Supporting Information Page

Prediction of Open-Framework Aluminophosphate Structures Using the AASBU
Method with Lowenstein's Constraints

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Table 1 Combinations of different kinds of Al and P atoms for $\text{Al}_8\text{P}_{10}\text{O}_{40}$ stoichiometry

No.	$\text{Al}(\text{O}_\text{b})_4$	$\text{Al}(\text{O}_\text{b})_5$	$\text{Al}(\text{O}_\text{b})_6$	$\text{P}(\text{O}_\text{b})_4$	$\text{P}(\text{O}_\text{b})_3(\text{O}_\text{t})$	$\text{P}(\text{O}_\text{b})_2(\text{O}_\text{t})_2$	$\text{P}(\text{O}_\text{b})(\text{O}_\text{t})_3$	$\text{O}_\text{b}/(\text{Al}+\text{P})$
1	0	8	0	10	0	0	0	2.22
2	1	6	1	10	0	0	0	2.22
3	1	7	0	9	1	0	0	2.17
4	2	4	2	10	0	0	0	2.22
5	2	5	1	9	1	0	0	2.17
6	2	6	0	8	2	0	0	2.11
7	2	6	0	9	0	1	0	2.11
8	3	2	3	10	0	0	0	2.22
9	3	3	2	9	1	0	0	2.17
10	3	4	1	8	2	0	0	2.11
11	3	4	1	9	0	1	0	2.11
12	3	5	0	7	3	0	0	2.06
13	3	5	0	8	1	1	0	2.06
14	3	5	0	9	0	0	1	2.06
15	4	0	4	10	0	0	0	2.22
16	4	1	3	9	1	0	0	2.17
17	4	2	2	8	2	0	0	2.11
18	4	2	2	9	0	1	0	2.11
19	4	3	1	7	3	0	0	2.06
20	4	3	1	8	1	1	0	2.06
21	4	3	1	9	0	0	1	2.06

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
22	4	4	0	6	4	0	0	2.00
23	4	4	0	7	2	1	0	2.00
24	4	4	0	8	0	2	0	2.00
25	4	4	0	8	1	0	1	2.00
26	5	0	3	8	2	0	0	2.11
27	5	0	3	9	0	1	0	2.11
28	5	1	2	7	3	0	0	2.06
29	5	1	2	8	1	1	0	2.06
30	5	1	2	9	0	0	1	2.06
31	5	2	1	6	4	0	0	2.00
32	5	2	1	7	2	1	0	2.00
33	5	2	1	8	0	2	0	2.00
34	5	2	1	8	1	0	1	2.00
35	5	3	0	5	5	0	0	1.94
36	5	3	0	6	3	1	0	1.94
37	5	3	0	7	1	2	0	1.94
38	5	3	0	7	2	0	1	1.94
39	5	3	0	8	0	1	1	1.94
40	6	0	2	6	4	0	0	2.00
41	6	0	2	7	2	1	0	2.00
42	6	0	2	8	0	2	0	2.00
43	6	0	2	8	1	0	1	2.00
44	6	1	1	5	5	0	0	1.94
45	6	1	1	6	3	1	0	1.94

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
46	6	1	1	7	1	2	0	1.94
47	6	1	1	7	2	0	1	1.94
48	6	1	1	8	0	1	1	1.94
49	6	2	0	4	6	0	0	1.89
50	6	2	0	5	4	1	0	1.89
51	6	2	0	6	2	2	0	1.89
52	6	2	0	6	3	0	1	1.89
53	6	2	0	7	0	3	0	1.89
54	6	2	0	7	1	1	1	1.89
55	6	2	0	8	0	0	2	1.89
56	7	0	1	4	6	0	0	1.89
57	7	0	1	5	4	1	0	1.89
58	7	0	1	6	2	2	0	1.89
59	7	0	1	6	3	0	1	1.89
60	7	0	1	7	0	3	0	1.89
61	7	0	1	7	1	1	1	1.89
62	7	0	1	8	0	0	2	1.89
63	7	1	0	3	7	0	0	1.83
64	7	1	0	4	5	1	0	1.83
65	7	1	0	5	3	2	0	1.83
66	7	1	0	5	4	0	1	1.83
67	7	1	0	6	1	3	0	1.83
68	7	1	0	6	2	1	1	1.83
69	7	1	0	7	0	2	1	1.83

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
70	7	1	0	7	1	0	2	1.83
71	8	0	0	2	8	0	0	1.78
72	8	0	0	3	6	1	0	1.78
73	8	0	0	4	4	2	0	1.78
74	8	0	0	4	5	0	1	1.78
75	8	0	0	5	2	3	0	1.78
76	8	0	0	5	3	1	1	1.78
77	8	0	0	6	0	4	0	1.78
78	8	0	0	6	1	2	1	1.78
79	8	0	0	6	2	0	2	1.78
80	8	0	0	7	0	1	2	1.78

Table 2 Combinations of different kinds of Al and Patoms for $\text{Al}_6\text{P}_8\text{O}_{32}$ stoichiometry

No.	$\text{Al}(\text{O}_\text{b})_4$	$\text{Al}(\text{O}_\text{b})_5$	$\text{Al}(\text{O}_\text{b})_6$	$\text{P}(\text{O}_\text{b})_4$	$\text{P}(\text{O}_\text{b})_3(\text{O}_\text{l})$	$\text{P}(\text{O}_\text{b})_2(\text{O}_\text{l})_2$	$\text{P}(\text{O}_\text{b})(\text{O}_\text{l})_3$	$\text{O}_\text{b}/(\text{Al}+\text{P})$
1	0	4	2	8	0	0	0	2.29
2	0	5	1	7	1	0	0	2.21
3	0	6	0	6	2	0	0	2.14
4	0	6	0	7	0	1	0	2.14
5	1	2	3	8	0	0	0	2.29
6	1	3	2	7	1	0	0	2.21
7	1	4	1	6	2	0	0	2.14
8	1	4	1	7	0	1	0	2.14
9	1	5	0	5	3	0	0	2.07
10	1	5	0	6	1	1	0	2.07
11	1	5	0	7	0	0	1	2.07
12	2	0	4	8	0	0	0	2.29
13	2	1	3	7	1	0	0	2.21
14	2	2	2	6	2	0	0	2.14
15	2	2	2	7	0	1	0	2.14
16	2	3	1	5	3	0	0	2.07
17	2	3	1	6	1	1	0	2.07
18	2	3	1	7	0	0	1	2.07
19	2	4	0	4	4	0	0	2.00
20	2	4	0	5	2	1	0	2.00
21	2	4	0	6	0	2	0	2.00

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
22	2	4	0	6	1	0	1	2.00
23	3	0	3	6	2	0	0	2.14
24	3	0	3	7	0	1	0	2.14
25	3	1	2	5	3	0	0	2.07
26	3	1	2	6	1	1	0	2.07
27	3	1	2	7	0	0	1	2.07
28	3	2	1	4	4	0	0	2.00
29	3	2	1	5	2	1	0	2.00
30	3	2	1	6	0	2	0	2.00
31	3	2	1	6	1	0	1	2.00
32	3	3	0	3	5	0	0	1.93
33	3	3	0	4	3	1	0	1.93
34	3	3	0	5	1	2	0	1.93
35	3	3	0	5	2	0	1	1.93
36	3	3	0	6	0	1	1	1.93
37	4	0	2	4	4	0	0	2.00
38	4	0	2	5	2	1	0	2.00
39	4	0	2	6	0	2	0	2.00
40	4	0	2	6	1	0	1	2.00
41	4	1	1	3	5	0	0	1.93
42	4	1	1	4	3	1	0	1.93
43	4	1	1	5	1	2	0	1.93
44	4	1	1	5	2	0	1	1.93
45	4	1	1	6	0	1	1	1.93

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
46	4	2	0	2	6	0	0	1.86
47	4	2	0	3	4	1	0	1.86
48	4	2	0	4	2	2	0	1.86
49	4	2	0	4	3	0	1	1.86
50	4	2	0	5	0	3	0	1.86
51	4	2	0	5	1	1	1	1.86
52	4	2	0	6	0	0	2	1.86
53	5	0	1	2	6	0	0	1.86
54	5	0	1	3	4	1	0	1.86
55	5	0	1	4	2	2	0	1.86
56	5	0	1	4	3	0	1	1.86
57	5	0	1	5	0	3	0	1.86
58	5	0	1	5	1	1	1	1.86
59	5	0	1	6	0	0	2	1.86
60	5	1	0	1	7	0	0	1.79
61	5	1	0	2	5	1	0	1.79
62	5	1	0	3	3	2	0	1.79
63	5	1	0	3	4	0	1	1.79
64	5	1	0	4	1	3	0	1.79
65	5	1	0	4	2	1	1	1.79
66	5	1	0	5	0	2	1	1.79
67	5	1	0	5	1	0	2	1.79
68	6	0	0	0	8	0	0	1.71
69	6	0	0	1	6	1	0	1.71

No.	Al(O _b) ₄	Al(O _b) ₅	Al(O _b) ₆	P(O _b) ₄	P(O _b) ₃ (O _t)	P(O _b) ₂ (O _t) ₂	P(O _b)(O _t) ₃	O _b /(Al+P)
70	6	0	0	2	4	2	0	1.71
71	6	0	0	2	5	0	1	1.71
72	6	0	0	3	2	3	0	1.71
73	6	0	0	3	3	1	1	1.71
74	6	0	0	4	0	4	0	1.71
75	6	0	0	4	1	2	1	1.71
76	6	0	0	4	2	0	2	1.71
77	6	0	0	5	0	1	2	1.71

Figure 1 The distribution of $O_b/(Al+P)$ in three dimensionalities

H-1

Space Group: $P-1$

Cell Parameters:

$$\begin{array}{lll} a = 8.8942 \text{ \AA} & b = 11.4596 \text{ \AA} & c = 12.4849 \text{ \AA} \\ \alpha = 67.6275^\circ & \beta = 103.7927^\circ & \gamma = 82.9911^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	0.72513	0.01813	-0.06850
AL2	0.99864	-0.33826	-0.15480
AL3	-0.04236	0.05051	-0.36662
AL4	0.50344	0.25727	-0.78944
P1	0.48602	0.18391	-1.00575
P2	0.24056	0.51269	-0.89527
P3	0.73319	-0.09496	-0.25445
P4	-0.02247	0.15102	-0.16492
P5	1.14380	-0.20150	-0.35657
O1	0.81654	0.13144	-0.15134
O2	0.01757	0.09646	-0.24978
O3	1.62499	-0.86039	-0.04217
O4	1.39290	-0.68192	-0.10063
O5	0.87655	-0.20280	-0.16153
O6	1.08612	-0.17603	-0.48964
O7	0.39659	0.15872	-0.70712
O8	0.66965	-0.01278	-0.19756
O9	0.67853	0.25947	-0.69455
O10	0.88529	-0.45118	-0.15163
O11	0.54797	0.18947	-0.88445
O12	0.10897	-0.07330	-0.06850
O13	1.09749	-0.91768	-0.15480
O14	0.78878	-0.01193	-0.36662
O15	0.97452	-0.70586	-0.78944
O16	1.05752	-0.29203	-1.00575
O17	1.16657	-0.39740	-0.89527
O18	0.37841	0.40968	-0.25445
O19	1.38039	-0.90976	-0.16492
O20	0.69841	-0.58949	-0.35657

H-2

Space Group: $P-1$

Cell Parameters:

$$\begin{array}{lll} a = 8.9228 \text{ \AA} & b = 9.6624 \text{ \AA} & c = 13.0091 \text{ \AA} \\ \alpha = 86.1747^\circ & \beta = 63.4588^\circ & \gamma = 96.9301^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	-0.30095	-0.01452	0.31328
AL2	-0.29602	0.40081	0.35066
AL3	0.17943	0.18532	0.24938
AL4	-0.13864	0.29473	-0.01132
P1	-0.17686	0.16983	0.45799
P2	-0.44954	0.20796	0.22464
P3	0.06658	-0.02954	0.12902
P4	-0.05379	0.60409	-0.12736
P5	-0.34162	-0.30709	0.43169
O1	-0.26348	0.05588	0.41974
O2	-0.43968	0.07307	0.28563
O3	-0.37548	0.33228	0.26137
O4	-0.23499	0.30627	0.44071
O5	0.01338	0.18524	0.38588
O6	0.14963	0.02422	0.20177
O7	-0.11530	-0.00534	0.18619
O8	0.16117	0.05633	0.01004
O9	-0.34046	0.21472	0.09476
O10	-0.63007	0.21634	0.25313
O11	-0.27741	0.58301	0.35240
O12	-0.38290	-0.19122	0.36859
O13	-0.15170	0.46025	-0.06276
O14	0.09303	0.58434	-0.23850
O15	-0.16998	0.68454	-0.15487
O16	-0.00623	0.31597	0.05321
O17	-0.07345	0.18344	-0.11709
O18	-0.20311	-0.24435	0.46012
O19	-0.49637	-0.37173	0.54101
O20	-0.22367	0.13267	0.58440

H-3

Space Group: $P-1$

Cell Parameters:

$$\begin{array}{lll} a = 8.6891 \text{ \AA} & b = 9.1954 \text{ \AA} & c = 13.4170 \text{ \AA} \\ \alpha = 82.9792^\circ & \beta = 70.4194^\circ & \gamma = 88.4699^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	-0.25460	-0.00809	0.31502
AL2	-0.30971	0.40785	0.35565
AL3	0.20161	0.22006	0.22961
AL4	-0.10665	0.25277	0.01234
P1	-0.09705	0.18056	0.43528
P2	-0.42267	0.23569	0.20910
P3	0.06436	0.00982	0.11893
P4	0.00242	0.53662	-0.15108
P5	-0.37848	-0.30182	0.45900
O1	-0.18112	0.06149	0.40397
O2	-0.39514	0.09946	0.27580
O3	-0.37795	0.36565	0.25389
O4	-0.18383	0.32282	0.42230
O5	0.07898	0.19573	0.36260
O6	0.17472	0.06606	0.17324
O7	-0.09608	-0.04199	0.20232
O8	0.03665	0.13683	0.04435
O9	-0.31123	0.23517	0.09526
O10	-0.59746	0.24474	0.21535
O11	-0.39164	0.57168	0.40051
O12	-0.36450	-0.16445	0.38273
O13	-0.05656	0.38357	-0.09950
O14	0.13179	0.52234	-0.25782
O15	-0.13788	0.62451	-0.16832
O16	-0.07318	0.38553	0.08407
O17	-0.14108	0.11740	-0.05929
O18	-0.23032	-0.31835	0.49361
O19	-0.53106	-0.29740	0.55502
O20	-0.10496	0.14481	0.54961

H-4

Space Group: $P-1$

Cell Parameters:

$$\begin{array}{lll} a = 10.7339 \text{ \AA} & b = 8.1852 \text{ \AA} & c = 10.0621 \text{ \AA} \\ \alpha = 82.7797^\circ & \beta = 99.4598^\circ & \gamma = 91.3910^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	0.66471	0.61988	0.61501
AL2	1.32829	-0.26861	-0.13433
AL3	1.42672	0.16072	-0.21617
AL4	0.87455	0.80128	-0.06744
P1	0.60159	-0.11296	-0.08568
P2	0.90250	0.01795	0.17856
P3	0.79605	0.44812	-0.09665
P4	0.69980	0.97611	0.48802
P5	0.60607	0.47458	0.34486
O1	1.36217	0.12566	-0.06722
O2	1.44402	0.36908	-0.25861
O3	0.50551	0.63342	0.62627
O4	1.31013	-0.38580	-0.27020
O5	1.21631	-0.11686	-0.16006
O6	1.35217	0.05978	-0.34671
O7	0.72555	0.81568	0.58097
O8	0.73787	0.50649	0.75999
O9	0.67918	0.51577	0.47802
O10	1.30485	-0.39993	0.00984
O11	1.48665	-0.21711	-0.11963
O12	1.57136	0.06338	-0.14916
O13	0.87572	0.58647	-0.03806
O14	0.71648	0.83696	-0.14085
O15	1.01633	0.13067	0.17077
O16	0.89859	-0.10041	0.07523
O17	0.92289	-0.08437	0.31691
O18	0.87732	0.30023	-0.09632
O19	0.60773	1.07622	0.54298
O20	0.82083	1.07490	0.48986

H-5

Space Group: $P2_1$

Cell Parameters:

$$\begin{array}{lll} a = 9.3217 \text{ \AA} & b = 9.7907 \text{ \AA} & c = 10.1301 \text{ \AA} \\ \alpha = 90.0000^\circ & \beta = 93.1450^\circ & \gamma = 90.0000^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	-0.95562	0.39310	0.07849
AL2	-0.62771	0.34057	0.41672
AL3	-0.54027	0.60969	0.91519
AL4	-0.87456	0.66192	0.58077
P1	-0.95007	0.42446	0.38771
P2	-0.62437	0.38226	0.11535
P3	-0.54909	0.57708	0.61009
P4	-0.87576	0.62176	0.87890
P5	-0.72818	-0.04943	-0.01788
O1	-0.47519	0.77600	-0.06304
O2	-0.95705	0.45084	0.24109
O3	-0.81112	0.35298	0.42961
O4	-1.07355	0.10526	0.26576
O5	-1.03592	0.23198	0.06032
O6	-1.07202	0.33208	0.42557
O7	-0.95777	0.55924	0.46046
O8	-0.41116	0.90123	0.73804
O9	-0.77883	0.33548	0.09723
O10	-0.60073	0.51594	0.04677
O11	-0.89294	0.48594	-0.05385
O12	-0.42967	0.67239	0.57244
O13	-0.54076	0.44531	0.53297
O14	-0.69058	0.64707	0.57788
O15	-0.53140	0.54385	0.75576
O16	-0.71799	0.65801	0.88111
O17	-0.70832	-0.16987	0.07451
O18	-0.68666	0.92372	0.84250
O19	-0.88716	-0.01671	-0.03107
O20	-0.63748	1.06451	1.04128

H-6

Space Group: Cc

Cell Parameters:

$$\begin{array}{lll} a = 13.7920 \text{ \AA} & b = 9.1952 \text{ \AA} & c = 13.4391 \text{ \AA} \\ \alpha = 90.0000^\circ & \beta = 79.8253^\circ & \gamma = 90.0000^\circ \end{array}$$

Atomic Coordinates:

<i>Atom</i>	<i>x</i>	<i>y</i>	<i>z</i>
AL1	-1.04012	0.22579	0.09926
AL2	-1.14012	-0.34174	0.92622
AL3	-0.48556	-0.27193	0.76994
AL4	0.67923	-0.09026	0.39310
P1	0.02156	-0.23958	0.03680
P2	-0.97078	-0.43660	0.75163
P3	-1.11489	-0.04955	0.79722
P4	-1.16556	0.32229	0.93903
P5	-0.86041	0.25542	0.92976
O1	-0.89065	-0.36575	0.79858
O2	-0.86396	0.41883	0.93530
O3	0.60152	-0.14860	0.50397
O4	-0.98594	0.36808	0.15373
O5	-1.13339	0.26504	0.03317
O6	-0.93901	0.18304	0.00762
O7	-1.11190	-0.17563	0.86749
O8	-1.06792	-0.42132	0.82222
O9	-1.26231	-0.29279	0.94926
O10	-0.94687	-0.59593	0.73435
O11	-1.09030	-0.09999	0.68848
O12	-1.03521	0.05951	0.81003
O13	-1.21504	0.02023	0.82000
O14	-0.88047	0.20649	0.82704
O15	-1.18490	0.48331	0.95703
O16	-1.08644	0.30344	0.84787
O17	-1.25567	0.24387	0.91846
O18	-0.47993	-0.31248	0.64297
O19	0.92384	-0.30859	0.02595
O20	0.04141	-0.11106	0.96576