

CHEMISTRY OF MATERIALS

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Table 1. Crystal data and structure refinement for $\text{Al}_2\text{P}_3\text{O}_{10}(\text{OH})_2\text{C}_6\text{NH}_8$

Empirical formula	$\text{C}_6\text{H}_{10}\text{Al}_2\text{NO}_{12}\text{P}_3$	
Formula weight	435.02	
Temperature	298(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	$P 2_1/c$	
Unit cell dimensions	$a = 8.686(3) \text{ \AA}$	$\alpha = 90^\circ$
	$b = 21.240(3) \text{ \AA}$	$\beta = 113.23(3)^\circ$
	$c = 8.799(2) \text{ \AA}$	$\gamma = 90^\circ$
Volume	$1491.8(6) \text{ \AA}^3$	
Z	4	
Density (calculated)	1.937 Mg/m^3	
Absorption coefficient	0.583 mm^{-1}	
F(000)	880	
Crystal size	$0.31 \times 0.14 \times 0.02 \text{ mm}$	
Theta range for data collection	$2.55 \text{ to } 30.00^\circ$	
Index ranges	$0 \leq h \leq 12, 0 \leq k \leq 29, -12 \leq l \leq 11$	
Reflections collected	4343	
Independent reflections	4343 [R(int) = 0.0556]	
Absorption correction	Integration	
Max. and min. transmission	0.9918 and 0.9300	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4343 / 2 / 190	
Goodness-of-fit on F^2	1.023	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0534, wR2 = 0.1164$	
R indices (all data)	$R1 = 0.1269, wR2 = 0.1357$	
Largest diff. peak and hole	$0.868 \text{ and } -0.893 \text{ e.\AA}^{-3}$	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Al}_2\text{P}_3\text{O}_{10}(\text{OH})_2\text{C}_6\text{NH}_8$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
P(1)	9557(1)	964(1)	-713(1)	11(1)
P(2)	4584(1)	2504(1)	-595(1)	11(1)
P(3)	9859(1)	1968(1)	3207(1)	11(1)
Al(1)	6971(1)	2072(1)	-2192(1)	11(1)
Al(2)	1937(1)	2089(1)	873(1)	11(1)
O(1)	9227(4)	652(1)	671(3)	18(1)
O(2)	9674(4)	445(1)	-1930(3)	19(1)
O(3)	8092(3)	1378(1)	-1790(3)	21(1)
O(4)	1175(3)	1344(1)	-112(3)	18(1)
O(5)	5417(3)	2028(1)	-4189(3)	16(1)
O(6)	3490(3)	2033(1)	-166(3)	15(1)
O(7)	5946(3)	2115(1)	-853(3)	16(1)
O(8)	3606(3)	2122(1)	2857(3)	17(1)
O(9)	9647(4)	1246(1)	3365(3)	21(1)
O(10)	283(3)	2104(1)	1737(3)	18(1)
O(11)	1195(3)	2824(1)	-147(3)	16(1)
O(12)	8198(3)	2725(1)	-2020(3)	19(1)
C(1)	3990(6)	-148(2)	-3328(6)	34(1)
C(2)	5292(6)	90(2)	-1947(6)	35(1)
C(3)	5065(6)	638(2)	-1215(6)	31(1)
N(1)	3596(5)	937(2)	-1870(5)	31(1)
C(4)	2353(6)	740(2)	-3239(6)	34(1)
C(5)	2519(7)	192(3)	-3981(7)	37(1)
C(6)	4167(8)	-763(3)	-4087(8)	59(2)
H(1)	10130(8)	71(16)	-1440(7)	73(7)
H(2)	9410(8)	1030(3)	2400(4)	73(7)
H(3)	6315	-119	-1516	73(7)
H(4)	5924	796	-278	73(7)
H(5)	3449	1270	-1387	73(7)
H(6)	1371	974	-3693	73(7)
H(7)	1640	49	-4925	73(7)
H(8)	3631	-1090	-3722	73(7)
H(9)	5334	-861	-3753	73(7)
H(10)	3650	-730	-5270	73(7)

Table 3 Bond lengths [Å] and angles [°] for $\text{Al}_2\text{P}_3\text{O}_{10}(\text{OH})_2\text{C}_6\text{NH}_8$

P(1)-O(1)	1.510(3)
P(1)-O(4)#1	1.524(3)
P(1)-O(3)	1.530(3)
P(1)-O(2)	1.567(3)
P(2)-O(8)#2	1.516(3)
P(2)-O(6)	1.527(3)
P(2)-O(5)#3	1.528(3)
P(2)-O(7)	1.532(3)
P(3)-O(10)#1	1.506(3)
P(3)-O(11)#4	1.521(3)
P(3)-O(12)#3	1.523(3)
P(3)-O(9)	1.558(3)
Al(1)-O(12)	1.718(3)
Al(1)-O(3)	1.726(3)
Al(1)-O(7)	1.737(3)
Al(1)-O(5)	1.746(3)
Al(2)-O(8)	1.777(3)
Al(2)-O(11)	1.789(3)
Al(2)-O(4)	1.800(3)
Al(2)-O(10)	1.872(3)
Al(2)-O(6)	1.908(3)
O(1)...O(9)	2.580(4)
O(2)...O(1)#5	2.594(4)
O(2)-H(2)	0.916(10)
O(4)-P(1)#6	1.524(3)
O(5)-P(2)#2	1.528(3)
O(6)...N(1)	2.790(5)
O(8)-P(2)#3	1.516(3)
O(9)-H(2)	0.917(10)
O(10)-P(3)#6	1.506(3)
O(11)-P(3)#7	1.521(3)
O(12)-P(3)#2	1.523(3)
C(1)-C(5)	1.380(7)
C(1)-C(2)	1.388(7)
C(1)-C(6)	1.501(8)
C(2)-C(3)	1.381(7)
C(2)-H(3)	0.9300
C(3)-N(1)	1.337(6)
C(3)-H(4)	0.9300
N(1)-C(4)	1.329(6)
N(1)-H(5)	0.8600
C(4)-C(5)	1.371(7)
C(4)-H(6)	0.9300
C(5)-H(7)	0.9300
C(6)-H(8)	0.9600
C(6)-H(9)	0.9600
C(6)-H(10)	0.9600
O(1)-P(1)-O(4)#1	113.28(16)
O(1)-P(1)-O(3)	112.10(16)

O(4)#1-P(1)-O(3)	109.75(16)
O(1)-P(1)-O(2)	109.09(16)
O(4)#1-P(1)-O(2)	108.07(16)
O(3)-P(1)-O(2)	104.07(16)
O(8)#2-P(2)-O(6)	112.53(15)
O(8)#2-P(2)-O(5)#3	107.80(15)
O(6)-P(2)-O(5)#3	111.59(15)
O(8)#2-P(2)-O(7)	110.02(15)
O(6)-P(2)-O(7)	105.95(15)
O(5)#3-P(2)-O(7)	108.92(15)
O(10)#1-P(3)-O(11)#4	114.13(15)
O(10)#1-P(3)-O(12)#3	110.20(15)
O(11)#4-P(3)-O(12)#3	109.11(15)
O(10)#1-P(3)-O(9)	110.05(16)
O(11)#4-P(3)-O(9)	105.92(16)
O(12)#3-P(3)-O(9)	107.12(17)
O(12)-Al(1)-O(3)	113.02(15)
O(12)-Al(1)-O(7)	111.41(14)
O(3)-Al(1)-O(7)	107.71(14)
O(12)-Al(1)-O(5)	109.77(13)
O(3)-Al(1)-O(5)	108.03(14)
O(7)-Al(1)-O(5)	106.63(13)
O(8)-Al(2)-O(11)	116.87(14)
O(8)-Al(2)-O(4)	120.63(14)
O(11)-Al(2)-O(4)	122.28(14)
O(8)-Al(2)-O(10)	93.42(13)
O(11)-Al(2)-O(10)	90.42(13)
O(4)-Al(2)-O(10)	90.88(13)
O(8)-Al(2)-O(6)	90.92(13)
O(11)-Al(2)-O(6)	89.80(12)
O(4)-Al(2)-O(6)	84.80(12)
O(10)-Al(2)-O(6)	175.02(13)
P(1)-O(1)-O(9)	121.57(16)
P(1)-O(2)...O(1)#5	116.84(15)
P(1)-O(2)-H(1)	115(4)
O(1)#5...O(2)-H(1)	4(4)
P(1)-O(3)-Al(1)	152.0(2)
P(1)#6-O(4)-Al(2)	138.30(18)
P(2)#2-O(5)-Al(1)	135.35(17)
P(2)-O(6)-Al(2)	134.77(17)
P(2)-O(6)...N(1)	104.96(15)
Al(2)-O(6)...N(1)	119.26(14)
P(2)-O(7)-Al(1)	139.52(18)
P(2)#3-O(8)-Al(2)	148.70(19)
P(3)-O(9)...O(1)	112.22(15)
P(3)-O(9)-H(2)	114(4)
O(1)...O(9)-H(2)	5(4)
P(3)#6-O(10)-Al(2)	146.36(18)
P(3)#7-O(11)-Al(2)	136.07(18)
P(3)#2-O(12)-Al(1)	151.6(2)
C(5)-C(1)-C(2)	118.3(5)
C(5)-C(1)-C(6)	120.7(5)
C(2)-C(1)-C(6)	121.0(5)
C(3)-C(2)-C(1)	119.9(5)

C(3)-C(2)-H(3)	120.1
C(1)-C(2)-H(3)	120.1
N(1)-C(3)-C(2)	119.2(5)
N(1)-C(3)-H(4)	120.4
C(2)-C(3)-H(4)	120.4
C(4)-N(1)-C(3)	122.5(4)
C(4)-N(1)...O(6)	124.2(3)
C(3)-N(1)...O(6)	113.2(3)
C(4)-N(1)-H(5)	118.8
C(3)-N(1)-H(5)	118.8
O(6)...N(1)-H(5)	6.1
N(1)-C(4)-C(5)	119.9(5)
N(1)-C(4)-H(6)	120.0
C(5)-C(4)-H(6)	120.0
C(4)-C(5)-C(1)	120.0(5)
C(4)-C(5)-H(7)	120.0
C(1)-C(5)-H(7)	120.0
C(1)-C(6)-H(8)	109.5
C(1)-C(6)-H(9)	109.5
H(8)-C(6)-H(9)	109.5
C(1)-C(6)-H(10)	109.5
H(8)-C(6)-H(10)	109.5
H(9)-C(6)-H(10)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 $x+1,y,z$ #2 $x,-y+1/2,z-1/2$ #3 $x,-y+1/2,z+1/2$
#4 $x+1,-y+1/2,z+1/2$ #5 $-x+2,-y,-z$
#6 $x-1,y,z$ #7 $x-1,-y+1/2,z-1/2$

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Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Al}_2\text{P}_3\text{O}_{10}(\text{OH})_2\text{C}_6\text{NH}_8$

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
P(1)	12(1)	10(1)	12(1)	-1(1)	5(1)	1(1)
P(2)	10(1)	15(1)	8(1)	-1(1)	4(1)	-1(1)
P(3)	12(1)	12(1)	11(1)	-1(1)	6(1)	0(1)
Al(1)	10(1)	15(1)	10(1)	1(1)	4(1)	1(1)
Al(2)	10(1)	13(1)	9(1)	-1(1)	3(1)	-1(1)
O(1)	30(2)	11(1)	19(1)	1(1)	15(1)	-2(1)
O(2)	28(2)	12(1)	17(1)	-2(1)	10(1)	2(1)
O(3)	21(1)	20(2)	19(1)	2(1)	6(1)	9(1)
O(4)	14(1)	17(1)	26(2)	-7(1)	10(1)	-5(1)
O(5)	17(1)	15(1)	11(1)	1(1)	2(1)	2(1)
O(6)	14(1)	17(1)	15(1)	0(1)	9(1)	-2(1)
O(7)	14(1)	22(1)	14(1)	1(1)	9(1)	0(1)
O(8)	14(1)	23(2)	10(1)	-2(1)	1(1)	0(1)
O(9)	38(2)	11(1)	15(1)	-1(1)	11(1)	-2(1)
O(10)	16(1)	26(2)	14(1)	0(1)	10(1)	-3(1)
O(11)	16(1)	19(1)	14(1)	5(1)	5(1)	2(1)
O(12)	17(1)	24(2)	20(1)	1(1)	11(1)	-6(1)