Electronic Supplementary Material (ESI) for Dalton Transactions.

Synthesis and characterization of two layered aluminophosphates $[R\text{-}C_8H_{12}N]_8[H_2O]_2\cdot[Al_8P_{12}O_{48}H_4]$ and $[S\text{-}C_8H_{12}N]_8[H_2O]_2\cdot[Al_8P_{12}O_{48}H_4]$ with mirror symmetric feature and their proton conductivity

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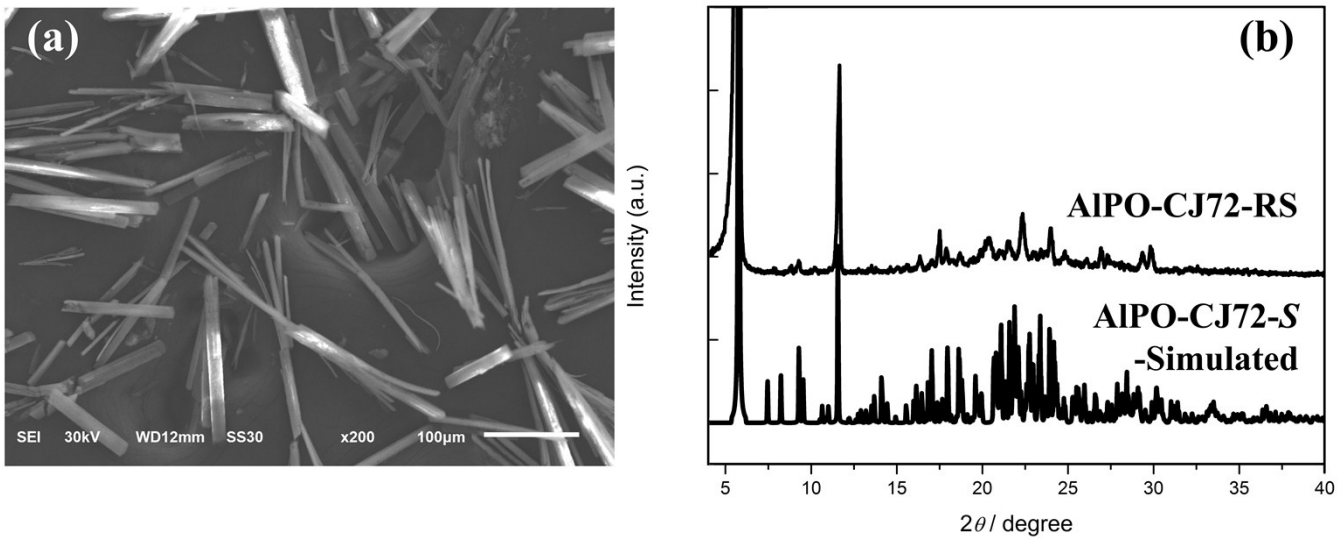

Fig. S1 (a) SEM image of AlPO-CJ72-*RS*. (b) Experimental powder X-ray diffraction PXRD pattern of AlPO-CJ72-*RS*.

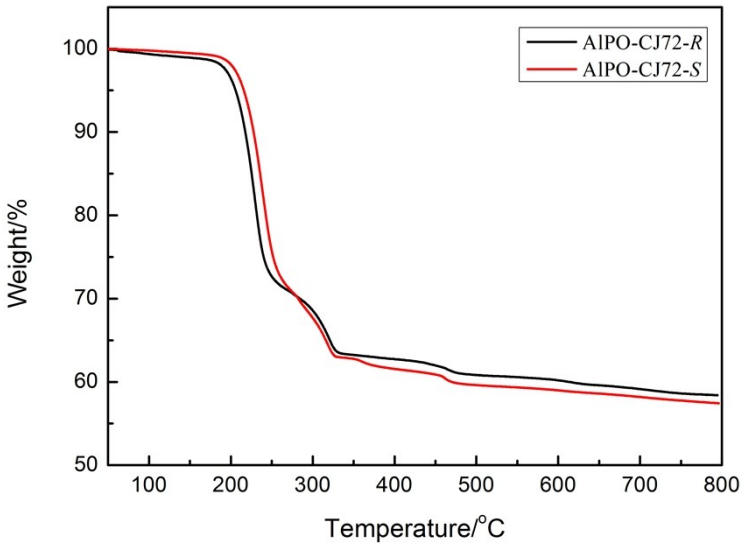

Fig. S2 TG analyses of AlPO-CJ72-*R* and AlPO-CJ-72-*S*.

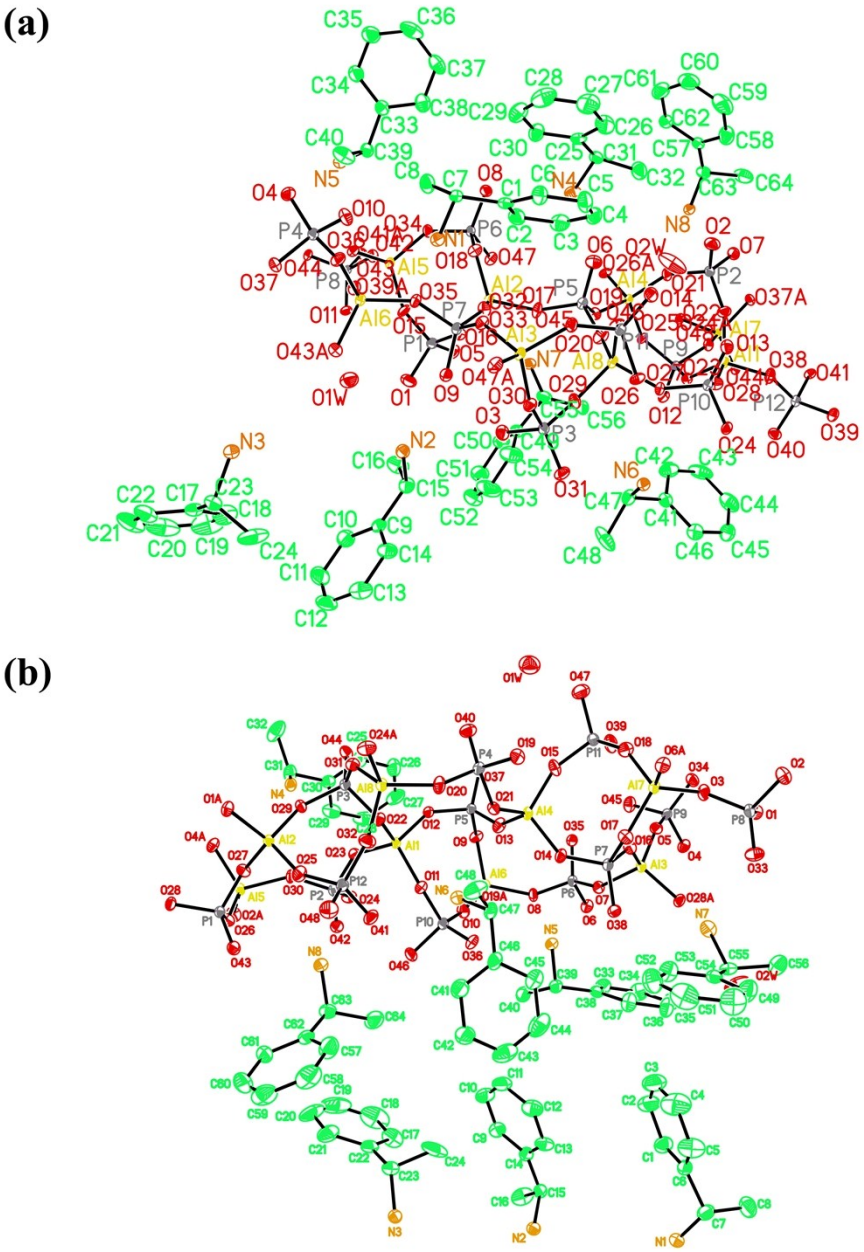

Fig. S3 Thermal ellipsoids of AlPO-CJ72-*R* (a) and AlPO-CJ72-*S* (b) given at 50% probability, showing the atomic labeling schemes of Al, P, O, C and N.

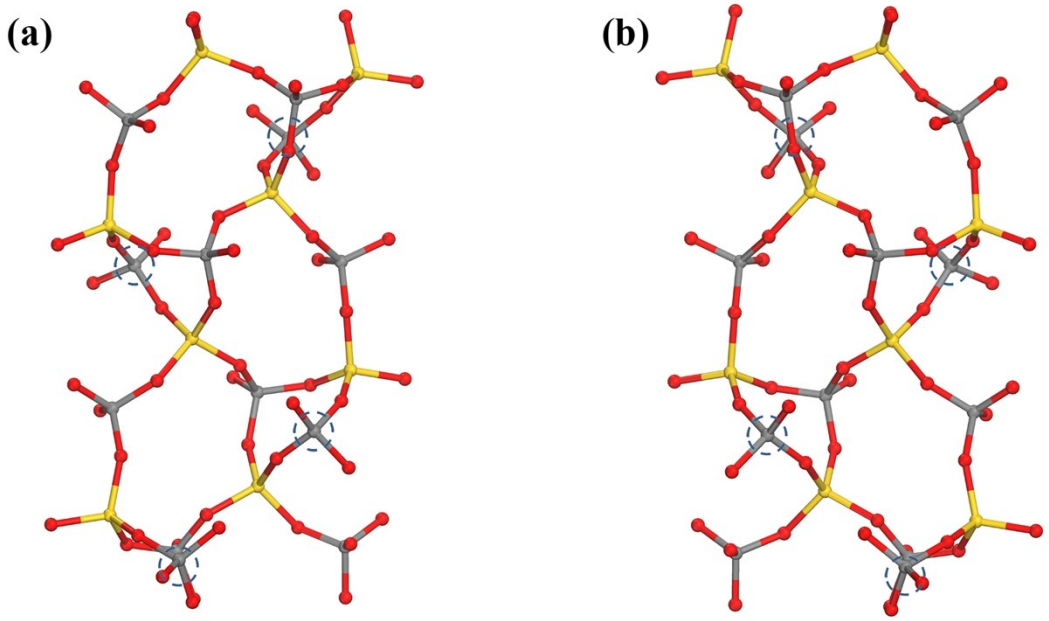

Fig. S4 The asymmetric units of AlPO-CJ72-*R* (a) and -*S* (b), P atoms in blue circle represent the ones with coordination state of $PO_2(=O)(OH)$. Color code: yellow, Al; grey, P; red, O.

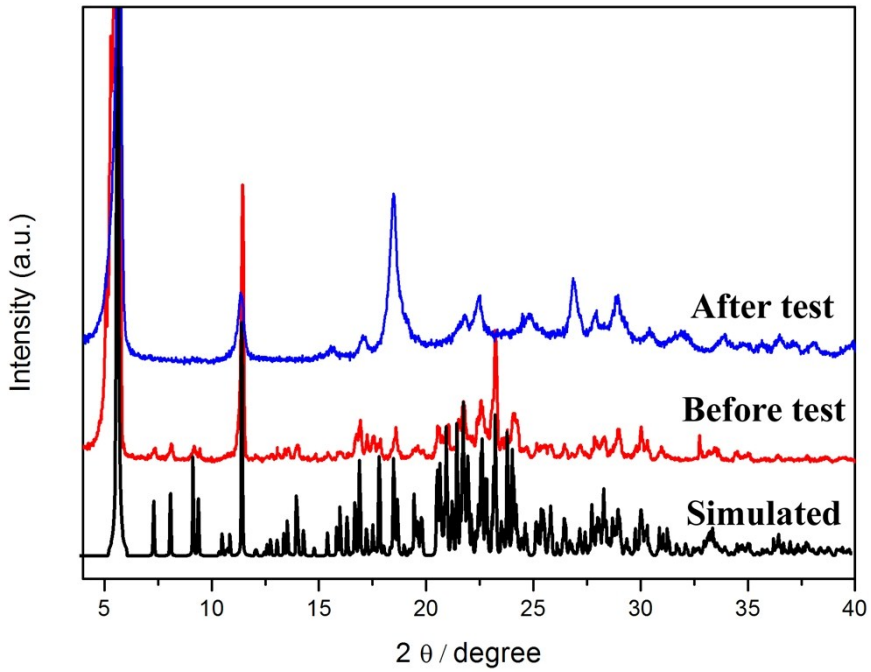

Fig. S5 Simulated and experimental PXRD pattern of AlPO-CJ72-*R* before and after the proton conductivity test.

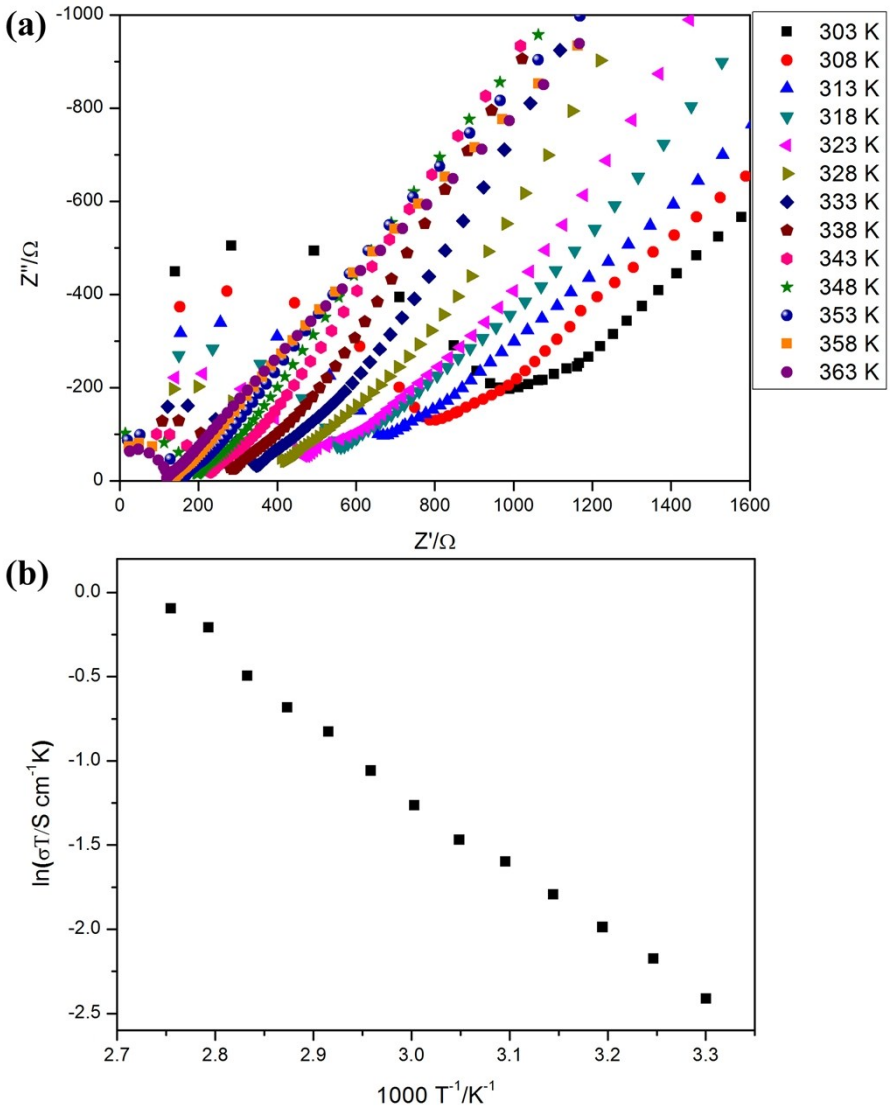

Fig. S6 (a) AC impedance plots of AlPO-CJ72-*S* and (b) Arrheniustype plots of AlPO-CJ72-*S* at different temperatures in 98% RH.

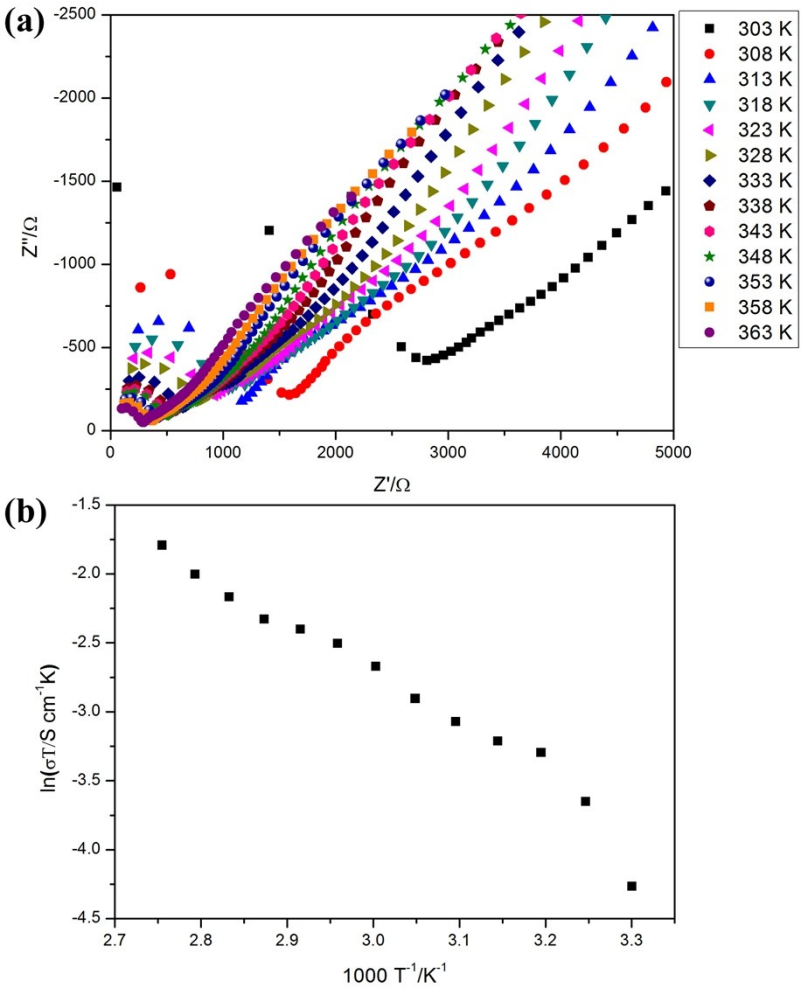

Fig. S7 (a) AC impedance plots of AlPO-CJ72-*RS* and (b) Arrheniustype plots of AlPO-CJ72-*RS* at different temperatures in 98% RH.

Table S1 Synthetic conditions and resulting products (SDA = α-methylbenzylamine).

No.	MO	Al(^{i}PrO)$_3$	H_3PO_4	SDA	Tetraethylene glycol	H_2O	Temp./ ^oC	Resulting products
1	-	1.0	10.2	7.5	11.2	32.6	110	Clear liquid
2	-	1.0	9.2	7.5	11.2	32.6	110	Few AlPO-CJ72
3	-	1.0	8.1	7.5	11.2	32.6	110	AlPO-CJ72
4	-	1.0	7.0	7.5	11.2	32.6	110	Few AlPO-CJ72
5	-	1.0	5.6	7.5	11.2	32.6	110	Clear liquid
6	-	1.0	8.1	8.2	11.2	32.6	110	Clear liquid
7	-	1.0	8.1	6.8	11.2	32.6	110	Clear liquid
8	-	1.0	8.1	7.5	11.2	32.6	90	Clear liquid
9	-	1.0	8.1	7.5	11.2	32.6	100	Few AlPO-CJ72
10	-	1.0	8.1	7.5	11.2	32.6	140	Few AlPO-CJ72
11	0.2 $Co(NO_3)_2$	1.0	8.1	7.5	11.2	32.6	110	Clear liquid
12	0.2 $CoCl_2$	1.0	8.1	7.5	11.2	32.6	110	Clear liquid
13	0.2 $FeCl_3$	1.0	8.1	7.5	11.2	32.6	110	Clear liquid
14	0.2 $Zn(NO_3)_2$	1.0	8.1	7.5	11.2	32.6	110	Clear liquid

Table S2 Different SDA and resulting products (SDA-*R*=*R*-α-methylbenzylamine, SDA-*S* = *S*-α-methylbenzylamine).

No.	Al(^{i}PrO)$_3$	H_3PO_4	SDA-*R*	SDA-*S*	Tetraethylene glycol	H_2O	Temp./ ^oC	resulting products
1	1.0	8.1	7.5	0	11.2	32.6	110	AlPO-CJ72-*R*
2	1.0	8.1	5.625	1.875	11.2	32.6	110	Clear liquid
3	1.0	8.1	3.75	3.75	11.2	32.6	110	AlPO-RS
4	1.0	8.1	1.875	5.625	11.2	32.6	110	Clear liquid
5	1.0	8.1	0	7.5	11.2	32.6	110	AlPO-CJ72-*S*

Table S3 Compositional analysis results for AlPO-CJ72-*R* and AlPO-CJ72-*S*.

Compds.	Contents (wt %)				
	Al	**P**	**C**	**N**	**H**
AlPO-CJ72-*R* obsd.	8.82	15.92	32.57	4.93	4.21
AlPO-CJ72-*S* obsd.	8.76	15.83	32.54	4.81	4.29
AlPO-CJ72-*R* and –*S* calcd.	9.10	15.66	32.39	4.72	4.42

Table S4 Selected bond lengths [Å] and bond angles [deg.] for the inorganic framework of AlPO-CJ72-*R*.

P(1)-O(5)	1.491(4)	P(12)-O(40)	1.492(4)
P(1)-O(15)	1.515(4)	P(12)-O(38)	1.535(3)
P(1)-O(16)	1.520(3)	P(12)-O(39)	1.536(3)
P(1)-O(1)	1.562(4)	P(12)-O(41)	1.543(3)
P(2)-O(7)	1.494(4)	Al(1)-O(28)	1.712(4)
P(2)-O(22)	1.518(4)	Al(1)-O(38)	1.714(3)
P(2)-O(21)	1.528(3)	Al(1)-O(22)	1.728(4)
P(2)-O(2)	1.564(4)	Al(1)-O(23)	1.753(3)
P(3)-O(31)	1.496(4)	Al(2)-O(32)	1.721(4)
P(3)-O(29)	1.528(4)	Al(2)-O(16)	1.726(4)
P(3)-O(30)	1.533(4)	Al(2)-O(17)	1.731(3)
P(3)-O(3)	1.565(4)	Al(2)-O(18)	1.753(4)
P(4)-O(10)	1.492(4)	Al(3)-O(47)#1	1.726(3)
P(4)-O(36)	1.518(4)	Al(3)-O(45)	1.734(3)
P(4)-O(37)	1.535(3)	Al(3)-O(33)	1.737(3)
P(4)-O(4)	1.563(4)	Al(3)-O(30)	1.739(4)
P(5)-O(6)	1.481(4)	Al(4)-O(26)#2	1.717(4)
P(5)-O(17)	1.533(3)	Al(4)-O(21)	1.735(3)
P(5)-O(19)	1.535(3)	Al(4)-O(25)	1.742(3)
P(5)-O(20)	1.548(4)	Al(4)-O(19)	1.749(3)
P(6)-O(8)	1.492(4)	Al(5)-O(42)	1.725(3)
P(6)-O(34)	1.531(3)	Al(5)-O(15)	1.733(4)
P(6)-O(18)	1.543(3)	Al(5)-O(34)	1.746(3)
P(6)-O(47)	1.547(3)	Al(5)-O(41)#3	1.755(3)
P(7)-O(9)	1.511(4)	Al(6)-O(39)#3	1.718(4)
P(7)-O(32)	1.522(3)	Al(6)-O(35)	1.728(3)
P(7)-O(33)	1.541(3)	Al(6)-O(36)	1.730(4)
P(7)-O(35)	1.550(3)	Al(6)-O(43)#1	1.754(4)
P(8)-O(11)	1.496(4)	Al(7)-O(44)#4	1.727(4)

P(8)-O(43)	1.535(3)	Al(7)-O(48)	1.732(3)
P(8)-O(44)	1.541(3)	Al(7)-O(24)#2	1.732(3)
P(8)-O(42)	1.545(3)	Al(7)-O(37)#5	1.736(3)
P(9)-O(12)	1.495(3)	Al(8)-O(20)	1.694(4)
P(9)-O(23)	1.533(3)	Al(8)-O(29)	1.739(4)
P(9)-O(25)	1.540(3)	Al(8)-O(27)	1.739(3)
P(9)-O(48)	1.548(3)	Al(8)-O(46)	1.742(4)
P(10)-O(13)	1.503(4)	O(24)-Al(7)#1	1.732(3)
P(10)-O(28)	1.513(4)	O(26)-Al(4)#1	1.717(4)
P(10)-O(27)	1.534(3)	O(37)-Al(7)#6	1.736(3)
P(10)-O(24)	1.546(4)	O(39)-Al(6)#4	1.718(4)
P(11)-O(14)	1.485(3)	O(41)-Al(5)#4	1.755(3)
P(11)-O(46)	1.535(3)	O(43)-Al(6)#2	1.754(4)
P(11)-O(26)	1.545(4)	O(44)-Al(7)#3	1.727(4)
P(11)-O(45)	1.547(3)	O(47)-Al(3)#2	1.726(3)
O(5)-P(1)-O(15)	112.1(2)	O(32)-Al(2)-O(16)	107.59(18)
O(5)-P(1)-O(16)	112.3(2)	O(32)-Al(2)-O(17)	109.90(18)
O(15)-P(1)-O(16)	109.2(2)	O(16)-Al(2)-O(17)	106.27(19)
O(5)-P(1)-O(1)	107.3(2)	O(32)-Al(2)-O(18)	108.13(18)
O(15)-P(1)-O(1)	108.0(2)	O(16)-Al(2)-O(18)	112.33(18)
O(16)-P(1)-O(1)	107.7(2)	O(17)-Al(2)-O(18)	112.51(19)
O(7)-P(2)-O(22)	113.0(2)	O(47)#1-Al(3)-O(45)	109.58(17)
O(7)-P(2)-O(21)	111.3(2)	O(47)#1-Al(3)-O(33)	107.60(17)
O(22)-P(2)-O(21)	109.0(2)	O(45)-Al(3)-O(33)	111.60(18)
O(7)-P(2)-O(2)	108.2(2)	O(47)#1-Al(3)-O(30)	107.96(19)
O(22)-P(2)-O(2)	107.0(2)	O(45)-Al(3)-O(30)	109.49(17)
O(21)-P(2)-O(2)	108.2(2)	O(33)-Al(3)-O(30)	110.51(17)
O(31)-P(3)-O(29)	112.2(2)	O(26)#2-Al(4)-O(21)	111.19(19)
O(31)-P(3)-O(30)	110.4(2)	O(26)#2-Al(4)-O(25)	104.21(18)
O(29)-P(3)-O(30)	110.3(2)	O(21)-Al(4)-O(25)	112.78(17)
O(31)-P(3)-O(3)	110.1(2)	O(26)#2-Al(4)-O(19)	108.35(17)
O(29)-P(3)-O(3)	107.1(2)	O(21)-Al(4)-O(19)	111.31(17)

O(30)-P(3)-O(3)	106.54(19)	O(25)-Al(4)-O(19)	108.67(18)
O(10)-P(4)-O(36)	112.2(2)	O(42)-Al(5)-O(15)	109.79(19)
O(10)-P(4)-O(37)	109.0(2)	O(42)-Al(5)-O(34)	108.37(18)
O(36)-P(4)-O(37)	110.9(2)	O(15)-Al(5)-O(34)	112.96(18)
O(10)-P(4)-O(4)	111.2(2)	O(42)-Al(5)-O(41)#3	108.84(16)
O(36)-P(4)-O(4)	106.0(2)	O(15)-Al(5)-O(41)#3	110.43(18)
O(37)-P(4)-O(4)	107.34(19)	O(34)-Al(5)-O(41)#3	106.32(17)
O(6)-P(5)-O(17)	113.4(2)	O(39)#3-Al(6)-O(35)	108.36(18)
O(6)-P(5)-O(19)	112.9(2)	O(39)#3-Al(6)-O(36)	111.69(19)
O(17)-P(5)-O(19)	104.61(18)	O(35)-Al(6)-O(36)	105.68(17)
O(6)-P(5)-O(20)	112.7(2)	O(39)#3-Al(6)-O(43)#1	109.18(17)
O(17)-P(5)-O(20)	106.5(2)	O(35)-Al(6)-O(43)#1	111.77(18)
O(19)-P(5)-O(20)	105.9(2)	O(36)-Al(6)-O(43)#1	110.14(18)
O(8)-P(6)-O(34)	109.4(2)	O(44)#4-Al(7)-O(48)	110.96(19)
O(8)-P(6)-O(18)	113.2(2)	O(44)#4-Al(7)-O(24)#2	111.20(18)
O(34)-P(6)-O(18)	108.5(2)	O(48)-Al(7)-O(24)#2	108.61(16)
O(8)-P(6)-O(47)	112.9(2)	O(44)#4-Al(7)-O(37)#5	109.41(17)
O(34)-P(6)-O(47)	107.53(19)	O(48)-Al(7)-O(37)#5	106.52(17)
O(18)-P(6)-O(47)	105.0(2)	O(24)#2-Al(7)-O(37)#5	110.03(18)
O(9)-P(7)-O(32)	112.7(2)	O(20)-Al(8)-O(29)	111.15(19)
O(9)-P(7)-O(33)	112.5(2)	O(20)-Al(8)-O(27)	107.37(18)
O(32)-P(7)-O(33)	106.01(18)	O(29)-Al(8)-O(27)	105.99(18)
O(9)-P(7)-O(35)	111.92(19)	O(20)-Al(8)-O(46)	109.11(19)
O(32)-P(7)-O(35)	109.2(2)	O(29)-Al(8)-O(46)	111.71(18)
O(33)-P(7)-O(35)	104.04(19)	O(27)-Al(8)-O(46)	111.41(17)
O(11)-P(8)-O(43)	112.2(2)	P(1)-O(1)-H(1O)	103.4
O(11)-P(8)-O(44)	109.83(19)	P(2)-O(2)-H(2O)	103.4
O(43)-P(8)-O(44)	108.4(2)	P(3)-O(3)-H(3O)	106
O(11)-P(8)-O(42)	112.4(2)	P(4)-O(4)-H(4O)	104
O(43)-P(8)-O(42)	105.77(18)	P(1)-O(15)-Al(5)	154.7(2)
O(44)-P(8)-O(42)	108.08(19)	P(1)-O(16)-Al(2)	151.4(3)
O(12)-P(9)-O(23)	113.2(2)	P(5)-O(17)-Al(2)	150.1(3)

O(12)-P(9)-O(25)	109.56(19)	P(6)-O(18)-Al(2)	128.7(2)
O(23)-P(9)-O(25)	107.02(19)	P(5)-O(19)-Al(4)	139.9(2)
O(12)-P(9)-O(48)	112.27(19)	P(5)-O(20)-Al(8)	156.6(3)
O(23)-P(9)-O(48)	106.37(18)	P(2)-O(21)-Al(4)	152.4(3)
O(25)-P(9)-O(48)	108.1(2)	P(2)-O(22)-Al(1)	155.4(2)
O(13)-P(10)-O(28)	111.8(2)	P(9)-O(23)-Al(1)	131.9(2)
O(13)-P(10)-O(27)	112.38(19)	P(10)-O(24)-Al(7)#1	138.7(2)
O(28)-P(10)-O(27)	108.27(19)	P(9)-O(25)-Al(4)	139.9(2)
O(13)-P(10)-O(24)	112.9(2)	P(11)-O(26)-Al(4)#1	143.1(2)
O(28)-P(10)-O(24)	106.8(2)	P(10)-O(27)-Al(8)	146.0(2)
O(27)-P(10)-O(24)	104.20(19)	P(10)-O(28)-Al(1)	157.5(3)
O(14)-P(11)-O(46)	114.0(2)	P(3)-O(29)-Al(8)	155.8(3)
O(14)-P(11)-O(26)	111.9(2)	P(3)-O(30)-Al(3)	148.8(3)
O(46)-P(11)-O(26)	105.78(19)	P(7)-O(32)-Al(2)	146.0(2)
O(14)-P(11)-O(45)	108.8(2)	P(7)-O(33)-Al(3)	137.8(2)
O(46)-P(11)-O(45)	108.0(2)	P(6)-O(34)-Al(5)	139.3(2)
O(26)-P(11)-O(45)	108.1(2)	P(7)-O(35)-Al(6)	144.2(2)
O(40)-P(12)-O(38)	113.5(2)	P(4)-O(36)-Al(6)	162.1(3)
O(40)-P(12)-O(39)	111.6(2)	P(4)-O(37)-Al(7)#6	144.0(2)
O(38)-P(12)-O(39)	107.1(2)	P(12)-O(38)-Al(1)	151.6(3)
O(40)-P(12)-O(41)	111.7(2)	P(12)-O(39)-Al(6)#4	150.5(2)
O(38)-P(12)-O(41)	105.3(2)	P(12)-O(41)-Al(5)#4	132.4(2)
O(39)-P(12)-O(41)	107.22(18)	P(8)-O(42)-Al(5)	145.7(2)
O(28)-Al(1)-O(38)	111.40(19)	P(8)-O(43)-Al(6)#2	132.9(2)
O(28)-Al(1)-O(22)	110.16(19)	P(8)-O(44)-Al(7)#3	142.4(2)
O(38)-Al(1)-O(22)	106.14(19)	P(11)-O(45)-Al(3)	138.0(2)
O(28)-Al(1)-O(23)	106.44(17)	P(11)-O(46)-Al(8)	132.6(2)
O(38)-Al(1)-O(23)	111.44(18)	P(6)-O(47)-Al(3)#2	134.6(2)
O(22)-Al(1)-O(23)	111.33(18)	P(9)-O(48)-Al(7)	131.4(2)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z #3 x,y,z+1
#4 x,y,z-1 #5 x+1,y,z-1 #6 x-1,y,z+1

Table S5 Hydrogen bonds for AlPO-CJ72-*R* [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A) ···O(33)	0.89	2.31	3.092(5)	146.3
N(1)-H(1A) ···O(35)	0.89	2.38	3.192(5)	151.2
N(1)-H(1B) ···O(10)	0.89	1.85	2.731(5)	168.5
N(1)-H(1C)···O(8)#1	0.89	2.03	2.895(6)	163.7
N(2)-H(2A)···O(11)#1	0.89	1.91	2.791(5)	169.2
N(2)-H(2B)···O(9)	0.89	1.98	2.868(6)	177.6
N(2)-H(2C)···O(5)#1	0.89	1.9	2.786(6)	176
N(3)-H(3A)···O(12)#6	0.89	1.96	2.839(5)	168.8
N(3)-H(3B)···O(11)#1	0.89	2.11	2.950(5)	158.1
N(3)-H(3C)···O(40)#6	0.89	1.88	2.767(5)	172.5
N(4)-H(4A)···O(8)	0.89	2.14	3.000(6)	160.9
N(4)-H(4B)···O(6)	0.89	1.91	2.791(6)	172.3
N(4)-H(4C)···O(14)#2	0.89	2.24	3.088(6)	158.6
N(4)-H(4C)···O(45)#2	0.89	2.38	3.083(5)	135.6
N(5)-H(5A)···O(7)#3	0.89	1.88	2.769(5)	173
N(5)-H(5B)···O(41)#3	0.89	2.19	3.028(6)	157.6
N(5)-H(5C)···O(10)#2	0.89	1.94	2.833(6)	176.7
N(5)-H(5C)···O(37)#2	0.89	2.56	3.015(5)	112.7
N(6)-H(6A)···O(27)	0.89	2.34	3.114(6)	146
N(6)-H(6A)···O(24)	0.89	2.35	3.158(5)	150.7
N(6)-H(6B)···O(12)#1	0.89	2	2.815(5)	152.6
N(6)-H(6C)···O(31)	0.89	1.86	2.722(5)	161.6
N(7)-H(7A)···O(5)	0.89	1.87	2.745(5)	165.4
N(7)-H(7B)···O(31)#2	0.89	1.95	2.807(6)	160.8
N(7)-H(7C)···O(19)	0.89	2.37	3.115(5)	141.2
N(7)-H(7C)···O(17)	0.89	2.43	3.138(5)	136.8
N(8)-H(8D)···O(14)#2	0.89	1.87	2.749(5)	167.2
N(8)-H(8E)···O(7)	0.89	1.94	2.809(6)	166.2
N(8)-H(8F)···O(13)#2	0.89	1.99	2.882(5)	176.4

O(1)-H(1O)···O(1W)	0.95	1.71	2.576(6)	149.7
O(4)-H(4O)···O(13)#3	0.95	1.95	2.660(5)	130
O(1W)-H(5W1)···O(43)#1	1	2.19	3.087(5)	148.9
O(1W)-H(5W2)···O(40)#3	0.97	1.78	2.734(6)	165.6
O(2W)-H(6W2)···O(6)	1	2.27	2.950(6)	124.5
O(2W)-H(6W2)···O(20)	1	2.45	3.438(6)	169.5
O(2W)-H(6W2)···O(46)	1	2.61	3.120(5)	111.9

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z #2 x+1,y,z #3 x,y,z+1 #4 x,y,z-1
#5 x+1,y,z-1 #6 x-1,y,z+1

Table S6 Selected bond lengths [Å] and bond angles [deg.] for the inorganic framework of AlPO-CJ72-*S*.

Al(1)-O(11)	1.727(4)	P(3)-O(22)	1.547(4)
Al(1)-O(22)	1.730(4)	P(4)-O(40)	1.492(5)
Al(1)-O(12)	1.732(4)	P(4)-O(20)	1.528(4)
Al(1)-O(23)	1.738(4)	P(4)-O(19)	1.538(4)
Al(2)-O(27)	1.723(4)	P(4)-O(21)	1.542(4)
Al(2)-O(30)	1.730(4)	P(5)-O(37)	1.494(4)
Al(2)-O(1)#1	1.732(4)	P(5)-O(12)	1.536(4)
Al(2)-O(29)	1.744(4)	P(5)-O(13)	1.541(4)
Al(3)-O(16)	1.729(4)	P(5)-O(9)	1.546(4)
Al(3)-O(5)	1.731(4)	P(6)-O(35)	1.509(4)
Al(3)-O(7)	1.734(4)	P(6)-O(6)	1.523(4)
Al(3)-O(28)#2	1.734(4)	P(6)-O(8)	1.533(4)
Al(4)-O(15)	1.720(5)	P(6)-O(7)	1.544(4)
Al(4)-O(13)	1.729(5)	P(7)-O(38)	1.492(4)
Al(4)-O(21)	1.747(4)	P(7)-O(14)	1.531(4)
Al(4)-O(14)	1.749(4)	P(7)-O(16)	1.546(4)
Al(5)-O(2)#3	1.708(5)	P(7)-O(17)	1.546(4)
Al(5)-O(26)	1.738(4)	P(8)-O(33)	1.483(5)
Al(5)-O(4)#1	1.740(5)	P(8)-O(3)	1.525(4)
Al(5)-O(25)	1.742(4)	P(8)-O(2)	1.539(5)

Al(6)-O(19)#4	1.716(5)	P(8)-O(1)	1.555(4)
Al(6)-O(10)	1.718(4)	P(9)-O(34)	1.485(5)
Al(6)-O(8)	1.738(4)	P(9)-O(5)	1.525(4)
Al(6)-O(9)	1.741(5)	P(9)-O(4)	1.531(5)
Al(7)-O(6)#5	1.720(4)	P(9)-O(45)	1.561(5)
Al(7)-O(18)	1.728(5)	P(10)-O(36)	1.483(4)
Al(7)-O(3)	1.738(4)	P(10)-O(10)	1.529(4)
Al(7)-O(17)	1.740(5)	P(10)-O(11)	1.539(5)
Al(8)-O(24)#5	1.708(5)	P(10)-O(46)	1.561(5)
Al(8)-O(32)	1.726(5)	P(11)-O(39)	1.488(5)
Al(8)-O(20)	1.726(5)	P(11)-O(15)	1.523(5)
Al(8)-O(31)	1.740(4)	P(11)-O(18)	1.524(4)
P(1)-O(43)	1.485(4)	P(11)-O(47)	1.563(5)
P(1)-O(27)	1.537(4)	P(12)-O(41)	1.494(5)
P(1)-O(28)	1.539(4)	P(12)-O(32)	1.526(5)
P(1)-O(26)	1.539(4)	P(12)-O(30)	1.528(4)
P(2)-O(42)	1.502(4)	P(12)-O(48)	1.553(5)
P(2)-O(24)	1.520(4)	O(1)-Al(2)#2	1.732(4)
P(2)-O(25)	1.523(4)	O(2)-Al(5)#6	1.708(5)
P(2)-O(23)	1.527(4)	O(4)-Al(5)#2	1.739(5)
P(3)-O(44)	1.499(4)	O(6)-Al(7)#4	1.720(4)
P(3)-O(31)	1.543(4)	O(19)-Al(6)#5	1.716(5)
P(3)-O(29)	1.545(4)	O(24)-Al(8)#4	1.708(5)
O(11)-Al(1)-O(22)	106.9(2)	O(28)-Al(3)#1	1.734(4)
O(11)-Al(1)-O(12)	109.1(2)	O(13)-P(5)-O(9)	105.2(2)
O(22)-Al(1)-O(12)	110.3(2)	O(35)-P(6)-O(6)	112.7(3)
O(11)-Al(1)-O(23)	109.5(2)	O(35)-P(6)-O(8)	112.1(2)
O(22)-Al(1)-O(23)	109.1(2)	O(6)-P(6)-O(8)	108.8(3)
O(12)-Al(1)-O(23)	111.7(2)	O(35)-P(6)-O(7)	112.0(2)
O(27)-Al(2)-O(30)	111.7(2)	O(6)-P(6)-O(7)	106.3(2)
O(27)-Al(2)-O(1)#1	108.3(2)	O(8)-P(6)-O(7)	104.4(2)
O(30)-Al(2)-O(1)#1	111.4(2)	O(38)-P(7)-O(14)	109.8(3)

O(27)-Al(2)-O(29)	104.0(2)	O(38)-P(7)-O(16)	112.5(3)
O(30)-Al(2)-O(29)	112.7(2)	O(14)-P(7)-O(16)	107.2(2)
O(1)#1-Al(2)-O(29)	108.6(2)	O(38)-P(7)-O(17)	113.7(2)
O(16)-Al(3)-O(5)	108.8(2)	O(14)-P(7)-O(17)	108.7(3)
O(16)-Al(3)-O(7)	107.3(2)	O(16)-P(7)-O(17)	104.6(2)
O(5)-Al(3)-O(7)	110.6(2)	O(33)-P(8)-O(3)	113.5(3)
O(16)-Al(3)-O(28)#2	109.6(2)	O(33)-P(8)-O(2)	112.4(3)
O(5)-Al(3)-O(28)#2	108.8(2)	O(3)-P(8)-O(2)	107.0(3)
O(7)-Al(3)-O(28)#2	111.8(2)	O(33)-P(8)-O(1)	112.6(3)
O(15)-Al(4)-O(13)	110.1(2)	O(3)-P(8)-O(1)	104.6(2)
O(15)-Al(4)-O(21)	110.5(2)	O(2)-P(8)-O(1)	106.2(2)
O(13)-Al(4)-O(21)	109.1(2)	O(34)-P(9)-O(5)	111.0(3)
O(15)-Al(4)-O(14)	112.2(2)	O(34)-P(9)-O(4)	112.2(3)
O(13)-Al(4)-O(14)	108.2(2)	O(5)-P(9)-O(4)	109.7(3)
O(21)-Al(4)-O(14)	106.6(2)	O(34)-P(9)-O(45)	109.6(3)
O(2)#3-Al(5)-O(26)	108.7(2)	O(5)-P(9)-O(45)	107.6(3)
O(2)#3-Al(5)-O(4)#1	111.3(2)	O(4)-P(9)-O(45)	106.5(3)
O(26)-Al(5)-O(4)#1	111.9(2)	O(36)-P(10)-O(10)	112.3(3)
O(2)#3-Al(5)-O(25)	107.2(2)	O(36)-P(10)-O(11)	109.8(3)
O(26)-Al(5)-O(25)	111.2(2)	O(10)-P(10)-O(11)	109.9(3)
O(4)#1-Al(5)-O(25)	106.6(2)	O(36)-P(10)-O(46)	110.9(3)
O(19)#4-Al(6)-O(10)	112.0(2)	O(10)-P(10)-O(46)	106.0(3)
O(19)#4-Al(6)-O(8)	107.9(2)	O(11)-P(10)-O(46)	107.8(3)
O(10)-Al(6)-O(8)	106.0(2)	O(39)-P(11)-O(15)	111.9(3)
O(19)#4-Al(6)-O(9)	109.7(2)	O(39)-P(11)-O(18)	112.1(3)
O(10)-Al(6)-O(9)	109.8(2)	O(15)-P(11)-O(18)	108.7(3)
O(8)-Al(6)-O(9)	111.5(2)	O(39)-P(11)-O(47)	106.9(3)
O(6)#5-Al(7)-O(18)	107.4(2)	O(15)-P(11)-O(47)	109.8(3)
O(6)#5-Al(7)-O(3)	110.1(2)	O(18)-P(11)-O(47)	107.4(3)
O(18)-Al(7)-O(3)	106.3(2)	O(41)-P(12)-O(32)	113.0(3)
O(6)#5-Al(7)-O(17)	108.1(2)	O(41)-P(12)-O(30)	112.0(3)
O(18)-Al(7)-O(17)	112.3(2)	O(32)-P(12)-O(30)	108.5(3)

O(3)-Al(7)-O(17)	112.6(2)	O(41)-P(12)-O(48)	107.0(3)
O(24)#5-Al(8)-O(32)	110.3(2)	O(32)-P(12)-O(48)	107.6(3)
O(24)#5-Al(8)-O(20)	111.1(2)	O(30)-P(12)-O(48)	108.6(3)
O(32)-Al(8)-O(20)	106.1(2)	P(8)-O(1)-Al(2)#2	139.9(3)
O(24)#5-Al(8)-O(31)	106.4(2)	P(8)-O(2)-Al(5)#6	156.6(3)
O(32)-Al(8)-O(31)	111.3(2)	P(8)-O(3)-Al(7)	149.9(3)
O(20)-Al(8)-O(31)	111.8(2)	P(9)-O(4)-Al(5)#2	155.2(3)
O(43)-P(1)-O(27)	112.6(2)	P(9)-O(5)-Al(3)	150.1(3)
O(43)-P(1)-O(28)	109.2(2)	P(6)-O(6)-Al(7)#4	146.5(3)
O(27)-P(1)-O(28)	108.0(3)	P(6)-O(7)-Al(3)	137.8(3)
O(43)-P(1)-O(26)	113.7(3)	P(6)-O(8)-Al(6)	144.7(3)
O(27)-P(1)-O(26)	105.4(2)	P(5)-O(9)-Al(6)	133.3(3)
O(28)-P(1)-O(26)	107.7(3)	P(10)-O(10)-Al(6)	163.0(4)
O(42)-P(2)-O(24)	111.4(3)	P(10)-O(11)-Al(1)	144.8(3)
O(42)-P(2)-O(25)	112.2(2)	P(5)-O(12)-Al(1)	142.3(3)
O(24)-P(2)-O(25)	108.7(3)	P(5)-O(13)-Al(4)	145.1(3)
O(42)-P(2)-O(23)	112.8(2)	P(7)-O(14)-Al(4)	139.4(3)
O(24)-P(2)-O(23)	106.6(3)	P(11)-O(15)-Al(4)	156.3(3)
O(25)-P(2)-O(23)	104.7(3)	P(7)-O(16)-Al(3)	135.1(3)
O(44)-P(3)-O(31)	113.3(3)	P(7)-O(17)-Al(7)	129.6(3)
O(44)-P(3)-O(29)	109.7(2)	P(11)-O(18)-Al(7)	151.2(3)
O(31)-P(3)-O(29)	107.4(2)	P(4)-O(19)-Al(6)#5	149.8(3)
O(44)-P(3)-O(22)	111.7(3)	P(4)-O(20)-Al(8)	150.9(3)
O(31)-P(3)-O(22)	106.2(2)	P(4)-O(21)-Al(4)	133.1(3)
O(29)-P(3)-O(22)	108.3(2)	P(3)-O(22)-Al(1)	131.6(3)
O(40)-P(4)-O(20)	113.9(3)	P(2)-O(23)-Al(1)	139.5(3)
O(40)-P(4)-O(19)	111.9(3)	P(2)-O(24)-Al(8)#4	157.0(3)
O(20)-P(4)-O(19)	106.9(2)	P(2)-O(25)-Al(5)	146.8(3)
O(40)-P(4)-O(21)	111.6(3)	P(1)-O(26)-Al(5)	132.8(3)
O(20)-P(4)-O(21)	105.5(3)	P(1)-O(27)-Al(2)	142.8(3)
O(19)-P(4)-O(21)	106.6(2)	P(1)-O(28)-Al(3)#1	138.6(3)
O(37)-P(5)-O(12)	109.9(2)	P(3)-O(29)-Al(2)	139.7(3)

O(37)-P(5)-O(13)	112.8(3)	P(12)-O(30)-Al(2)	152.9(3)
O(12)-P(5)-O(13)	107.7(2)	P(3)-O(31)-Al(8)	132.2(3)
O(37)-P(5)-O(9)	112.2(2)	P(12)-O(32)-Al(8)	155.4(3)
O(12)-P(5)-O(9)	108.8(3)		

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 x,y,z+1 #3 x-1,y,z-1
#4 x-1,y,z #5 x+1,y,z #6 x+1,y,z+1

Table S7 Hydrogen bonds for AlPO-CJ72-*S* [Å and deg.].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A)···O(39)#7	0.89	1.87	2.741(7)	165.2
N(1)-H(1B)···O(1)#7	0.89	2.33	3.116(7)	147.9
N(1)-H(1B)···O(3)#7	0.89	2.51	3.141(7)	128.3
N(1)-H(1C)···O(34)#7	0.89	1.96	2.801(8)	157
N(2)-H(2A)···O(37)#7	0.89	1.91	2.789(7)	168.4
N(2)-H(2B)···O(39)#7	0.89	1.92	2.806(7)	179
N(2)-H(2C)···O(35)#7	0.89	1.97	2.854(7)	175.5
N(3)-H(3A)···O(44)#7	0.89	1.96	2.842(7)	172.5
N(3)-H(3B)···O(40)#7	0.89	1.9	2.776(7)	169.3
N(3)-H(3C)···O(37)#7	0.89	2.13	2.960(7)	154.7
N(4)-H(4A)···O(25)	0.89	2.31	3.128(7)	153.5
N(4)-H(4A)···O(23)	0.89	2.41	3.172(7)	143.5
N(4)-H(4B)···O(34)#1	0.89	1.87	2.724(7)	161.3
N(4)-H(4C)···O(44)	0.89	1.98	2.818(7)	156.6
N(5)-H(5A)···O(7)	0.89	2.34	3.089(7)	142.1
N(5)-H(5A)···O(8)	0.89	2.36	3.195(7)	155.6
N(5)-H(5B)···O(38)	0.89	2.03	2.903(7)	166.2
N(5)-H(5C)···O(36)	0.89	1.86	2.736(7)	166.5
N(6)-H(6A)···O(36)	0.89	1.95	2.843(7)	177.4
N(6)-H(6A)···O(11)	0.89	2.56	3.023(6)	113
N(6)-H(6B)···O(21)	0.89	2.21	3.046(7)	156.3
N(6)-H(6C)···O(41)	0.89	1.87	2.759(7)	172.1

N(7)-H(7A)···O(38)	0.89	2.13	2.991(7)	162.1
N(7)-H(7B)···O(43)#2	0.89	2.24	3.096(8)	162.4
N(7)-H(7B)···O(28)#2	0.89	2.41	3.085(7)	132.9
N(7)-H(7C)···O(33)	0.89	1.91	2.769(8)	161.7
N(8)-H(8D)···O(41)	0.89	1.94	2.813(7)	165.6
N(8)-H(8E)···O(43)	0.89	1.88	2.757(7)	170.3
N(8)-H(8F)···O(42)	0.89	2	2.890(6)	173.5
O(45)-H(1P)···O(35)	1.07	1.54	2.575(6)	162.3
O(46)-H(2P)···O(42)	0.94	1.78	2.663(6)	154.4
O(47)-H(3P)···O(1W)	1.04	1.74	2.588(8)	136.4
O(48)-H(4P)···O(2W)#8	0.99	1.62	2.594(8)	165.8
O(1W)-H(1W1)···O(40)	1.02	1.75	2.733(8)	162.1
O(1W)-H(1W1)···O(19)	1.02	2.55	3.160(7)	117.9
O(1W)-H(2W1)···O(9)#5	1.01	2.25	3.085(7)	139.4
O(2W)-H(1W2)···O(33)#4	1	2.14	2.939(8)	134.9
O(2W)-H(1W2)···O(26)#2	1	2.62	3.152(7)	112.9
O(2W)-H(2W2)···O(42)#2	1.01	2.62	3.236(9)	119.5

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 x,y,z+1 #3 x-1,y,z-1 #4 x-1,y,z
#5 x+1,y,z #6 x+1,y,z+1 #7 x,y+1,z #8 x+1,y,z-1