A novel 2-(Aminomethyl)pyridineH_2PO_4 crystal with second-order nonlinear optical performance

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Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for x11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	5420(1)	8249(1)	5892(1)	27(1)
O(4)	5115(1)	6509(3)	6819(3)	35(1)
O(1)	6369(1)	8444(3)	6148(3)	45(1)
O(2)	5048(2)	10118(3)	6403(3)	44(1)
N(2)	9386(1)	6521(3)	5128(3)	28(1)
O(3)	5286(1)	7812(3)	3964(3)	42(1)
N(1)	7178(1)	5437(4)	4783(4)	37(1)
C(2)	7989(2)	5189(4)	4602(3)	29(1)
C(3)	8308(2)	3584(5)	3813(5)	38(1)
C(1)	8493(2)	6809(4)	5305(4)	34(1)
C(4)	7782(2)	2186(5)	3206(4)	42(1)
C(5)	6951(2)	2432(5)	3398(5)	45(1)
C(6)	6684(2)	4059(5)	4185(5)	49(1)

Table S2. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for x11.

	x	y	z	U(eq)
H(1)	6602	7558	5665	68
H(2A)	9511	6373	4040	34
H(2B)	9536	5479	5700	34
H(2C)	9650	7537	5538	34
H(3A)	5209	8819	3452	63
H(3)	8872	3445	3691	46
H(1A)	8341	7985	4731	41
H(1B)	8363	6964	6495	41
H(4)	7988	1097	2677	50
H(5)	6582	1519	3004	54
H(6)	6122	4222	4315	58

Table S3. Bond lengths [Å] and angles [°] for 11.

P(1)-O(4)	1.502(2)	H(2A)-N(2)-H(2B)	109.5
P(1)-O(1)	1.568(2)	H(2A)-N(2)-H(2C)	109.5
P(1)-O(2)	1.494(2)	H(2B)-N(2)-H(2C)	109.5
P(1)-O(3)	1.570(2)	C(1)-N(2)-H(2A)	109.5
O(1)-H(1)	0.8200	C(1)-N(2)-H(2B)	109.5
N(2)-H(2A)	0.8900	C(1)-N(2)-H(2C)	109.5
N(2)-H(2B)	0.8900	P(1)-O(3)-H(3A)	109.5
N(2)-H(2C)	0.8900	C(6)-N(1)-C(2)	117.6(3)
N(2)-C(1)	1.478(3)	N(1)-C(2)-C(3)	121.6(3)
O(3)-H(3A)	0.8200	N(1)-C(2)-C(1)	113.8(3)
N(1)-C(2)	1.342(3)	C(3)-C(2)-C(1)	124.7(3)
N(1)-C(6)	1.340(4)	C(2)-C(3)-H(3)	120.2
C(2)-C(3)	1.384(4)	C(2)-C(3)-C(4)	119.5(3)
C(2)-C(1)	1.504(4)	C(4)-C(3)-H(3)	120.2
C(3)-H(3)	0.9300	N(2)-C(1)-C(2)	113.7(2)
C(3)-C(4)	1.385(4)	N(2)-C(1)-H(1A)	108.8
C(1)-H(1A)	0.9700	N(2)-C(1)-H(1B)	108.8
C(1)-H(1B)	0.9700	C(2)-C(1)-H(1A)	108.8
C(4)-H(4)	0.9300	C(2)-C(1)-H(1B)	108.8
C(4)-C(5)	1.374(5)	H(1A)-C(1)-H(1B)	107.7
C(5)-H(5)	0.9300	C(3)-C(4)-H(4)	120.5
C(5)-C(6)	1.366(5)	C(5)-C(4)-C(3)	119.0(3)
C(6)-H(6)	0.9300	C(5)-C(4)-H(4)	120.5
O(4)-P(1)-O(1)	109.53(13)	C(4)-C(5)-H(5)	121.0
O(4)-P(1)-O(3)	105.70(12)	C(6)-C(5)-C(4)	117.9(3)
O(1)-P(1)-O(3)	106.22(13)	C(6)-C(5)-H(5)	121.0
O(2)-P(1)-O(4)	116.03(14)	N(1)-C(6)-C(5)	124.4(3)
O(2)-P(1)-O(1)	106.92(13)	N(1)-C(6)-H(6)	117.8
O(2)-P(1)-O(3)	112.04(13)	C(5)-C(6)-H(6)	117.8
P(1)-O(1)-H(1)	109.5		