1(7)	Eu(1)-O(1W)-H(1WA)	141.4
C(24)-C(19)-P(1)	116.6(7)	Eu(1)-O(1W)-H(1WB)	98.5
C(21)-C(20)-C(19)	119.6(10)	H(1WA)-O(1W)-H(1WB)	111.9
C(21)-C(20)-H(20A)	120.2	C(1A)-O(1A)-Eu(1)	138.7(6)

C(1C)-O(1C)-Eu(1)	142.5(6)	F(3C)-C(2C)-F(2C)	109.4(16)
C(1B)-O(1B)-Eu(1)	174.9(6)	F(3C)-C(2C)-F(1C)	109.2(10)
O(2C)-C(1C)-O(1C)	128.9(9)	F(2C)-C(2C)-F(1C)	104.8(12)
O(2C)-C(1C)-C(2C)	117.2(7)	F(2C')-C(2C)-F(3C')	105.4(14)
O(1C)-C(1C)-C(2C)	114.0(8)	F(1C')-C(2C)-F(3C')	105.2(9)
O(2A)-C(1A)-O(1A)	131.0(8)	F(3C)-C(2C)-C(1C)	117.1(9)
O(2A)-C(1A)-C(2A)	113.9(7)	F(2C')-C(2C)-C(1C)	114.6(19)
O(1A)-C(1A)-C(2A)	115.1(7)	F(1C')-C(2C)-C(1C)	112.1(8)
O(2B)-C(1B)-O(1B)	129.3(9)	F(2C)-C(2C)-C(1C)	107.8(18)
O(2B)-C(1B)-C(2B)	116.3(8)	F(1C)-C(2C)-C(1C)	107.9(8)
O(1B)-C(1B)-C(2B)	114.3(7)	F(3C')-C(2C)-C(1C)	106.2(8)
F(1B)-C(2B)-F(3B)	107.7(19)	F(2A)-C(2A)-F(3A)	111.3(17)
F(1B')-C(2B)-F(3B')	106.8(18)	F(1A')-C(2A)-F(3A')	111.4(18)
F(1B')-C(2B)-F(2B')	108.2(19)	F(1A')-C(2A)-F(2A')	107.3(10)
F(3B')-C(2B)-F(2B')	105.8(17)	F(3A')-C(2A)-F(2A')	105.4(15)
F(1B)-C(2B)-F(2B)	107.7(18)	F(2A)-C(2A)-F(1A)	102.8(9)
F(3B)-C(2B)-F(2B)	106.5(17)	F(3A)-C(2A)-F(1A)	104.2(15)
F(1B')-C(2B)-C(1B)	114(4)	F(1A')-C(2A)-C(1A)	114.6(10)
F(1B)-C(2B)-C(1B)	113(4)	F(2A)-C(2A)-C(1A)	114.1(8)
F(3B)-C(2B)-C(1B)	114(3)	F(3A)-C(2A)-C(1A)	114(2)
F(3B')-C(2B)-C(1B)	109(3)	F(3A')-C(2A)-C(1A)	112(2)
F(2B')-C(2B)-C(1B)	112(3)	F(2A')-C(2A)-C(1A)	105.3(9)
F(2B)-C(2B)-C(1B)	107(3)	F(1A)-C(2A)-C(1A)	108.9(8)
F(2C')-C(2C)-F(1C')	112.4(13)	H(1SA)-O(1S)-H(1SB)	106.5

Symmetry transformations used to generate equivalent atoms:

Table 36 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for PnPPOEu(TFA)3H2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Eu(1)	17(1)	18(1)	17(1)	1(1)	0(1)	1(1)
P(1)	22(1)	22(1)	21(1)	-2(1)	-3(1)	-2(1)
P(2)	25(1)	24(1)	26(1)	-4(1)	-6(1)	1(1)
O(1)	18(3)	33(4)	25(3)	-2(3)	4(3)	-2(3)
O(2)	23(3)	21(3)	23(3)	-2(3)	-1(3)	2(3)
N(1)	20(3)	16(3)	20(3)	3(3)	0(3)	0(3)
N(2)	21(2)	19(3)	19(3)	1(4)	1(4)	-2(2)
C(1)	18(4)	19(4)	21(4)	3(3)	3(3)	2(3)
C(2)	22(4)	25(4)	23(4)	2(3)	-3(3)	-1(3)
C(3)	25(5)	30(5)	23(4)	-2(3)	2(4)	-1(4)
C(4)	35(5)	20(4)	25(4)	-7(3)	6(4)	4(4)
C(5)	23(4)	24(4)	27(4)	-1(3)	5(3)	3(3)
C(6)	33(5)	38(5)	29(5)	-3(4)	14(4)	2(4)
C(7)	19(4)	37(5)	45(6)	0(4)	5(4)	3(4)
C(8)	21(4)	19(5)	41(5)	0(4)	1(4)	2(3)
C(9)	14(3)	32(4)	49(8)	7(5)	2(5)	0(3)
C(10)	20(4)	29(5)	33(5)	-3(4)	-6(4)	-1(4)
C(11)	19(4)	21(4)	27(4)	3(3)	-4(3)	0(3)
C(12)	21(4)	22(5)	20(4)	2(3)	4(3)	1(3)
C(13)	23(4)	30(5)	26(4)	1(4)	-4(4)	9(4)
C(14)	54(6)	30(6)	26(4)	-4(4)	-7(4)	-3(4)
C(15)	60(7)	20(5)	40(5)	3(4)	5(5)	6(5)
C(16)	41(6)	52(6)	29(5)	10(4)	-8(4)	10(5)
C(17)	48(7)	40(7)	58(7)	9(6)	-16(6)	-22(5)
C(18)	32(5)	44(6)	35(5)	11(4)	-11(4)	-13(4)
C(19)	24(5)	33(5)	28(5)	0(4)	0(4)	-6(4)
C(20)	32(5)	36(6)	47(6)	7(4)	1(4)	1(4)
C(21)	52(7)	35(6)	73(9)	6(6)	-14(6)	-9(5)
C(22)	77(9)	38(7)	85(10)	27(7)	-11(8)	-19(6)
C(23)	64(7)	60(7)	49(9)	28(6)	-9(6)	-18(5)
C(24)	44(6)	45(6)	37(6)	6(5)	3(5)	-10(5)
C(25)	32(5)	37(5)	23(4)	-7(4)	-5(4)	7(4)
C(26)	43(6)	50(6)	40(6)	12(5)	-13(5)	-7(5)
C(27)	43(6)	44(6)	49(6)	8(5)	-17(5)	6(5)
C(28)	73(8)	50(7)	36(6)	12(5)	-2(6)	21(6)
C(29)	56(8)	66(8)	45(7)	26(6)	9(6)	7(6)
C(30)	32(5)	67(7)	35(5)	8(5)	2(4)	11(5)
C(31)	26(5)	31(5)	40(5)	-8(4)	-9(4)	4(4)
C(32)	36(5)	22(5)	50(6)	-6(4)	1(5)	-3(4)
C(33)	66(8)	28(6)	92(10)	-7(6)	19(7)	-5(5)
C(34)	65(8)	26(6)	113(13)	-23(7)	-8(8)	-9(6)
C(35)	82(10)	46(8)	77(10)	-29(7)	-24(8)	12(7)
C(36)	60(7)	41(7)	47(8)	-22(6)	-21(6)	8(5)
O(1W)	33(4)	27(4)	25(3)	9(3)	8(3)	4(3)
F(1A)	56(4)	50(3)	49(3)	3(2)	-3(3)	9(3)
F(1B)	46(17)	26(9)	54(9)	5(10)	5(10)	6(9)
F(2B)	87(15)	90(20)	45(13)	-32(12)	-22(14)	41(8)

F(2A)	56(3)	58(3)	60(4)	1(3)	-7(3)	7(2)
F(3B)	63(10)	53(4)	88(19)	32(16)	54(11)	26(9)
F(3A)	77(17)	30(5)	44(7)	-5(6)	4(8)	9(7)
F(3B')	63(10)	53(4)	88(19)	32(16)	54(11)	26(9)
F(2A')	56(3)	58(3)	60(4)	1(3)	-7(3)	7(2)
F(2B')	87(15)	90(20)	45(13)	-32(12)	-22(14)	41(8)
F(1A')	56(4)	50(3)	49(3)	3(2)	-3(3)	9(3)
F(1B')	46(17)	26(9)	54(9)	5(10)	5(10)	6(9)
F(3A')	77(17)	30(5)	44(7)	-5(6)	4(8)	9(7)
F(1C)	59(4)	57(3)	56(3)	-8(2)	3(3)	0(3)
F(2C)	47(4)	62(5)	28(12)	7(10)	-17(4)	-15(3)
F(3C)	47(3)	38(3)	53(4)	1(3)	0(3)	3(2)
F(1C')	59(4)	57(3)	56(3)	-8(2)	3(3)	0(3)
F(2C')	47(4)	62(5)	28(12)	7(10)	-17(4)	-15(3)
F(3C')	47(3)	38(3)	53(4)	1(3)	0(3)	3(2)
O(1A)	24(2)	25(3)	32(3)	3(4)	2(4)	3(2)
O(1C)	33(4)	31(4)	38(4)	14(3)	11(3)	10(3)
O(1B)	32(3)	27(3)	26(3)	9(3)	6(3)	3(3)
O(2A)	44(4)	34(4)	39(4)	-3(3)	14(3)	10(3)
O(2B)	103(6)	47(4)	34(4)	15(3)	22(4)	35(4)
O(2C)	72(5)	32(4)	51(5)	-1(3)	-28(4)	4(3)
C(1C)	34(5)	22(4)	29(5)	4(3)	5(4)	1(4)
C(1A)	23(4)	23(5)	32(5)	-1(4)	-3(4)	-3(4)
C(1B)	36(5)	20(5)	30(5)	5(4)	1(4)	-1(4)
C(2B)	33(6)	27(5)	40(5)	2(4)	-4(5)	8(4)
C(2C)	42(6)	43(6)	28(5)	-4(4)	4(4)	-1(5)
C(2A)	32(6)	40(6)	36(6)	-1(4)	-6(4)	10(4)
O(1S)	76(6)	55(5)	59(5)	30(4)	36(5)	10(4)

Table 37 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for PnPPOEu(TFA)3H2O.

	x	y	z	U(eq)
H(3A)	6388	4677	3124	31
H(4A)	5233	4654	3261	32
H(6A)	4109	4082	2757	40
H(7A)	3479	3304	1787	40
H(9A)	3436	2333	481	38
H(10A)	3991	1634	-589	33
H(14A)	7332	2103	2763	44
H(15A)	7831	1557	3945	48
H(16A)	8491	2640	4694	49
H(17A)	8655	4256	4268	58
H(18A)	8182	4803	3065	45
H(20A)	7237	5838	2553	46
H(21A)	7524	7405	2044	64
H(22A)	7982	7540	757	80
H(23A)	8154	6151	-15	69
H(24A)	7890	4569	481	50
H(26A)	4341	2097	-1991	53
H(27A)	4270	3163	-3087	54
H(28A)	5228	3926	-3582	63
H(29A)	6253	3652	-2987	67
H(30A)	6352	2559	-1898	54
H(32A)	4953	-102	15	43
H(33A)	4555	-1703	-198	74
H(34A)	4469	-2335	-1474	82
H(35A)	4789	-1370	-2562	82
H(36A)	5191	257	-2400	59
H(1WA)	7531	3100	-1050	34
H(1WB)	7635	2210	-726	34
H(1SA)	7054	4282	8319	76
H(1SB)	7574	4431	7878	76

Table 38 Hydrogen bonds for PnPPOEu(TFA)3H2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WA)...O(1S)#1	0.80	1.88	2.652(10)	162
O(1W)-H(1WB)...O(1A)#2	0.80	2.33	2.788(9)	117
O(1W)-H(1WB)...O(2A)#2	0.80	1.91	2.713(9)	180
O(1S)-H(1SA)...O(2B)#3	0.80	1.95	2.746(11)	179
O(1S)-H(1SB)...O(2C)#4	0.80	2.01	2.811(10)	179

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 x,y,z #3 x,y,z+1 #4 -x+3/2,y+1/2,z+1/2

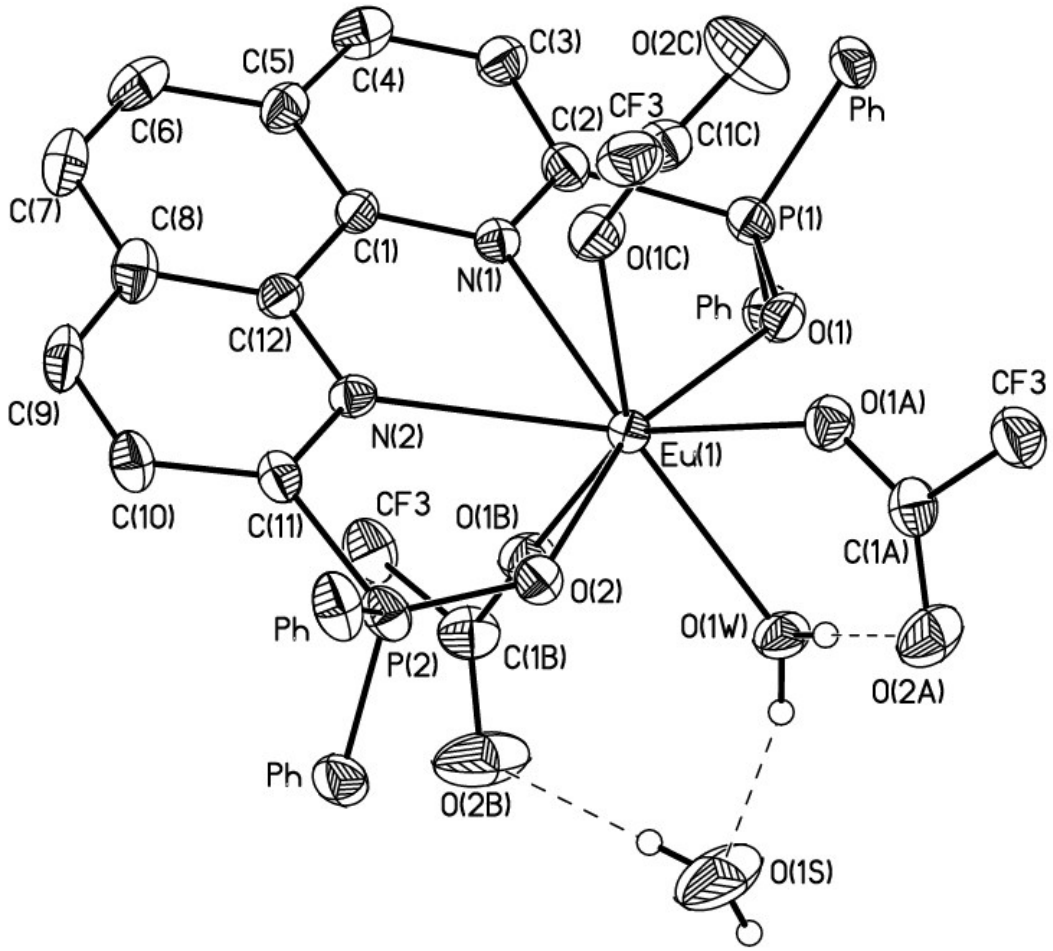

Figure 10 The independent part of the PnPPOEu(TFA)3H2O unit cell. Non-hydrogen atoms are given as probability ellipsoids of atomic displacements, hydrogen atoms at carbon atoms are omitted for clarity. The hydrogen bonds are shown by dashed lines.

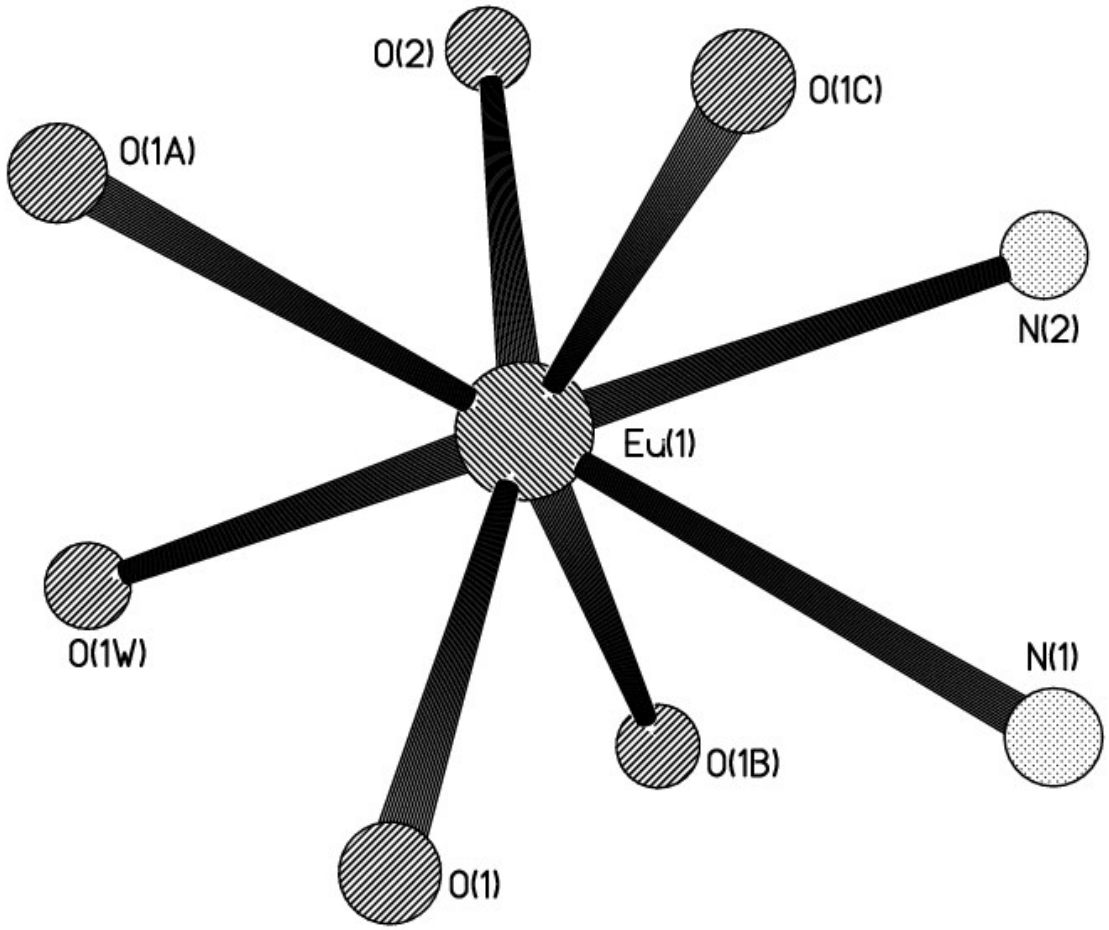

Figure 11 The distorted bicapped-trigonalaniprismatic environment of the Eu ion within the PnPPOEu(TFA)3H2O crystal: the O(2), O(1B), O(1W) and O(1A), O(1C), O(1) atoms form two bases of prism while the nitrogen atoms serve as two caps.

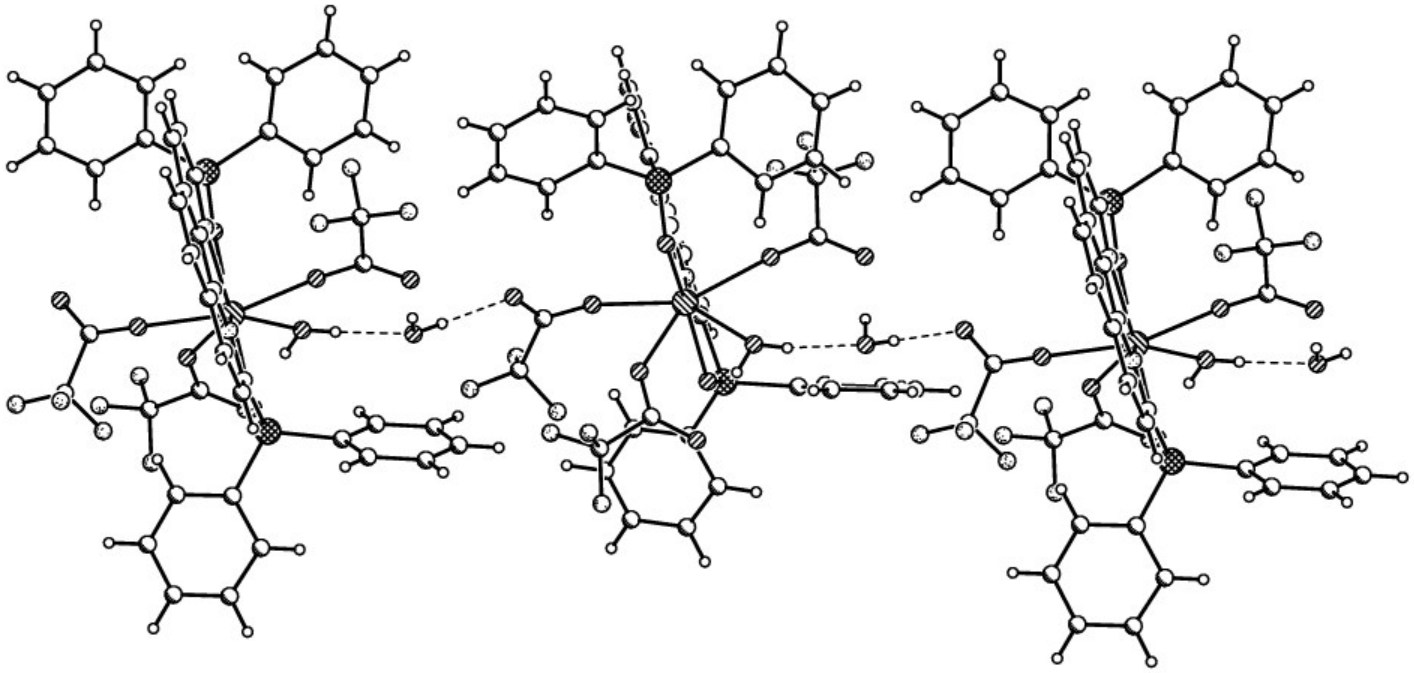

Figure 12 A fragment of H-bonded chain within the PnPPOEu(TFA)3H2O crystal.