Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information

Thermodynamic Rules for Zeolite Formation from Machine Learning based Global Optimization

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Supplementary Method

Ab-initio thermodynamics analyses

To determine the Gibbs formation energy of SiAlPOH and SiAlPONa, the *ab-initio* thermodynamics analyses have been performed where the formula (1,2) are used to compute the free energy change.

$Si_xAl_yP_zO_2H_{y-z} = x*SiO_2 + (y-z)/2*Al_2O_3 + z*AlPO_4 + (y-z)/2*H_2O$ (1)

$Si_xAl_yP_zO_2Na_{y-z} = x*SiO_2 + (y-z)/2*Al_2O_3 + z*AlPO_4 + (y-z)*NaOH(aq) - (y-z)/2*H_2O$ (2)

To determine the Gibbs free energy change (***ΔG***) per formula unit (f.u.) for the above reactions, one needs to compute

$$\Delta G(p,T) = G[Si_xAl_yP_zO_2H_{y-z}](p,T) - x*G[SiO_2](p,T) - \frac{y-z}{2}*G[Al_2O_3](p,T) - z*G[AlPO_4](p,T) - \frac{y-z}{2}*\mu[H_2O](p,T) \quad (3)$$

$$\Delta G(p,T) = G[Si_xAl_yP_zO_2H_{y-z}](p,T) - x*G[SiO_2](p,T) - \frac{y-z}{2}*G[Al_2O_3](p,T) - z*G[AlPO_4](p,T) - (y-z)*G[NaOH(aq)](p,T) + \frac{y-z}{2}*\mu[H_2O](p,T) \quad (4)$$

where G is the Gibbs free energy of bulks/surfaces and μ is the chemical potential for molecules. The $G[X]$ can be approximated by their DFT total energy $E[X]$ with appropriate inclusion of zero-point-energy (***ZPE***), since it is known that the vibration entropy and the ***pV*** term contributions of solid phases are negligibly small. The chemical potential for molecules $\mu[X]$ can be calculated as follows:

$$\mu[X](p,T) = E[X] + ZPE[X] + [H[X](p^0,T) - H[X](p^0,0K) - TS[X](p^0,T) + k_BTln\frac{p}{p^0}] \quad (5)$$

where enthalpy (***H***) and entropy (***S***) terms are taken from the standard thermodynamics data.

The chemical potential of $G[NaOH(aq)]$ is calculated as follows.

According to formula (6,7),the chemical potential of NaOH(aq) can be written as the function of the chemical potentials of H_2, H_2O and Na(s), see Eq. (9).

$Na(s) + H_2O(l) = NaOH(s) + 1/2*H_2(g)$ (6)

$Na(s) + H_2O(l) = NaOH(aq) + 1/2*H_2(g)$ (7)

Reaction of Eq. 7 is strongly exothermic and the heat release amount is about 141 kJ/mol and more if NaOH is dissolved in excess water (188 kJ/mol, Eq. 8).[1]

Here we assume that the $G[NaOH(aq)]$ at hydrothermal condition is equal to that at standard condition.

$$G[NaOH(aq)](473\ K, 15.53\ bar) = G^o[NaOH(aq)]\ at\ 298.15\ K, 1\ bar \quad (8)$$

Therefore,

$$G^o[NaOH(aq)] = G^o[Na(s)] + \mu^o[H_2O(l)] - \frac{1}{2}*\mu^o[H_2] - 188 \quad (9)$$

where

$$G^o[Na(s)] = E[Na(metal)] \quad (10)$$

$$\mu^o[H_2O(l)] = \mu^o[H_2O(g)](298.15K, 0.013\ bar) \quad (11)$$

Table S1 | Structure information in the first principles global dataset utilized in G-NN training. Listed data is the number of structures, as distinguished by the chemical formula, the number of atoms per supercell (N_{atom}), the type of structures (cluster, bulk and layer). In this work we build G-NN potential mainly from bulk systems as required for zeolite PES.

Species	N_{atom}	cluster	layer	bulk	total
O16-Si8	24	0	4	731	735
O16-Al1-Si7	24	0	0	11	11
O16-Al2-Si5-P1	24	0	0	17	17
O24-Si12	36	0	6	809	815
O24-Al1-Si10-P1	36	0	0	51	51
O24-Al1-Si11	36	0	0	6	6
O24-Al2-Si8-P2	36	0	0	57	57
O24-Al2-Si9-P1	36	0	0	14	14
O24-Al3-Si6-P3	36	0	0	54	54
O24-Al3-Si7-P2	36	0	0	10	10
O24-Al4-Si4-P4	36	0	0	52	52
O24-Al5-Si2-P5	36	0	0	55	55
O24-Al6-P6	36	0	2	330	332
O24-Al6-Si1-P5	36	0	1	10	11
O28-Al1-Si13	42	0	0	13	13
O28-Al2-Si11-P1	42	0	0	5	5
O28-Al4-Si6-P4	42	0	0	223	223
O28-Al5-Si4-P5	42	0	0	228	228
O32-Si16	48	0	0	513	513
O32-Al3-Si13	48	0	0	18	18
O32-Al4-Si8-P4	48	0	0	534	534
O32-Al5-Si6-P5	48	0	0	274	274
O32-Al5-Si7-P4	48	0	0	12	12
O32-Al6-Si4-P6	48	0	0	219	219
O32-Al7-Si2-P7	48	0	0	244	244
O32-Al8-P8	48	0	0	249	249
O32-Al8-Si1-P7	48	0	0	11	11
O36-Si18	54	0	1	24	25
O40-Si20	60	0	0	328	328
O40-Al1-Si19	60	0	0	7	7
O40-Al2-Si17-P1	60	0	0	2	2
O40-Al3-Si15-P2	60	0	0	12	12
O40-Al4-Si13-P3	60	0	0	2	2
O40-Al5-Si11-P4	60	0	0	3	3
O48-Si24	72	1	0	93	94
O108-Al27-Si1-P26	162	0	0	10	10
O128-Si64	192	0	0	8	8
O144-Si72	216	0	0	4	4

H1-O16-Al1-Si7	25	0	0	449	449
H1-O16-Al2-Si5-P1	25	0	1	252	253
H1-O24-Al1-Si11	37	0	2	1298	1300
H1-O24-Al2-Si9-P1	37	0	0	702	702
H1-O24-Al3-Si7-P2	37	0	0	924	924
H1-O24-Al6-Si1-P5	37	0	10	356	366
H1-O28-Al1-Si13	43	0	0	511	511
H1-O28-Al2-Si11-P1	43	0	0	218	218
H1-O28-Al2-Si12	43	0	0	9	9
H1-O32-Al1-Si15	49	0	0	489	489
H1-O32-Al2-Si13-P1	49	0	0	251	251
H1-O32-Al3-Si11-P2	49	0	0	245	245
H1-O32-Al4-Si9-P3	49	0	0	253	253
H1-O32-Al5-Si7-P4	49	0	0	230	230
H1-O32-Al6-Si6-P4	49	0	0	12	12
H1-O32-Al8-Si1-P7	49	0	0	229	229
H1-O32-Al8-Si2-P6	49	0	0	18	18
H1-O36-Al1-Si17	55	0	0	21	21
H1-O36-Al4-Si11-P3	55	0	0	28	28
H1-O36-Al5-Si9-P4	55	0	1	25	26
H1-O40-Al1-Si19	61	0	0	104	104
H1-O40-Al2-Si17-P1	61	0	0	691	691
H1-O40-Al2-Si18	61	0	0	5	5
H1-O40-Al3-Si15-P2	61	0	0	615	615
H1-O40-Al4-Si13-P3	61	0	0	284	284
H1-O40-Al5-Si11-P4	61	0	0	262	262
H1-O40-Al5-Si12-P3	61	0	0	9	9
H1-O48-Al1-Si23	73	0	0	8	8
H1-O96-Al1-Si47	145	0	0	44	44
H1-O96-Al24-Si1-P23	145	0	0	76	76
H1-O108-Al27-Si1-P26	163	0	0	127	127
H1-O128-Al1-Si63	193	0	0	35	35
H1-O144-Al36-Si1-P35	217	0	0	72	72
H1-O160-Al40-Si1-P39	241	0	0	59	59
H1-O216-Al54-Si1-P53	325	0	0	10	10
H2-O24-Al2-Si10	38	0	3	1304	1307
H2-O24-Al3-Si8-P1	38	0	0	466	466
H2-O24-Al4-Si6-P2	38	0	0	218	218
H2-O24-Al5-Si4-P3	38	0	0	235	235
H2-O24-Al6-Si1-P5	38	0	0	30	30
H2-O24-Al6-Si2-P4	38	0	1	513	514
H2-O24-Al8-P4	38	0	0	11	11
H2-O28-Al1-Si13	44	0	0	32	32
H2-O28-Al2-Si12	44	0	0	490	490

H2-O32-Al2-Si14	50	0	0	272	272
H2-O32-Al3-Si12-P1	50	0	0	492	492
H2-O32-Al3-Si13	50	0	0	17	17
H2-O32-Al6-Si6-P4	50	0	0	254	254
H2-O32-Al7-Si5-P4	50	0	0	8	8
H2-O32-Al8-Si2-P6	50	0	0	219	219
H2-O32-Al8-Si3-P5	50	0	0	6	6
H2-O32-Al8-Si4-P4	50	0	0	17	17
H2-O36-Al2-Si16	56	0	0	32	32
H2-O36-Al4-Si12-P2	56	0	0	30	30
H2-O40-Al2-Si18	62	0	0	289	289
H2-O40-Al5-Si12-P3	62	0	0	263	263
H2-O40-Al5-Si13-P2	62	0	0	14	14
H2-O48-Al5-Si19	74	0	0	6	6
H2-O96-Al2-Si46	146	0	0	41	41
H2-O96-Al12-Si26-P10	146	0	0	40	40
H3-O24-Al3-Si9	39	0	1	1003	1004
H3-O24-Al4-Si7-P1	39	0	0	234	234
H3-O24-Al6-Si3-P3	39	0	1	286	287
H3-O28-Al3-Si11	45	0	0	238	238
H3-O28-Al4-Si9-P1	45	0	0	229	229
H3-O32-Al3-Si13	51	0	0	545	545
H3-O32-Al7-Si5-P4	51	0	0	238	238
H3-O32-Al8-Si3-P5	51	0	0	223	223
H3-O32-Al8-Si4-P4	51	0	0	18	18
H3-O36-Al3-Si15	57	0	0	52	52
H3-O36-Al4-Si13-P1	57	0	0	27	27
H3-O36-Al5-Si11-P2	57	0	0	21	21
H3-O40-Al5-Si13-P2	63	0	0	246	246
H3-O40-Al5-Si14-P1	63	0	0	4	4
H3-O48-Al5-Si19	75	0	0	14	14
H3-O96-Al3-Si45	147	0	0	49	49
H4-O24-Al4-Si8	40	0	1	615	616
H4-O24-Al6-Si4-P2	40	0	2	58	60
H4-O24-Al10-P2	40	0	0	11	11
H4-O28-Al4-Si10	46	0	0	250	250
H4-O32-Al8-Si4-P4	52	0	0	299	299
H4-O36-Al4-Si14	58	0	0	30	30
H4-O40-Al5-Si14-P1	64	0	0	256	256
H4-O48-Al5-Si19	76	0	0	3	3
H4-O96-Al4-Si44	148	0	0	115	115
H5-O24-Al5-Si7	41	0	0	56	56
H5-O24-Al6-Si5-P1	41	0	0	61	61
H5-O24-Al11-P1	41	0	0	10	10

H5-O48-Al5-Si19	77	0	0	17	17
H5-O96-Al5-Si43	149	0	0	215	215
H6-O24-Al6-Si6	42	0	1	108	109
H6-O96-Al6-Si42	150	0	0	31	31
H7-O96-Al7-Si41	151	0	0	207	207
H8-O24-Al8-Si4	44	0	0	68	68
H8-O96-Al8-Si40	152	0	0	167	167
H9-O96-Al9-Si39	153	0	0	236	236
H10-O24-Al10-Si2	46	0	0	68	68
H10-O96-Al10-Si38	154	0	0	176	176
H10-O96-Al16-Si26-P6	154	0	0	39	39
H11-O96-Al11-Si37	155	0	0	130	130
H12-O24-Al12	48	0	0	59	59
H12-O96-Al12-Si36	156	0	0	98	98
H14-O96-Al14-Si34	158	0	0	100	100
H16-O96-Al16-Si32	160	0	0	158	158
H16-O96-Al20-Si24-P4	160	0	0	82	82
H16-O96-Al32-P16	160	0	0	36	36
H18-O96-Al18-Si30	162	0	0	61	61
H19-O96-Al19-Si29	163	0	0	69	69
H22-O96-Al22-Si26	166	0	0	122	122
H23-O96-Al23-Si25	167	0	0	54	54
H27-O96-Al27-Si21	171	0	0	47	47
H29-O96-Al29-Si19	173	0	0	42	42
H34-O96-Al34-Si14	178	0	0	52	52
total	--	1	38	27096	27135

Table S2 | Benchmark of G-NN calculations as compared with DFT results for low energy zeolites encountered in this work. Listed data include the compositions, total atom number per cell (N_{atom}), DFT energy, NN energy and energy differences between DFT energy and NN energy (ΔE, meV/atom).

ID	Composition	E_{DFT} (eV)	E_{NN} (eV)	N_{Atom}	ΔE (eV/f.u.)
1	P1Si10Al1O24	-247.36	-247.418	36	0.005
2	P1Si10Al1O24	-246.007	-245.976	36	-0.003
3	P1Si5Al6O24H5	-256.338	-256.19	41	-0.012
4	P1Si5Al6O24H5	-257.949	-257.969	41	0.002
5	P1Si6Al5O24H4	-254.112	-254.059	40	-0.004
6	P1Si6Al5O24H4	-255.558	-255.47	40	-0.007
7	P1Si7Al4O24H3	-253.926	-253.911	39	-0.001
8	P1Si7Al4O24H3	-251.782	-251.627	39	-0.013
9	P1Si8Al3O24H2	-249.616	-249.453	38	-0.014
10	P1Si8Al3O24H2	-251.433	-251.285	38	-0.012
11	P1Si9Al2O24H1	-249.537	-249.574	37	0.003

12	P1Si9Al2O24H1	-248.026	-247.992	37	-0.003
13	P2Si4Al6O24H4	-251.643	-251.644	40	0.000
14	P2Si4Al6O24H4	-253.244	-253.136	40	-0.009
15	P2Si5Al5O24H3	-249.446	-249.468	39	0.002
16	P2Si5Al5O24H3	-250.793	-250.644	39	-0.012
17	P2Si6Al4O24H2	-248.61	-248.503	38	-0.009
18	P2Si6Al4O24H2	-247.356	-247.356	38	0.000
19	P2Si7Al3O24H1	-245.349	-245.261	37	-0.007
20	P2Si7Al3O24H1	-246.463	-246.372	37	-0.008
21	P2Si8Al2O24	-244.75	-244.879	36	0.011
22	P2Si8Al2O24	-243.401	-243.362	36	-0.003
23	P3Si3Al6O24H3	-247.39	-247.332	39	-0.005
24	P3Si3Al6O24H3	-248.398	-248.142	39	-0.021
25	P3Si4Al5O24H2	-245.821	-245.735	38	-0.007
26	P3Si4Al5O24H2	-244.699	-244.73	38	0.003
27	P3Si5Al4O24H1	-242.761	-242.859	37	0.008
28	P3Si5Al4O24H1	-244.249	-244.348	37	0.008
29	P3Si6Al3O24	-240.163	-240.181	36	0.002
30	P3Si6Al3O24	-242.065	-242.084	36	0.002
31	P4Si2Al6O24H2	-244.234	-244.106	38	-0.011
32	P4Si2Al6O24H2	-242.956	-242.92	38	-0.003
33	P4Si3Al5O24H1	-240.282	-240.269	37	-0.001
34	P4Si3Al5O24H1	-241.489	-241.517	37	0.002
35	P4Si4Al4O24	-238.105	-238.156	36	0.004
36	P4Si4Al4O24	-239.792	-239.844	36	0.004
37	P5Si1Al6O24H1	-239.632	-239.55	37	-0.007
38	P5Si1Al6O24H1	-238.349	-238.228	37	-0.010
39	P5Si2Al5O24	-235.478	-235.45	36	-0.002
40	P5Si2Al5O24	-237.169	-237.205	36	0.003
41	P6Al6O24	-234.98	-234.939	36	-0.003
42	P6Al6O24	-233.967	-234.034	36	0.006
43	P6Al6O24	-234.547	-234.566	36	0.002
44	P6Al6O24	-233.944	-233.949	36	0.000
45	P6Al6O24	-233.944	-233.953	36	0.001
46	P6Al6O24	-233.935	-233.928	36	-0.001
47	P6Al6O24	-235.321	-235.319	36	0.000
48	Si10Al2O24H2	-253.189	-253.2	38	0.001
49	Si10Al2O24H2	-254.846	-254.839	38	-0.001
50	Si11Al1O24H1	-251.361	-251.417	37	0.005
51	Si11Al1O24H1	-252.966	-252.914	37	-0.004
52	Si12O24	-250.304	-250.357	36	0.004
53	Si12O24	-249.821	-249.835	36	0.001
54	Si12O24	-250.581	-250.498	36	-0.007
55	Si12O24	-248.753	-248.908	36	0.013

56	Si12O24	-249.812	-249.854	36	0.004
57	Si12O24	-251.147	-251.092	36	-0.005
58	Si12O24	-250.192	-250.222	36	0.003
59	Si6Al6O24H6	-262.448	-262.354	42	-0.008
60	Si6Al6O24H6	-257.613	-257.483	42	-0.011
61	Si6Al6O24H6	-262.64	-262.576	42	-0.005
62	Si6Al6O24H6	-262.774	-262.607	42	-0.014
63	Si6Al6O24H6	-260.934	-260.865	42	-0.006
64	Si6Al6O24H6	-260.523	-260.317	42	-0.017
65	Si6Al6O24H6	-261.586	-261.485	42	-0.008
66	Si6Al6O24H6	-261.916	-261.922	42	0.001
67	Si7Al5O24H5	-260.504	-260.403	41	-0.008
68	Si7Al5O24H5	-259.323	-259.275	41	-0.004
69	Si8Al4O24H4	-257.348	-257.173	40	-0.015
70	Si8Al4O24H4	-258.439	-258.441	40	0.000
71	Si9Al3O24H3	-256.46	-256.407	39	-0.004
72	Si9Al3O24H3	-255.345	-255.303	39	-0.004
Root mean square error					0.007

Table S3 | Benchmark of G-NN and DFT formation Gibbs free energy (G_f) of CHA-type $Si_xAl_yP_zO_2H_{y-z}$ (x + y + z = 1) compositions. G_f is the free energy of zeolite (without rigid body) relative to the free energies of quartz-SiO_2, quartz-AlPO, α-Al_2O_3 solids and H_2O at 200 °C and 15.53 bar. Also see Figure 2 for details.

Composition	DFT G_f (ev/f.u.)	NN G_f (eV/f.u.)	Δ*E*(eV/f.u.)
Si0Al6P6H0	0.114	0.113	0.001
Si10Al1P1H0	0.200	0.199	0.001
Si10Al2P0H2	0.182	0.171	0.011
Si11Al1P0H1	0.169	0.161	0.008
Si12Al0P0H0	0.110	0.105	0.005
Si1Al6P5H1	0.155	0.162	-0.007
Si2Al5P5H0	0.203	0.200	0.003
Si2Al6P4H2	0.178	0.177	0.001
Si3Al5P4H1	0.203	0.189	0.014
Si3Al6P3H3	0.216	0.217	-0.001
Si4Al4P4H0	0.207	0.200	0.007
Si4Al5P3H2	0.231	0.227	0.004
Si4Al6P2H4	0.240	0.239	0.001
Si5Al4P3H1	0.226	0.215	0.011
Si5Al5P2H3	0.232	0.235	-0.003
Si5Al6P1H5	0.276	0.271	0.005
Si6Al3P3H0	0.247	0.246	0.001
Si6Al4P2H2	0.231	0.220	0.011

Si6Al5P1H4	0.231	0.234	-0.003
Si6Al6P0H6	0.304	0.296	0.008
Si7Al3P2H1	0.231	0.234	-0.003
Si7Al4P1H3	0.286	0.288	-0.002
Si7Al5P0H5	0.256	0.253	0.003
Si8Al2P2H0	0.206	0.207	-0.001
Si8Al3P1H2	0.269	0.271	-0.002
Si8Al4P0H4	0.233	0.241	-0.008
Si9Al2P1H1	0.205	0.198	0.007
Si9Al3P0H3	0.212	0.210	0.002
Root mean square error	--	--	0.005

Table S4. The energy difference between G-NN and DFT calculations for 30 different zeolite structures with AlPO and SiO_2 compositions.*

	name	Δ*E*(eV/f.u.) of AlPO	Δ*E*(eV/f.u.) SiO_2		name	Δ*E*(eV/f.u.) AlPO	Δ*E*(eV/f.u.) SiO_2		name	Δ*E*(eV/f.u.) AlPO	Δ*E*(eV/f.u.) SiO_2
1	ACO	-0.002	0.006	11	AVE	0.001	-0.003	21	GME	-0.001	0.008
2	AEI	0.002	0.008	12	AWO	-0.001	0.000	22	MVY	0.011	0.009
3	AFG	0.002	-0.010	13	CGS	0.003	0.007	23	PON	0.003	0.005
4	AFI	0.003	0.008	14	CHA	0.001	0.006	24	quartz	-0.003	0.006
5	AFN	0.000	-0.007	15	CZP	0.010	0.016	25	RHO	0.005	0.009
6	AHT	0.003	0.002	16	DL	-0.003	0.010	26	SAF	0.003	0.006
7	ATN	-0.003	-0.010	17	EAB	0.002	0.003	27	SAT	0.002	-0.003
8	ATO	0.000	-0.012	18	ERI	0.000	-0.001	28	SAV	0.003	0.008
9	ATS	-0.004	-0.003	19	EZT	0.001	-0.002	29	TOL	0.000	-0.011
10	ATV	0.000	0.002	20	FAU	0.006	0.014	30	VFI	0.001	0.002

*The root mean square errors are 0.003 and 0.007 eV/f.u. for AlPO and SiO_2, respectively.

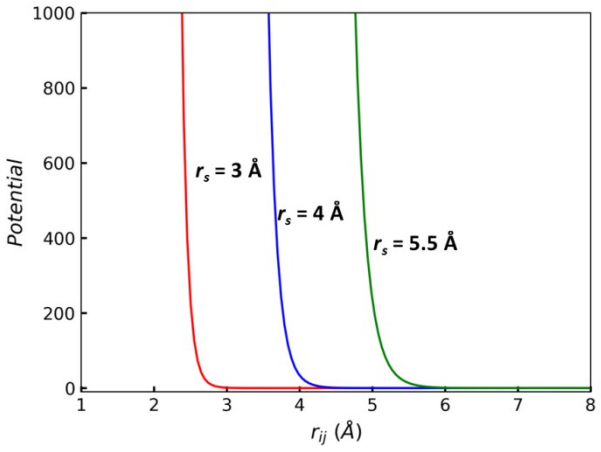


Figure S1 | The power-type repulsive potential profile with different r_s.

Supplementary Note 1

All experiment results in Table S5, S6, S7 and S10 are collected from the IZC-SC bank,[2] which are related to the as-synthesized AlPO, SiO_2, SAPO and aluminosilicate zeolites, respectively. By using G-NN calculations, we can facilely optimize and compute the energy of these known framework for AlPO and SiO_2 zeolites.

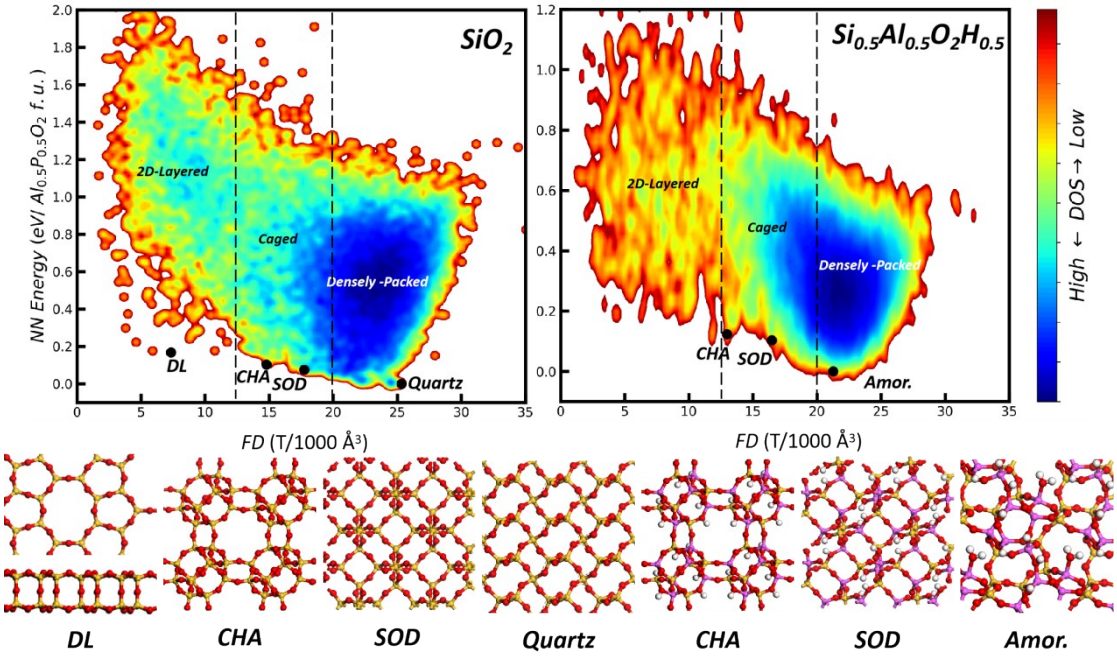


Figure S2 | Global PES contour plots for SiO_2 and $Si_{0.5}Al_{0.5}O_2H_{0.5}$ minima as determined from E-SSW-NN global. Each plot contains more than 25,000 minima. The **x** axis is the framework density (FD) of structure, and the **y** axis is the relative G-NN energy of minima (GM is set as energy zero). For the structure snapshots, the yellow, pink, red and white balls represent the Si, Al, O and H atoms, respectively.

Table S5 | The G-NN energies, FD values and n_T of 66 zeolites from 252 zeolite bank. 63 of them are predicted to be possible for AlPO zeolite. Others (186=252-66) do not satisfy the bonding pattern rules, e.g. no P-O-P or Al-O-Al bonding patterns. 29 kinds of AlPO zeolites have been synthesized in experiment as indicated by the reference.

	name	energy	FD	n_T	material	reference
	quartz	**0**	**24.57**	**12**		
1	PSI	0.046	19.16	72	*PST-6	Angew. Chem. Int. Ed., 53, 7480-7483 (2014)
2	SAF	0.053	17.83	32	*STA-15	Chem. Mater., 22, 338-346 (2010)
3	AFO	0.054	18.12	20	AlPO-41	Zeolites, 14, 523-528 (1994)
4	AEL	0.06	18.11	20	AlPO-11	Zeolites, 7, 160-162 (1987)
5	ATO	0.062	17.73	12	AlPO-31	Zeolites, 12, 338-342 (1992)
6	ATV	0.071	18.03	12	AlPO-25	J. Phys. Chem., 94, 3365-3367 (1990)
7	AFI	0.072	16.02	24	AlPO-5	ACS Sym. Ser., 218, 109-118 (1983)
8	IFO	0.077	16.13	32	*ITQ-51	Proc. Natl. Acad. Sci., 110, 3749-3754 (2013)
9	OSI	0.077	16.72	16	*UiO-6	Chem. Commun., , 1553-1554 (1996)
10	ATN	0.079	16.9	8	SAPO-39	Zeolites, 18, 350-355 (1997)
11	AET	0.083	16.72	36	AlPO-8	Zeolites, 10, 522-524 (1990)
12	FRA	0.084	16.29	60		
13	AWO	0.085	17.28	24	AlPO-21	Inorg. Chem., 24, 188-193 (1985)
14	FAR	0.086	16.07	84		
15	GIU	0.086	16.19	96		
16	LTN	0.086	15.81	192		
17	AFG	0.087	16.09	48		
18	JSW	0.087	17.45	48		
19	MAR	0.087	16.05	72		
20	CAN	0.088	15.95	12		
21	ATS	0.089	15.24	12	AlPO-36	Microporous Mesoporous Mat., 32, 241-250 (1999)
22	LIO	0.089	15.99	36		
23	MVY	0.089	19.62	12		
24	SAT	0.089	15.59	24		
25	TOL	0.089	16.07	72		
26	AST	0.091	15.04	10	AlPO-16	Zeolites, 11, 502-506 (1991)
27	AVE	0.091	15.6	48	AlPO-78	Chem. Mater., 30, 582-586 (2018)
28	EZT	0.092	16.21	24	*EMM-3	Chem. Mater., 18, 1697-1704 (2006)
29	PON	0.092	17.1	24	*IST-1	Microporous Mesoporous Mat., 65, 43-57 (2003)
30	LOS	0.092	16.02	24		
31	ERI	0.097	15.14	36	AlPO-17	Acta Crystallogr., C42, 283-286 (1986)
32	EAB	0.097	15.11	36		
33	SWY	0.098	15.14	72	*STA-20	Chem. Mater., 29, 2180-2190 (2017)
34	ANA	0.098	18.26	24	AlPO-24	J. Am. Chem. Soc., 104, 1146-1147 (1982)
35	LTJ	0.099	17.67	16		

36	PHI	0.102	15.53	16		
37	AEI	0.103	14.25	24	AlPO-18	Zeolites, 11, 654-661 (1991)
38	CHA	0.103	14.26	12	AlPO-34	Acta Crystallogr., C50, 852-854 (1994)
39	GIS	0.103	15.56	8	AlPO-43	Chem. Commun., , 1293-1294 (1996)
40	SIV	0.103	15.54	32		
41	AFT	0.104	14.28	72	AlPO-52	Zeolites, 15, 460-469 (1995)
42	AFX	0.104	14.26	48		
43	GME	0.105	14.25	24		
44	MWF	0.105	15.23	720		
45	SAV	0.105	14.26	48		
46	SFW	0.105	14.28	36		
47	PAU	0.106	15.09	336		
48	PWN	0.106	14.78	120		
49	FAU	0.107	12.51	48	AlPO-37	J. Am. Chem. Soc., 106, 6092-6093 (1984)
50	CGS	0.107	15.94	32		
51	JNT	0.107	18.89	32		
52	TSC	0.107	12.46	96		
53	AFN	0.108	16.74	16	AlPO-14	Microporous Mesoporous Mat., 57, 211-214 (2003)
54	RHO	0.109	13.62	24		
55	SBT	0.109	12.92	48		
56	SBS	0.11	12.92	96		
57	AFS	0.111	13.71	56		
58	BPH	0.111	13.72	28		
59	ETR	0.114	14.54	48		
60	POR	0.116	16.46	64	*PST-14	Angew. Chem. Int. Ed., 57, 3727-3732 (2018)
61	ACO	0.117	15.6	8		
62	AHT	0.134	17.39	12	AlPO-H2	Solid State Nucl. Mag. Res., 4, 173-178 (1995)
63	VFI	0.138	13.31	36	*VPI-5	Nature, 331, 698-699 (1988)
	DL	**0.166**	**5.71**	**12**		
64	**AFY**	**0.17**	**13.15**	**16**		**Only observed in CoAlPO material**
65	**BSV**	**0.187**	**17.2**	**48**		**Only observed in GaGeO material**
66	**CZP**	**0.198**	**18.75**	**24**		**Only observed in ZnPO material**

Table S6 | The G-NN energies, FD values and n_T of 233 zeolites from 252 zeolite bank. 225 of them are predicted to be possible for SiO_2 composition. Others (19=252-233) do not satisfy the Si:O ratio of 1:2. 60 kinds of pure silica zeolites have been synthesized in experiment as indicated by the reference.

	name	energy	FD	Tatoms	material	reference
	quartz	**0.000**	**22.85**	**12**		
1	VET	0.043	19.41	17	*VPI-8	J. Am. Chem. Soc., 118, 7299-7310 (1996)
2	PSI	0.045	19.83	72		
3	MRE	0.049	19.03	24	*ZSM-48	Zeolites, 5, 355-358 (1985)
4	MTF	0.050	19.67	22	*MCM-35	Chem. Mater., 11, 2919-2927 (1999)
5	GON	0.052	18.80	16	*GUS-1	Chem. Commun., , 2363-2364 (2000)
6	STO	0.054	18.10	112	*SSZ-31 polymorph	J. Phys. Chem. B, 107, 10983-10989 (2003)
7	AFO	0.054	18.84	20		
8	SAF	0.056	18.49	32		
9	AEL	0.059	18.72	20		
10	MSO	0.063	17.64	30		
11	PCR	0.067	18.48	30	*IPC-4	Nature Chemistry, , 628-633 (2013)
12	IHW	0.069	18.07	56	*ITQ-32	J. Am. Chem. Soc., 127, 11560-11561 (2005)
13	SFG	0.070	17.25	74		
14	SFV	0.070	16.97	784	*SSZ-57	Science, 333, 1134-1137 (2011)
15	MEL	0.070	16.99	48		
16	MFI	0.071	17.32	96	Silicalite	Nature, 271, 512-516 (1978)
17	DON	0.071	16.64	32	UTD-1	J. Am. Chem. Soc., 119, 8474-8484 (1997)
18	TER	0.072	16.83	40		
19	MTT	0.072	17.98	24		
20	TON	0.073	17.92	12	ZSM-22	Zeolites, 5, 349-351 (1985)
21	AFI	0.073	16.62	24	SSZ-24	Zeolites, 11, 438-442 (1991)
22	DDR	0.074	17.11	40	*Deca-dodecasil 3R	Z. Kristallogr., 175, 93-104 (1986)
23	TUN	0.074	17.03	96		
24	ATV	0.074	18.68	12		
25	IMF	0.074	17.08	144	*IM-5	Science, 315, 1113-1116 (2007)
26	SVV	0.075	17.24	28		
27	RUT	0.076	17.40	18	|TMA-|[Si-O]-RUT	J. Phys. Chem. Solids, 56, 1363-1368 (1995)
28	SGT	0.076	17.09	32	*Sigma-2	J. Appl. Crystallogr., 21, 305-310 (1988)
29	JBW	0.076	18.53	6		
30	ITR	0.076	16.82	56		
31	JRY	0.076	18.17	12		
32	ITH	0.076	16.89	28	*ITQ-13	Angew. Chem. Int. Ed., 42, 1156-1159 (2003)
33	SFS	0.076	16.19	56		
34	MEP	0.077	17.68	46	*Melanophlogite	Z. Kristallogr., 164, 247-257 (1983)
35	BOF	0.077	17.76	24		
36	SSF	0.078	16.21	54		

37	ATO	0.078	18.44	12		
38	MTW	0.079	17.59	14		
39	YFI	0.080	16.11	60		
40	BIK	0.080	18.45	6		
41	MFS	0.081	17.30	18		
42	HEU	0.081	17.21	18	K-Heulandite	Acta Cryst., B39, 189-197 (1983)
43	MOR	0.082	16.83	24	Mordenite, de-al	Chem. Lett., , 1547-1550 (1983)
44	FER	0.082	17.38	18	[Si-O]-FER	Zeolites, 7, 442-445 (1987)
45	RTE	0.082	16.78	12	*RUB-3	Microporous Mesoporous Mat., 26, 49-59 (1998)
46	UWY	0.082	15.93	60		
47	NSI	0.082	18.55	6	*Nu-6(2)	Angew. Chem. Int. Ed., 43, 4933-4937 (2004)
48	BOG	0.084	15.50	48		
49	STI	0.084	16.46	18		
50	CAS	0.084	18.56	12	EU-20b	Microporous Mesoporous Mat., 90, 87-101 (2006)
51	IFR	0.084	16.56	16	ITQ-4	J. Am. Chem. Soc., 123, 5453-5459 (2001)
52	LAU	0.085	17.63	12		
53	ETL	0.085	17.87	36	*H-EU-12	Angew. Chem. Int. Ed., 55, 7369-7373 (2016)
54	OSI	0.086	17.37	16		
55	BCT	0.086	18.74	4		
56	DAC	0.086	17.26	12		
57	BRE	0.087	17.82	16		
58	SEW	0.087	15.97	66		
59	RWR	0.088	18.92	16	*RUB-24	Microporous Mesoporous Mat., 83, 201-211 (2005)
60	PCS	0.088	17.63	64	*IPC-6	Nature Chem., 9, 1012-1018 (2017)
61	ESV	0.088	17.26	48		
62	IFO	0.088	16.66	32		
63	ITE	0.089	15.64	32	*ITQ-3	Angew. Chem. Int. Ed., 36, 2659-2661 (1997)
64	EEI	0.089	17.70	50	*ERS-18	Microporous Mesoporous Mat., 143, 6-13 (2011)
65	SZR	0.089	17.42	18		
66	RTH	0.089	15.67	16		
67	IWW	0.089	15.97	112		
68	MSE	0.089	15.87	112	YNU-2	Angew. Chem. Int. Ed., 47, 1042-1046 (2008)
69	IFW	0.090	15.53	32		
70	NON	0.090	17.43	22	*Nonasil	J. Incl. Phenom., 4, 339-349 (1986)
71	ATN	0.090	17.56	8		
72	ITG	0.090	15.94	56		
73	AET	0.090	17.39	36		
74	AWW	0.090	16.62	24		
75	EPI	0.091	17.42	12		
76	POS	0.092	15.08	64		
77	SFN	0.092	16.08	16		
78	JSW	0.092	17.91	48		
79	ITW	0.093	17.52	12	*ITQ-12	Chem. Commun., , 2114-2115 (2003)

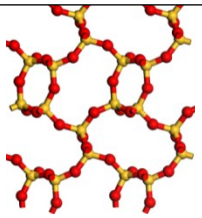
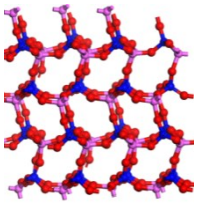
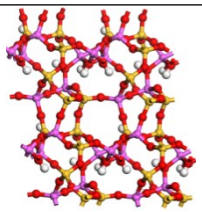
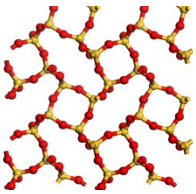
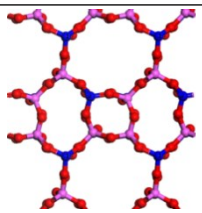
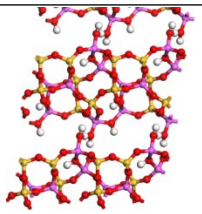
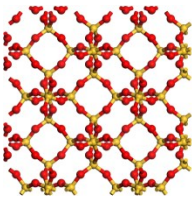
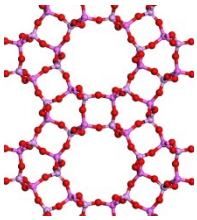
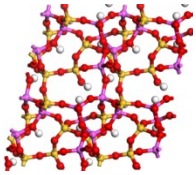
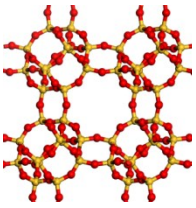
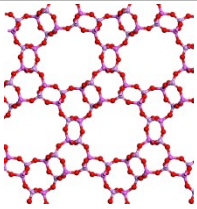
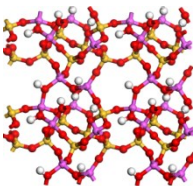
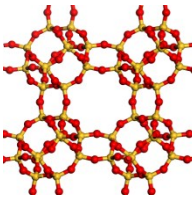
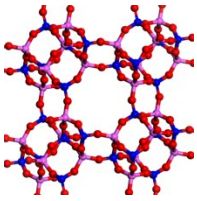
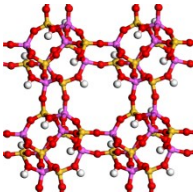
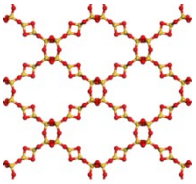
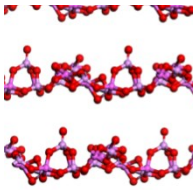
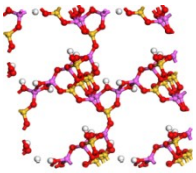
80	ATS	0.093	15.85	12	SSZ-55	J. Phys. Chem. B, 106, 264-270 (2002)
81	IWR	0.093	15.22	28		
82	SFE	0.093	16.67	14	*SSZ-48	J. Phys. Chem. B, 103, 8245-8250 (1999)
83	EUO	0.093	17.00	56	o-FDBDM-ZSM-50	Chem. Mater., 17, 4374-4385 (2005)
84	UOV	0.093	15.75	88	*IM-17	RSC Adv., 4, 19440-19449 (2014)
85	MWW	0.093	15.67	72	ITQ-1	Chem. Mater., 8, 2415-2417 (1996)
86	UTL	0.093	15.13	38		
87	BEA	0.094	14.96	64	pure silica beta	Chem. Commun., , 2365-2366 (1996)
88	ANA	0.094	18.92	24	|Cs-Fe|[Si-O]-ANA	Am. Mineral., 48, 100-109 (1963)
89	DOH	0.094	16.79	34	*Dodecasil 1H	Z. Kristallogr., 166, 11-22 (1984)
90	APD	0.094	17.73	16		
91	SFF	0.094	16.67	32	*SSZ-44	Angew. Chem. Int. Ed., 38, 1269-1272 (1999)
92	EON	0.094	16.68	60		
93	SFH	0.095	16.07	32		
94	SSY	0.095	16.62	28		
95	AWO	0.095	17.63	24		
96	AST	0.095	15.64	10	Octadecasil	Eur. J. Solid State Inorg. Chem., 28, 345-361 (1991)
97	PWW	0.095	16.80	20		
98	YUG	0.095	17.67	8		
99	PON	0.095	17.76	24		
100	SOV	0.096	14.89	64		
101	STF	0.096	16.40	16	*SSZ-35	Angew. Chem. Int. Ed., 38, 1269-1272 (1999)
102	UEI	0.096	17.68	12		
103	OWE	0.097	16.91	16		
104	STT	0.097	16.15	64	*SSZ-23	Angew. Chem. Int. Ed., 37, 2122-2126 (1998)
105	UOE	0.098	17.36	12		
106	LTN	0.098	16.40	192		
107	UOS	0.098	17.35	24		
108	BEC	0.098	14.77	32	ITQ-14 overgrowth	J. Am. Chem. Soc., 123, 5370-5371 (2001)
109	UOZ	0.098	18.82	40		
110	EAB	0.098	15.75	36		
111	CSV	0.099	15.69	20	*CIT-7	Chem. Sci., 6, 1728-1734 (2015)
112	ABW	0.099	17.37	4		
113	JSN	0.099	17.32	16		
114	FRA	0.099	16.74	60		
115	SOD	0.099	16.45	6	Silica sodalite	Nature, 317, 157-158 (1985)
116	ATT	0.100	16.90	12		
117	ZON	0.100	17.34	32		
118	CGF	0.100	18.43	18		
119	SOR	0.100	16.88	24		
120	OFF	0.100	15.83	18		
121	LEV	0.100	15.73	18	NU-3	Mater. Sci. Forum, 133-136, 423-433 (1993)
122	FAR	0.100	16.67	84		
123	KFI	0.101	14.74	48		

124	GIU	0.101	16.82	96		
125	MER	0.101	16.13	16		
126	SFO	0.101	14.87	16		
127	AVE	0.101	16.13	48		
128	SWY	0.101	15.82	72		
129	AEN	0.101	19.32	24		
130	IRN	0.101	15.09	46		
131	MRT	0.101	16.91	24		
132	MAR	0.101	16.60	72		
133	SAT	0.101	16.19	24		
134	LTF	0.101	16.71	108	*LZ-135	J. Phys. Chem. C, 113, 9838-9850 (2009)
135	CFI	0.102	16.33	16	*CIT-5	Chem. Commun., , 2179-2180 (1997)
136	ASV	0.102	19.45	20		
137	AFR	0.102	14.88	32		
138	LTL	0.102	16.48	36		
139	OKO	0.102	16.87	34	*COK-14	Nature Mater., 11, 1059-1064 (2012)
140	ERI	0.102	15.80	36		
141	MOZ	0.102	16.70	108		
142	PHI	0.103	16.13	16		
143	EZT	0.103	16.89	24		
144	SAS	0.103	15.17	16	SSZ-73	U.S. Patent 7,138,099, (2006)
145	AEI	0.103	14.81	24		
146	MAZ	0.103	16.53	36		
147	PWO	0.103	16.78	20		
148	TSC	0.103	12.97	96		
149	SIV	0.104	16.10	32		
150	GME	0.104	14.81	24		
151	EMT	0.104	13.03	96		
152	FAU	0.104	13.03	48		
153	GIS	0.104	16.14	8		
154	SAV	0.104	14.83	48		
155	PAU	0.104	15.71	336		
156	SFW	0.104	14.81	36		
157	MWF	0.104	15.84	720		
158	PWN	0.104	15.38	120		
159	AFX	0.104	14.81	48		
160	CTH	0.104	15.72	64		
161	AFT	0.105	14.82	72		
162	CHA	0.105	14.80	12	[Si-O]-CHA	Chem. Commun., , 1881-1882 (1998)
163	IWS	0.105	14.34	68		
164	AFG	0.105	16.60	48		
165	RHO	0.105	14.23	24		
166	TOL	0.105	16.62	72		
167	LIO	0.106	16.57	36		

168	MTN	0.107	16.98	34	CF-4	J. Incl. Phenom., 5, 355-362 (1987)
169	CAN	0.107	16.57	12		
170	EWS	0.107	16.63	48		
171	NPO	0.107	19.90	6		
172	DFO	0.108	14.57	132		
173	LOS	0.108	16.53	24		
174	ISV	0.108	14.63	64	*ITQ-7	Angew. Chem. Int. Ed., 38, 1997-2000 (1999)
175	SOF	0.109	16.12	20		
176	CGS	0.110	16.52	32		
177	LTJ	0.110	18.08	16		
178	MEI	0.110	14.21	34	ZSM-18	Zeolites, 14, 635-642 (1994)
179	SBE	0.110	13.48	64		
180	AFV	0.111	15.41	30		
181	SBS	0.111	13.45	96		
182	IWV	0.111	14.67	38		
183	SBT	0.112	13.45	48		
184	APC	0.112	17.28	16		
185	UFI	0.112	14.80	32		
186	USI	0.113	15.57	20		
187	RRO	0.114	17.19	18	RUB-41	Chem. Mater., 17, 43-49 (2005)
188	AVL	0.114	15.23	42		
189	ITT	0.115	12.44	46		
190	ACO	0.115	16.26	8		
191	AFS	0.116	14.31	56		
192	ETR	0.117	15.15	48		
193	BPH	0.117	14.34	28		
194	JNT	0.118	19.61	32		
195	MON	0.118	17.42	8		
196	DFT	0.119	17.38	8		
197	IFY	0.120	16.82	48	*ITQ-50	Angew. Chem. Int. Ed., 52, 10458-10462 (2013)
198	STW	0.120	15.87	60		
199	SAO	0.120	13.66	28		
200	LTA	0.121	13.96	24		
201	AFN	0.122	17.43	16		
202	POR	0.123	17.06	64		
203	VNI	0.128	17.23	60		
204	CDO	0.130	17.80	18	UZM-25	Stud. Surf. Sci. Catal., 170A, 338-346 (2007)
205	NES	0.131	16.26	34		
206	IRR	0.132	11.33	52		
207	GOO	0.136	17.92	16		
208	LOV	0.141	16.44	18		
209	RSN	0.143	16.44	18		
210	VSV	0.144	16.45	18		
211	EDI	0.151	16.04	5		

212	THO	0.151	16.01	10	
213	NAT	0.152	16.01	10	
214	AHT	0.153	18.00	12	
215	VFI	0.157	13.79	36	
216	PUN	0.159	14.50	36	
217	SBN	0.160	15.87	10	
218	NAB	0.167	15.76	5	
219	MVY	0.168	20.20	12	
220	WEI	0.169	15.58	10	
221	NPT	0.169	13.12	36	
222	AFY	0.174	13.63	16	
223	BOZ	0.177	12.47	46	
224	JOZ	0.178	15.90	20	
225	OBW	0.178	12.33	38	
	DL	**0.181**	**3.78**	**12**	
226	BSV	0.214	17.88	48	**Observed in GaGeO material**
227	JSR	0.217	11.76	96	**Observed in GaGeO material**
228	JST	0.229	13.70	48	**Observed in GaGeO material**
229	OSO	0.230	12.69	9	**Observed in BeSiO material**
230	CZP	0.239	19.65	24	**Observed in ZnPO material**
231	SOS	0.247	16.49	24	**Observed in BGeO material**
232	RWY	0.468	8.26	24	**Observed in GaGeO material**
233	CLO	1.236	11.11	196	**Observed in GaPO material**

Table S7 | The identified global minima structures and G-NN energies from E-SSW-NN simulation with different repulsive potential radius r_s.

r_s	SAPO compositions (energy eV/f.u.)		
	SiO_2	AlPO	$Si_{0.5}Al_{0.5}O_2H_{0.5}$
3			
	0.046	0.027	0.002
3.5			
	0.062	0.071 ATV	0.026
4			
	0.099 SOD	**0.062 ATO**	0.06
4.5			
	0.105 CHA	**0.071 ATS**	0.094
5~5.5			
	0.105 CHA	**0.103 CHA**	**0.147 CHA**
6			
	0.398	0.739	0.407

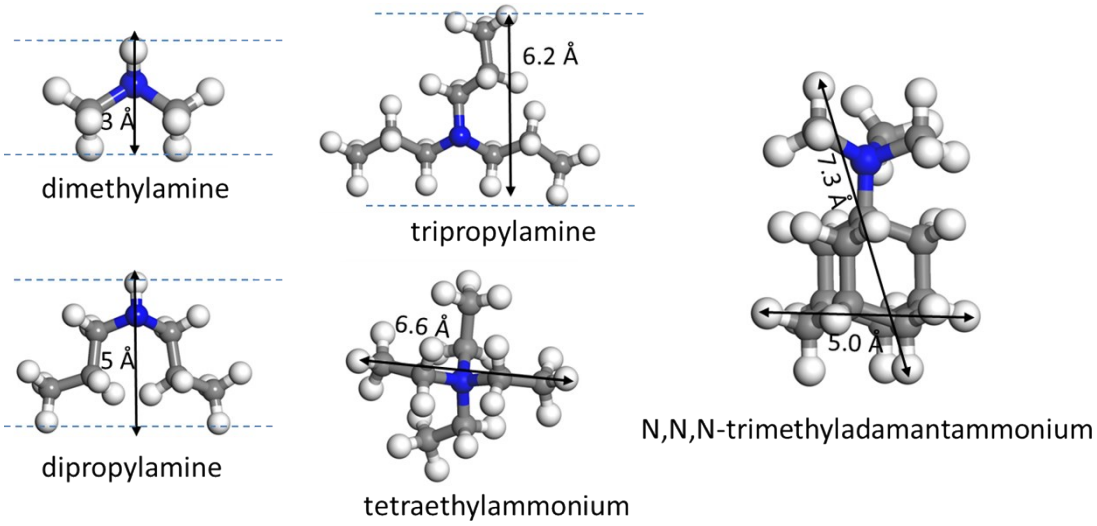


Figure S3 | The experimentally used SDAs for synthesizing *ATV*, *ATO, ATS* and *CHA* zeolites.

Experimentally, the SDAs for synthesizing *ATV*, *ATO, ATS* and *CHA* zeolites are dimethylamine, dipropylamine, tripropylamine and tetraethylammonium (or N,N,N-trimethyladamantammonium) whose molecular diameters are around 6, 8, 9.2 and 9.6 Å (plus 3 Å for distances between H in SDAs and O in zeolite skeleton), respectively.[3-6]

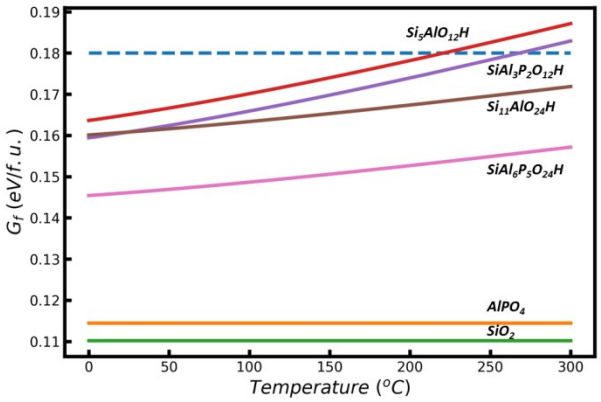


Figure S4. The Gibbs formation energy profiles at different hydrothermal temperature and water saturated vapor pressures for CHA-type zeolite with different compositions.

The temperature effect in the formation of CHA-type zeolite with different compositions is examined, as shown in Figure S4. The hydrothermal temperature does not affect the stabilities of AlPO and SiO_2 zeolites (both have no extra H in framework), but significantly affects the stabilities of SAPO and aluminosilicates zeolites. By comparing to the upper bounds of 0.18 eV/f.u., $Si_5AlO_{12}H$ and $SiAl_3P_2O_{12}H$ compositions can only be thermodynamically accessible at the temperature lower than 200 and 250 °C, respectively. Decreasing the hydrothermal temperature is conducive to the formation of zeolites, but too low temperature will slow crystallization rate. This may explain the common hydrothermal temperature region in experiment of 100 ~ 200 °C. Therefore, we choose 200 °C as the reference in manuscript.

Table S8 | The 23 kinds of as-synthesized SAPO zeolites from 252 zeolite bank (IZC-SC), showing the limited n_P:n_{Si} ratio (>2 in general).

	code	material	Material composition	n_P:n_{Si}	reference
1	AEI	SAPO-18	[Al-Si-P-O]-AEI		Catalysis Letters, 28, 241-248 (1994)
2	AEL	SAPO-11	$[Al_{17.6}Si_{5.6}P_{16.8}O_{80}]$-AEL	3.00	Pure Appl. Chem., 58, 1351-1358 (1986)
3	AEN	CFSAPO-1A	$\|(MA)_{12.28}\|[Al_{22.33}P_{22.10}Si_{3.57}O_{96}]$-AEN	6.19	J. Incl. Phenom., 5, 591-599 (1987)
4	AET	MCM-37	[Al-Si-P-O]-AET		U.S. Patent 5091073,(1992)
5	AFI	SAPO-5	$[Al_{10.8}Si_{3.36}P_{9.84}O_{48}]$-AFI	2.93	Pure Appl. Chem., 58, 1351-1358 (1986)
6	AFO	SAPO-41	$[Si_{0.8}Al_{20.4}P_{18.8}O_{80}]$-AFO	17.50	J. Chem. Soc., Faraday Trans., 94, 723-727 (1998)
7	AFR	*SAPO-40	$[Si_4Al_{14}P_{14}O_{64}]_2$-AFR		J. Appl. Crystallogr., 25, 539-543 (1992)
8	AFV	SAPO-57	[Al-Si-P-O]-AFV		Microporous Mesoporous Mat., 189, 49-63 (2014)
9	AFX	*SAPO-56	$[Al_{23}Si_5P_{20}O_{96}]$-AFX	4.00	private communication, , (1994)
10	ANA	[Al-Si-P-O]	$[Al_{24}Si_{13}P_{11}O_{96}]$-ANA	0.85	Acta Crystallogr., C40, 214-217 (1984)
11	ATN	SAPO-39	$[Si_{1.12}Al_{7.84}P_{7.2}O_{32}]$-ATN	6.43	Zeolites, 18, 350-355 (1997)
12	ATO	SAPO-31	$[Al_{18}Si_2P_{16}O_{72}]$-ATO	8.00	Acta Crystallogr., B50, 290-294 (1994)
13	AVL	SAPO-59	$[Al_{21}P_{14.49}Si_{5.88}O_{84}]$-AVL	2.46	Microporous Mesoporous Mat., 189, 49-63 (2014)
14	CHA	ZYT-6	$[Al_{20}Si_5P_{15}O_{80}]$-CHA	3.00	Acta Crystallogr., C41, 1698-1700 (1985)
15	CHA	SAPO-47	$[Al_{18}Si_{4.2}P_{13.8}O_{72}]$-CHA	3.29	J. Phys. Chem., 93, 6516-6520 (1989)
16	FAU	SAPO-37	[Al-Si-P-O]-FAU		J. Am. Chem. Soc., 106, 6092-6093 (1984)
17	GIS	SAPO-43	[Al-Si-P-O]-GIS		Acta Crystallogr., B49, 413-420 (1993)
18	IFO	*ITQ-51	$[Si_{2.6}Al_{14.7}P_{14.7}O_{64}]$-IFO	5.65	Proc. Natl. Acad. Sci., 110, 3749-3754 (2013)
19	LEV	SAPO-67	$[Al_{27}P_{21.87}Si_{5.94}O_{108}]$-LEV	3.68	Microporous Mesoporous Mat., 189, 49-63 (2014)
20	LTA	SAPO-42	[Al-Si-P-O]-LTA		J. Am. Chem. Soc., 106, 6092-6093 (1984)
21	MEI	ECR-40	$[Al_{15.95}Si_{5.85}P_{12.21}O_{68}]$-MEI	2.09	Stud. Surf. Sci. Catal., 154, 1274-1281 (2004)
22	SWY	*STA-20	$[Al_{36}P_{30.4}Si_{5.6}O_{144}]$-SWY	5.43	Chem. Mater., 29, 2180-2190 (2017)
23	VFI	MCM-9	[Al-Si-P-O]-VFI		Appl. Catal., 51, L13-L20 (1989)

*$[Al_{24}Si_{13}P_{11}O_{96}]$-ANA material with the low Si:P = 0.85 is synthesized under alkaline condition, while other materials are synthesized under neutral or acidic condition.

Table S9 | The formation free energy (G_f) and proportions of TO_4 (monomer, P_T) and their linkages (T-O-T', $P_{TT'}$) for each CHA-type SAPO compositions.

name	G_f	P_{Si}	P_{Al}	P_P	P_{SiAl}	P_{SiSi}	P_{SiP}	P_{AlAl}	P_{AlP}
Si0Al6P6H0	0.114	0.000	0.500	0.500	0.000	0.000	0.000	0.000	1.000
Si10Al1P1H0	0.200	0.833	0.083	0.083	0.125	0.708	0.125	0.000	0.042
Si10Al2P0H2	0.182	0.833	0.167	0.000	0.333	0.667	0.000	0.000	0.000
Si11Al1P0H1	0.169	0.917	0.083	0.000	0.167	0.833	0.000	0.000	0.000
Si12Al0P0H0	0.110	1.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000
Si1Al6P5H1	0.155	0.083	0.500	0.417	0.167	0.000	0.000	0.000	0.833
Si2Al5P5H0	0.203	0.167	0.417	0.417	0.125	0.042	0.125	0.000	0.708
Si2Al6P4H2	0.178	0.167	0.500	0.333	0.333	0.000	0.000	0.000	0.667
Si3Al5P4H1	0.203	0.250	0.417	0.333	0.250	0.083	0.083	0.000	0.583
Si3Al6P3H3	0.216	0.250	0.500	0.250	0.500	0.000	0.000	0.000	0.500
Si4Al4P4H0	0.207	0.333	0.333	0.333	0.167	0.167	0.167	0.000	0.500
Si4Al5P3H2	0.231	0.333	0.417	0.250	0.375	0.125	0.042	0.000	0.458
Si4Al6P2H4	0.240	0.333	0.500	0.167	0.667	0.000	0.000	0.000	0.333
Si5Al4P3H1	0.226	0.417	0.333	0.250	0.292	0.208	0.125	0.000	0.375
Si5Al5P2H3	0.232	0.417	0.417	0.167	0.500	0.167	0.000	0.000	0.333
Si5Al6P1H5	0.276	0.417	0.500	0.083	0.583	0.125	0.000	0.125	0.167
Si6Al3P3H0	0.247	0.500	0.250	0.250	0.208	0.292	0.208	0.000	0.292
Si6Al4P2H2	0.231	0.500	0.333	0.167	0.417	0.250	0.083	0.000	0.250
Si6Al5P1H4	0.231	0.500	0.417	0.083	0.500	0.250	0.000	0.083	0.167
Si6Al6P0H6	0.304	0.500	0.500	0.000	0.750	0.125	0.000	0.125	0.000
Si7Al3P2H1	0.231	0.583	0.250	0.167	0.292	0.375	0.125	0.000	0.208
Si7Al4P1H3	0.286	0.583	0.333	0.083	0.542	0.250	0.125	0.042	0.042
Si7Al5P0H5	0.256	0.583	0.417	0.000	0.500	0.333	0.000	0.167	0.000
Si8Al2P2H0	0.206	0.667	0.167	0.167	0.167	0.500	0.167	0.000	0.167
Si8Al3P1H2	0.269	0.667	0.250	0.083	0.458	0.375	0.125	0.000	0.042
Si8Al4P0H4	0.233	0.667	0.333	0.000	0.500	0.417	0.000	0.083	0.000
Si9Al2P1H1	0.205	0.750	0.167	0.083	0.250	0.583	0.083	0.000	0.083
Si9Al3P0H3	0.212	0.750	0.250	0.000	0.333	0.583	0.000	0.083	0.000

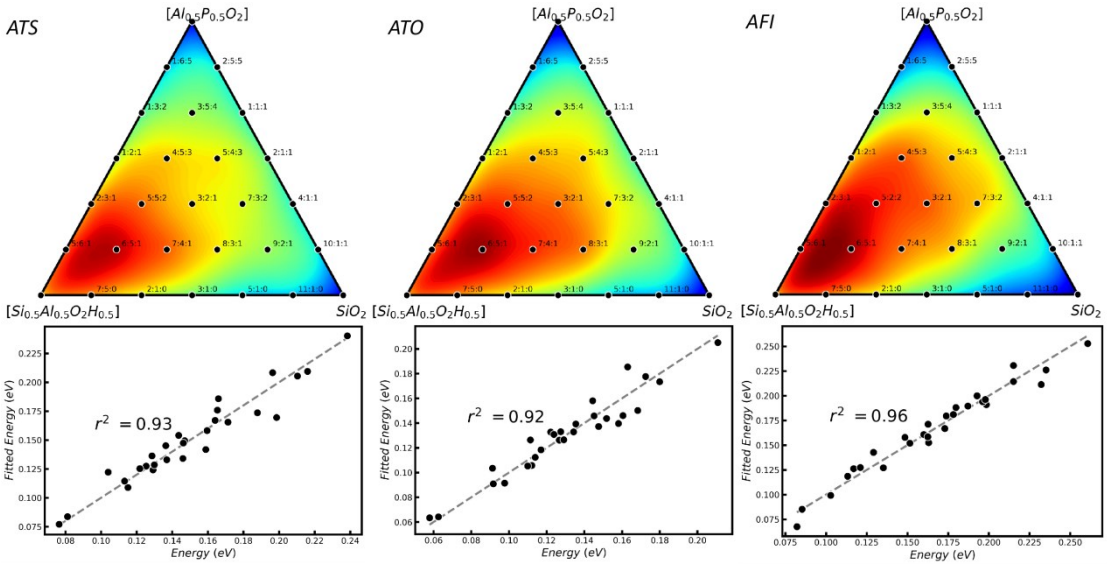


Figure S5 | Thermodynamics for *ATS*-, *ATO*- and *AFI*-type zeolites with different Si:Al:P compositions. The formation energy thermodynamic ternary phase diagram of different SAPO compositions with the energies of pure SiO_2, AlPO and Si:Al = 1:1 compositions as the energy references. The relationship between the calculated $G_{f,DFT}$ and the fitted $G_{f,fit}$ obtained from the following equations.

$$G_f = (0.15 * P_{Si} + 0.14 * P_{Al} + 0.13 * P_P) + (0.31 * P_{SiP} + 0.10 * P_{AlAl} + 0.13 * P_{SiAl} - 0.07 * P_{SiSi} - 0.05 * P_{AlP}) \quad \textbf{ATS}$$

$$G_f = (0.13 * P_{Si} + 0.12 * P_{Al} + 0.11 * P_P) + (0.28 * P_{SiP} + 0.09 * P_{AlAl} + 0.11 * P_{SiAl} - 0.06 * P_{SiSi} - 0.05 * P_{AlP}) \quad \textbf{ATO}$$

$$G_f = (0.14 * P_{Si} + 0.16 * P_{Al} + 0.12 * P_P) + (0.28 * P_{SiP} + 0.12 * P_{AlAl} + 0.14 * P_{SiAl} - 0.07 * P_{SiSi} - 0.05 * P_{AlP}) \quad \textbf{AFI}$$

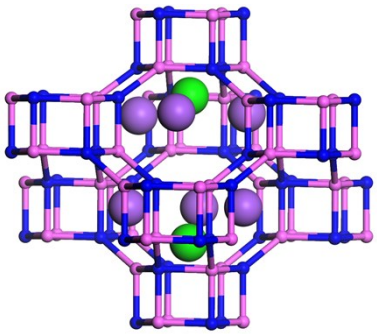


Figure S6. The possible Na ion positions in *cha* cage of CHA-type zeolite.

For the position of the Na, it locates at extra framework sites in the *cha* cage of CHA-type zeolite. The possible positions for Na ions are shown in Figure S6 above, i.e. at the centers of 6- and 8-membered ring. The most stable structure for Na-containing CHA is determined by Metropolis Monte Carlo sampling in the fixed *CHA*-type framework where all the likely positions of Na atoms are utilized as the pool of sites for random selection. From Metropolis Monte Carlo sampling, we found that Na ion prefers to first occupy the top and lower sites of 6-membered ring, as labeled by green balls in Figure S6, and then occupy the center of 8-membered ring, as labeled by purple ball in Figure S6.

Table S10 | The 93 kinds of as-synthesized aluminosilicates zeolites from 252 zeolite bank (IZC-SC).

	Name	Material	Material composition	Reference
1	ABW	*Li-A	$\|Li_4(H_2O)_4\|[Al_4Si_4O_{16}]$-ABW	Z. Kristallogr., 139, 186-195 (1974)
2	AEI	SSZ-39, calcined	$[Al_{0.8}Si_{47.2}O_{96}]$-AEI	J. Am. Chem. Soc., 122, 263-273 (2000)
3	AFG	*Afghanite	$\|Ca_{9.8}Na_{22}Cl_2(SO_4)_{5.3}CO_3(H_2O)_4\|[Al_{24}Si_{24}O_{96}]$-AFG	Dokl. Akad. Nauk SSSR, 320, 882-886 (1991)
4	AFX	SSZ-16	$[Si_{41.1}Al_{6.9}O_{96}]$-AFX	Chem. Mater., 8, 2409-2411 (1996)
5	ANA	*Analcime	$\|Na_{16}(H_2O)_{16}\|[Al_{16}Si_{32}O_{96}]$-ANA	Z. Kristallogr., 135, 240-252 (1972)
6	ATT	synthetic Rb-RMA-3	$\|Rb\text{-}H_2O\|[Al_{5.2}Si_{18.8}O_{48}]$-ATT	Micropor. Mesopor. Mater., 114, 495-506 (2008)
7	BCT	|Ca-|[Al-Si-O]-BCT	$[Al_4Si_4O_{16}]$-BCT	Z. Kristallogr., 137, 380-398 (1973)
8	BEA	*Beta	$\|Na_7\|[Al_7Si_{57}O_{128}]$-*BEA	Proc. R. Soc. Lond. A, 420, 375-405 (1988)
9	BIK	*Bikitaite	$\|Li_4(H_2O)_4\|_{1/2}[Al_4Si_8O_{24}]_{1/2}$-BIK	Zeolites, 9, 303-311 (1989)
10	BOG	*Boggsite	$\|Ca_7Na_4(H_2O)_{74}\|[Al_{18}Si_{78}O_{192}]$-BOG	Am. Mineral., 75, 501-507 (1990)
11	BPH	Linde Q	$[Al_{16}Si_{16}O_{56}]$-BPH	Zeolites, 11, 124-131 (1991)
12	BRE	*Brewsterite	$\|Ba_{0.5}Sr_{1.5}(H_2O)_{10}\|[Al_4Si_{12}O_{32}]$-BRE	Acta Crystallogr., B33, 2907-2910 (1977)
13	CAN	*Cancrinite	$\|Na_6CaCO_3(H_2O)_2\|[Al_6Si_6O_{24}]$-CAN	Z. Kristallogr., 122, 407-422 (1965)
14	CAS	*Cesium Aluminosilicate	$\|Cs_4\|[Al_4Si_{20}O_{48}]$-CAS	Z. Kristallogr., 152, 207-213 (1980)
15	CHA	*Chabazite	$\|Ca_6(H_2O)_{40}\|_{1/3}[Al_{12}Si_{24}O_{72}]_{1/3}$-CHA	Acta Crystallogr., 16, 45-53 (1963)
16	CON	SSZ-26	[Al-Si-O]-CON	Science, 262, 1543-1546 (1993)
17	DAC	*Dachiardite	$\|(Ca_{0.5},K,Na)_5(H_2O)_{12}\|[Al_5Si_{19}O_{48}]$-DAC	Z. Kristallogr., 166, 63-71 (1984)
18	DDR	Sigma-1	[Al-Si-O]-DDR	Stud. Surf. Sci. Catal., 37, 57-64 (1988)
19	EAB	*TMA-E	$\|(TMA+)_2Na_7(H_2O)_{26}\|[Al_9Si_{27}O_{72}]$-EAB	J. Solid State Chem., 37, 204-218 (1981)
20	EDI	*Edingtonite	$\|Ba(H_2O)_4\|_2[Al_2Si_3O_{10}]_2$-EDI	Acta Crystallogr., B32, 1623-1627 (1976)
21	EMT	*EMC-2	$\|Na_{21}(18\text{-crown-}6)_4\|[Al_{21}Si_{75}O_{192}]$-EMT	Microporous Materials, 2, 269-280 (1994)
22	EON	*ECR-1	$\|Na_{10.97}Ca_{0.38}(H_2O)_{35.0}\|[Al_xSi_{60\text{-}x}O_{120}]$-EON(x=3.6-11.4)	Chem. Mater., 18, 76-84 (2006)
23	EPI	*Epistilbite	$\|Ca_3(H_2O)_{16}\|[Al_6Si_{18}O_{48}]$-EPI	Mineral. Mag., 36, 480-490 (1967)
24	ERI	*Erionite	$\|(Ca,Na_2)_{3.5}K_2(H_2O)_{27}\|[Al_9Si_{27}O_{72}]$-ERI	Proc. 3rd Int. Conf. Molecular Sieves, , pp. 94-99 (1973)
25	ESV	*ERS-7	$\|H_{5.06}Na_{0.07}\|[Al_{5.13}Si_{42.87}O_{96}]$-ESV	Proc. 12th Int. Zeolite Conf., I, pp. 541-548 (1999)

26	ETV	*EMM-37	|BDMP|$[Si_{12}Al_2O_{28}]$-ETV	Inorg. Chem, 58, 12854-12858 (2019)
27	EUO	*EU-1	|$Na_{3.6}(H_2O)_{26}$|$[Al_{3.6}Si_{108.4}O_{224}]$-EUO	Zeolites, 8, 74-76 (1988)
28	FAR	*Farneseite	|$(Na,K)_{46}Ca_{10}(SO_4)_{12}(H_2O)_6$|$[Al_{42}Si_{42}O_{168}]$-FAR	Eur. J. Mineral., 17, 839-846 (2005)
29	FAU	*Faujasite	|$(Ca,Mg,Na_2)_{29}(H_2O)_{240}$|$[Al_{58}Si_{134}O_{384}]$-FAU	Am. Mineral., 49, 697-704 (1964)
30	FER	*Ferrierite	|$Mg_2Na_2(H_2O)_{18}$|$[Al_6Si_{30}O_{72}]$-FER	Acta Crystallogr., 21, 983-990 (1966)
31	FRA	*Franzinite	|$(Na,K)_{30}Ca_{10}(SO_4)_{10}(H_2O)_2$|$[Al_{30}Si_{30}O_{120}]$-FRA	Can. Mineral., 38, 657-668 (2000)
32	GIS	*Gismondine	|$Ca_4(H_2O)_{16}$|$[Al_8Si_8O_{32}]$-GIS	Adv. Chem. Ser. , 101, 250-258 (1971)
33	GIU	*Giuseppettite	|$Na_{42}K_{16}Ca_6(SO_4)_{10}Cl_2(H_2O)_5$|$[Si_{48}Al_{48}O_{192}]$-GIU	Microporous Mesoporous Mat., 73, 129-136 (2004)
34	GME	natural gmelinite	|$Na_{6.92}Ca_{0.45}H_2O_x$|$[Al_{7.6}Si_{16.4}O_{48}]$-GME	J. Phys. Chem. B, 104, 4074-4079 (2000)
35	GOO	*Goosecreekite	|$Ca_4(H_2O)_{20}$|$_{1/2}[Al_8Si_{24}O_{64}]_{1/2}$-GOO	Am. Mineral., 71, 1494-1501 (1986)
36	HEU	*Heulandite	|$Ca_4(H_2O)_{24}$|$[Al_8Si_{28}O_{72}]$-HEU	Tschermaks Min. Petr. Mitt., 18, 129-146 (1972)
37	IFR	MCM-58	[Al-Si-O]-IFR	WOP 9511196,(1995)
38	ITE	Mu-14	$[Al_xSi_{64-x}O_{128}]$-ITE (x=2-3.4)	Microporous Mesoporous Mat., 38, 177-185 (2000)
39	IWV	*ITQ-27	$[Al_5Si_{147}O_{304}]$-IWV	J. Am. Chem. Soc., 128, 8862-8867 (2006)
40	JBW	*Na-J	|$Na_3(H_2O)_{1.5}$|$_4[Al_3Si_3O_{12}]_4$-JBW	Zeolites, 2, 162-166 (1982)
41	KFI	*ZK-5	|$Na_{30}(H_2O)_{98}$|$[Al_{30}Si_{66}O_{192}]$-KFI	Z. Kristallogr., 121, 211-219 (1965)
42	LAU	*Laumontite	|$Ca_4(H_2O)_{16}$|$[Al_8Si_{16}O_{48}]$-LAU	Adv. Chem. Ser. , 101, 259-265 (1971)
43	LEV	*Levyne	|$Ca_9(H_2O)_{50}$|$[Al_{18}Si_{36}O_{108}]$-LEV	Tschermaks Min. Petr. Mitt., 22, 117-129 (1975)
44	LIO	*Liottite	|$Ca_8(K,Na)_{16}(SO_4)_5Cl_4$|$[Al_{18}Si_{18}O_{72}]$-LIO	Can. Mineral., 34, 1021-1030 (1996)
45	LIT	*Lithosite	|K_{12}|$_2[Al_{16}Si_{32}O_{88}OH_{16}]_2$--LIT	Sov. Phys. Dokl., 31, 941-942 (1986)
46	LOS	*Losod	|$Na_{12}(H_2O)_{18}$|$[Al_{12}Si_{12}O_{48}]$-LOS	Ph.D. Thesis, ETH, Zurich, Switzerland, , (1988)
47	LTA	*Linde Type A	|$Na_{12}(H_2O)_{278}$|$_8[Al_{12}Si_{12}O_{48}]_8$-LTA	Z. Kristallogr., 133, 134-149 (1971)

48	LTJ	*Linde Type J	$\|X_8(H_2O)_4\|[Si_8Al_8O_{32}]$-LTJ	Microporous Mesoporous Mat., 143, 398-400 (2011)
49	LTL	*Linde Type L	$\|K_6Na_3(H_2O)_{21}\|[Al_9Si_{27}O_{72}]$-LTL	Z. Kristallogr., 128, 352-370 (1969)
50	LTN	*Linde Type N	$\|Na_{384}(H_2O)_{518}\|[Al_{384}Si_{384}O_{1536}]$-LTN	Z. Kristallogr., 160, 313-316 (1982)
51	MAR	*Marinellite	$\|Na_{31}K_{11}Ca_6(SO_4)_8Cl_2(H_2O)_{3.4}\|[Al_{36}Si_{36}O_{144}]$-MAR	Eur. J. Mineral., 15, 1019-1027 (2003)
52	MAZ	*Mazzite	$\|(Na_2,K_2,Ca,Mg)_5(H_2O)_{28}\|[Al_{10}Si_{26}O_{72}]$-MAZ	Rend. Soc. Ital. Mineral. Petrol., 31, 599-612 (1975)
53	MEI	*ZSM-18	$\|Na_x(H_2O)_{28}\|[Al_xSi_{34-x}O_{68}]$-MEI (x=2.1-5.7)	Science, 247, 1319-1321 (1990)
54	MER	RMA-2	$\|Rb\text{-}H_2O_x\|[Al_{6.6}Si_{25.4}O_{64}]$-MER	Microporous Mesoporous Mat., 114, 495-506 (2008)
55	MFI	*ZSM-5	$\|Na_x(H_2O)_{16}\|[Al_xSi_{96-x}O_{192}]$-MFI (x<27)	J. Phys. Chem., 85, 2238-2243 (1981)
56	MFS	*ZSM-57	$\|H_{1.5}\|[Al_{1.5}Si_{34.5}O_{72}]$-MFS	Zeolites, 10, 293-296 (1990)
57	MON	*Montesommaite	$\|(K,Na)_{4.5}(H_2O)_5\|[Al_{4.5}Si_{11.5}O_{32}]$-MON	Am. Mineral., 75, 1415-1420 (1990)
58	MOZ	*ZSM-10	$\|K_{24}\|[Al_{24}Si_{84}O_{216}]$-MOZ	Z. Kristallogr., 221, 260-265 (2006)
59	MRT	*ZSM-43	$\|Cs_{2.4}K_{0.35}(H_2O)_{10.6}\|_4[Al_{3.8}Si_{20.2}O_{48}]_4$-MRT	Inorg. Chem, 56, 8856-8864 (2017)
60	MSE	*MCM-68	$[Al_{11.4}Si_{100.6}O_{224}]$-MSE	J. Phys. Chem. B, 110, 2045-2050 (2006)
61	MSO	*MCM-61	$\|K_{6.3}(_{18}\text{-crown-}_6)_3\|_{1/3}[Al_{6.3}Si_{83.7}O_{180}]_{1/3}$-MSO	Microporous Mesoporous Mat., 31, 61-73 (1999)
62	MTT	*ZSM-23	$\|Nax(H_2O)_4\|[AlxSi_{24}\text{-}xO_{48}]$-MTT(x<2)	private communication, , (0)
63	MTW	*ZSM-12	$\|Nax(H_2O)_4\|_2[AlxSi_{28}\text{-}xO_{56}]_2$-MTW(x<2.5)	J. Phys. Chem., 94, 3718-3721 (1990)
64	MWF	*ZSM-25	$\|(TEA+)_{38}(H_2O)_{812}\|[Al_{334}Si_{1106}O_{2880}]$-MWF	Nature, 524, 74-78 (2015)
65	MWW	SSZ-25	[Al-Si-O]-MWW	Chemistry - A European Journal, 7, 1990-2001 (2001)
66	NAT	*Natrolite	$\|Na_8(H_2O)_8\|_2[Al_8Si_{12}O_{40}]_2$-NAT	Z. Kristallogr., 113, 430-444 (1960)
67	NES	*NU-87	$\|H_8(H_2O)x\|_{1/2}[Al_8Si_{128}O_{272}]_{1/2}$-NES	Nature, 353, 417-420 (1991)
68	NON	CF-3	[Al-Si-O]-NON	J. Incl. Phenom., 4, 121-127 (1986)
69	OFF	*Offretite	$\|(Ca,Mg)_{1.5}K(H_2O)_{14}\|[Al_4Si_{14}O_{36}]$-OFF	Acta Crystallogr., B28, 825-834 (1972)

70	PAR	*Partheite	$\|Ca_8(H_2O)_{16}\|[Al_{16}Si_{16}O_{60}(OH)_8]$--PAR	Z. Kristallogr., 169, 165-175 (1984)
71	PAU	*Paulingite	$\|(Ca,K_2,Na_2)_{76}(H_2O)_{700}\|[Al_{152}Si_{520}O_{1344}]$-PAU	Science, 154, 1004-1007 (1966)
72	PHI	*Phillipsite	$\|K_4(Ca,Na_2)_4(H_2O)_{24}\|_{1/2}[Al_{12}Si_{20}O_{64}]_{1/2}$-PHI	Acta Crystallogr., B30, 2426-2433 (1974)
73	PTY	*PST-30, calcined	$\|H_{0.8}(H_2O)_{4.2}\|[Al_{0.8}Si_{9.2}O_{20}]$-PTY	Angew. Chem. Int. Ed., 58, 13845-13848 (2019)
74	PWN	*PST-29	$\|(Me_2\text{-}DABCO^{+}{}_2)_{11}Na_{32}(H_2O)_{120}\|[Al_{54}Si_{186}O_{480}]$-PWN	Chem. Mater., 30, 6619-6623 (2018)
75	PWO	*PST-21	$\|H_{1.8}(H_2O)_{6.9}\|[Al_{1.8}Si_{18.2}O_{40}]$-PWO	Angew. Chem. Int. Ed., 57, 2199-2203 (2018)
76	PWW	*PST-22	$\|H_{3.3}(H_2O)_{13.8}\|[Al_{3.3}Si_{36.7}O_{80}]$-PWW	Angew. Chem. Int. Ed., 57, 2199-2203 (2018)
77	RHO	*Rho	$\|(Na,Cs)_{12}(H_2O)_{44}\|[Al_{12}Si_{36}O_{96}]$-RHO	Proc. 6th Int. Zeolite Conf., , pp. 812-822 (1984)
78	RTH	SSZ-50 ([Al-Si-O]-RTH)	[Al-Si-O]-RTH	J. Solid State Chem., 167, 289-298 (2002)
79	RUT	Al-Nu-1	[Al-Si-O]-RUT	Zeolites, 10, 642-649 (1990)
80	SFW	*SSZ-52	$\|(DEDMAB^{+})_6Na_6(H_2O)_{18}\|[Al_{12}Si_{96}O_{216}]$-SFW	J. Am. Chem. Soc., 135, 10519-10524 (2013)
81	SOD	*Sodalite	$\|Na_8Cl_2\|[Al_6Si_6O_{24}]$-SOD	Acta Crystallogr., 23, 434-436 (1967)
82	STI	*Stilbite	$\|Na_4Ca_8(H_2O)_{56}\|_{1/2}[Al_{20}Si_{52}O_{144}]_{1/2}$-STI	Acta Crystallogr., B27, 833-841 (1971)
83	SZR	*SUZ-4	$\|K_4\|[Al_4Si_{32}O_{72}]$-SZR	Z. Kristallogr., 221, 689-698 (2006)
84	TER	*Terranovaite	$\|Na_{4.2}K_{0.2}Mg_{0.2}Ca_{3.7}(H_2O)_{29}\|[Al_{12.3}Si_{67.7}O_{160}]$-TER	Am. Mineral., 82, 423-429 (1997)
85	THO	*Thomsonite	$\|NaCa_2(H_2O)_6\|_4[Al_5Si_5O_{20}]_4$-THO	Zeolites, 5, 74-80 (1985)
86	TOL	*Tounkite-like mineral	$\|Na_{31.1}Ca_{15.94}K_{0.96}Cl_8(SO_4)_{9.3}(SO_3)_{0.7}\|[Al_{36}Si_{36}O_{144}]$-TOL	Crystallogr. Reports, 4, 635-642 (2004)
87	TON	*Theta-1	$\|Na_n(H_2O)_4\|$[AlxSi$_{24}$-xO$_{48}$]-TON (x<2)	Nature, 312, 533-534 (1984)
88	TSC	*Tschörtnerite	$\|Ca_{64}(K_2,Ca,Sr,Ba)_{48}Cu_{48}(OH)_{128}(H_2O)x\|[Al_{192}Si_{192}O_{768}]$-TSC	Am. Mineral., 83, 607-617 (1998)
89	TUN	*TNU-9	$\|H_{9.3}\|[Al_{9.3}Si_{182.7}O_{384}]$-TUN	Nature, 444, 79-81 (2006)
90	UFI	*UZM-5	$\|K_8\|[Al_8Si_{56}O_{128}]$-UFI	Angew. Chem. Int. Ed., 42, 1737-1740 (2003)
91	WEN	*Wenkite	$\|Ba_4(Ca,Na_2)_3(SO_4)_3H_2O\|[Al_8Si_{12}O_{39}(OH)_2]$--WEN	Acta Crystallogr., B30, 1262-1266 (1974)

92	YFI	*YNU-5	$\|K_{6.3}(H_2O)_{0.72}\|[Al_{12}Si_{108}O_{240}]$-YFI	J. Am. Chem. Soc., 139, 7989-7997 (2017)
93	YUG	*Yugawaralite	$\|Ca_2(H_2O)_8\|[Al_4Si_{12}O_{32}]$-YUG	Acta Crystallogr., B25, 1183-1190 (1969)

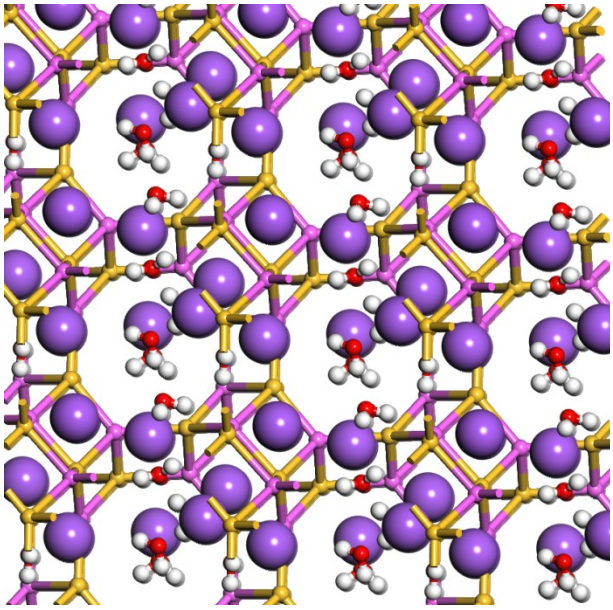


Figure S7 | The structure of $Si_6Al_6O_{24}Na_6(H_2O)_6$ in CHA-type structural skeleton. The formation Gibbs free energy of this structure with respect to the energies of quartz-SiO_2, α-Al_2O_3, H_2O and NaOH(aq) compositions at common hydrothermal conditions of 200 ^oC and 15.53 bar is -0.17 eV/f.u. The structure is the most stable configuration via DFT calculation from a number of manually configured structures for Na/H_2O in CHA. The purple ball represents the Na atom. Structural coordinates can be found in Supplementary Structural Coordinates.

Supplementary References

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Supplementary Structural Coordinates (.arc format)

GM in Table S6 at r_s = 3 for AlPO

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P          0.293214635     5.995489220     1.109812075 CORE     2 P    P      0.0000      2
P          6.043988105     3.079282793     2.545793440 CORE     3 P    P      0.0000      3
P          1.514198469     1.644760766     3.516968462 CORE     4 P    P      0.0000      4
P          3.480184831     6.630377058     5.073441007 CORE     5 P    P      0.0000      5
P         -1.133013028     5.118118672     5.926495812 CORE     6 P    P      0.0000      6
Al         7.036543854     5.224089009     0.555352883 CORE     7 Al Al     0.0000      7
Al         3.724678761     1.211205657     1.301664519 CORE     8 Al Al     0.0000      8
Al         4.410150511     8.708562150     2.941233518 CORE     9 Al Al     0.0000      9
Al         1.133367386     4.745759555     3.813030781 CORE    10 Al Al     0.0000     10
Al         5.608958855     4.348835218     5.347127182 CORE    11 Al Al     0.0000     11
Al        -1.405792688     8.244479731     6.224728434 CORE    12 Al Al     0.0000     12
O          6.173632596     6.692455076     0.122742579 CORE    13 O    O      0.0000     13
O         -1.187217809     5.645826507     0.990967852 CORE    14 O    O      0.0000     14
O          0.441579355     7.430296326     1.645434767 CORE    15 O    O      0.0000     15
O          4.994806195     2.320419715     1.734543361 CORE    16 O    O      0.0000     16
O          4.333364931     7.570760369     1.601472374 CORE    17 O    O      0.0000     17
O          6.245618223     4.474793256     1.936862820 CORE    18 O    O      0.0000     18
O          0.986450212     5.030180229     2.083346893 CORE    19 O    O      0.0000     19
O          2.234982995     1.559817260     2.166644167 CORE    20 O    O      0.0000     20
O          7.383690216     2.326473986     2.518095353 CORE    21 O    O      0.0000     21
O         -3.785007080     9.104378330     3.321752811 CORE    22 O    O      0.0000     22
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O          1.608120231     3.074986882     4.075108498 CORE    24 O    O      0.0000     24
O          3.620053818     7.964899951     4.325922258 CORE    25 O    O      0.0000     25
O         -0.429681177     5.042014562     4.564628301 CORE    26 O    O      0.0000     26
O         -1.645534930     8.535190542     4.507005131 CORE    27 O    O      0.0000     27
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O          4.795261871     5.846509052     4.932550823 CORE    29 O    O      0.0000     29
O         -2.590199159     4.701470631     5.754345817 CORE    30 O    O      0.0000     30
O         -1.059463512     6.546760952     6.485871357 CORE    31 O    O      0.0000     31
O          3.187286046     6.907029576     6.551191998 CORE    32 O    O      0.0000     32
O          4.785200632     3.604189165     6.711086953 CORE    33 O    O      0.0000     33
O         -0.435729632     4.166253040     6.909425861 CORE    34 O    O      0.0000     34
O         -0.056627576     9.157829617     6.838316363 CORE    35 O    O      0.0000     35
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GM in Table S6 at r_s = 3 for SiO_2

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Si        -1.724931888     7.495459794     0.269832544 CORE     2 Si Si     0.0000      2
Si         2.550251242     0.916020652     0.528166528 CORE     3 Si Si     0.0000      3
Si         0.764721806     5.701744229     0.526007015 CORE     4 Si Si     0.0000      4
Si         5.011218586     1.898140655     2.157830624 CORE     5 Si Si     0.0000      5
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Si 4.514521591 4.438720888 3.888650102 CORE 8 Si Si 0.0000 8
Si 1.504724096 0.525550547 5.518620967 CORE 9 Si Si 0.0000 9
Si -0.284887416 5.311812462 5.522152512 CORE 10 Si Si 0.0000 10
Si 3.995446804 -1.275591990 5.779164178 CORE 11 Si Si 0.0000 11
Si 2.206873403 3.510686475 5.777524066 CORE 12 Si Si 0.0000 12
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O 3.501965672 1.631674223 1.619860466 CORE 19 O O 0.0000 19
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O 5.659746917 0.499071888 2.660582425 CORE 21 O O 0.0000 21
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O 0.317367657 0.440039439 4.426634725 CORE 25 O O 0.0000 25
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O 2.562130726 -0.685822552 5.274500527 CORE 30 O O 0.0000 30
O 2.295525638 1.940393004 5.364820430 CORE 31 O O 0.0000 31
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GM in Table S6 at r_s = 3 for [$SiAlO_4H$]

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Si 0.939869972 6.210616506 3.704706022 CORE 2 Si Si 0.0000 2
Si 6.798770125 -0.373185966 4.247484718 CORE 3 Si Si 0.0000 3
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Si 3.628780931 1.014751518 6.921397898 CORE 5 Si Si 0.0000 5
Si 5.527787513 -1.404969244 6.993289928 CORE 6 Si Si 0.0000 6
Al 0.248609274 5.181056850 0.679935015 CORE 7 Al Al 0.0000 7
Al 4.798131234 1.282102196 2.486816763 CORE 8 Al Al 0.0000 8
Al 6.080023934 4.387066858 2.704883954 CORE 9 Al Al 0.0000 9
Al 2.266529478 -0.307197600 4.208388257 CORE 10 Al Al 0.0000 10
Al -0.227712364 3.858907825 5.428642140 CORE 11 Al Al 0.0000 11
Al 2.271176816 5.313400827 6.364201600 CORE 12 Al Al 0.0000 12
O 3.350385631 2.159193210 0.035456184 CORE 13 O O 0.0000 13
O 0.470507934 7.066229582 0.406727977 CORE 14 O O 0.0000 14
O 1.639490437 4.133201480 0.599799534 CORE 15 O O 0.0000 15
O 6.485754801 4.285417687 0.951177585 CORE 16 O O 0.0000 16
O 5.404322497 0.866750893 0.917342145 CORE 17 O O 0.0000 17
O 3.729659223 6.680978791 1.081641055 CORE 18 O O 0.0000 18
O 0.008331322 5.470360971 2.562949090 CORE 19 O O 0.0000 19

O 4.658676863 3.088372497 2.651815697 CORE 20 O O 0.0000 20
O 3.100490749 0.576955957 2.746876105 CORE 21 O O 0.0000 21
O 5.119918674 5.731871737 3.184803069 CORE 22 O O 0.0000 22
O 4.087530895 8.157715185 3.247792672 CORE 23 O O 0.0000 23
O 2.497136047 6.062140869 3.298519181 CORE 24 O O 0.0000 24
O 6.988394548 3.302487311 3.858744894 CORE 25 O O 0.0000 25
O 5.916573618 0.929713941 3.783336343 CORE 26 O O 0.0000 26
O 0.499766822 7.727007131 3.982400873 CORE 27 O O 0.0000 27
O 0.553688816 -0.066700439 4.089610366 CORE 28 O O 0.0000 28
O 0.893695594 5.240120715 5.107773535 CORE 29 O O 0.0000 29
O 2.877160911 0.688676981 5.515787133 CORE 30 O O 0.0000 30
O 6.436447813 -0.735410289 5.808612711 CORE 31 O O 0.0000 31
O 3.629945234 4.314093242 6.069772437 CORE 32 O O 0.0000 32
O 0.852570276 2.666193527 6.204609650 CORE 33 O O 0.0000 33
O 6.301834790 4.300589174 6.444051549 CORE 34 O O 0.0000 34
O 2.571060110 6.975749433 6.497362441 CORE 35 O O 0.0000 35
O 4.871347037 2.101924192 6.766256157 CORE 36 O O 0.0000 36
H 5.876187742 4.001452921 0.258261187 CORE 37 H H 0.0000 37
H 0.419244316 7.593041836 1.216193764 CORE 38 H H 0.0000 38
H 2.515114585 0.848362478 2.021445029 CORE 39 H H 0.0000 39
H 3.781182741 3.463390590 2.505018731 CORE 40 H H 0.0000 40
H 6.640330601 2.356542738 3.885362317 CORE 41 H H 0.0000 41
H 1.364477866 1.974947041 5.738218954 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 3.5 for AlPO

!BIOSYM archive 2
PBC=ON
Energy 0 0.0194 -234.611725 C2
!DATE
PBC 9.73679867 8.45852032 8.73085948 61.05262773 89.82676220 90.02937972
P 3.740866964 2.239830322 0.775992103 CORE 1 P P 0.0000 1
P 0.706775056 6.482445820 0.995206311 CORE 2 P P 0.0000 2
P 5.565123031 6.501742208 3.077038754 CORE 3 P P 0.0000 3
P 8.692995763 2.253316297 3.320093866 CORE 4 P P 0.0000 4
P 3.876105761 10.692754316 5.464167324 CORE 5 P P 0.0000 5
P 0.815549452 6.452976441 5.671708093 CORE 6 P P 0.0000 6
Al 3.691418524 5.413721207 0.785425419 CORE 7 Al Al 0.0000 7
Al 0.773153952 1.185991442 0.998235528 CORE 8 Al Al 0.0000 8
Al 5.630901397 9.645539482 3.059869580 CORE 9 Al Al 0.0000 9
Al 8.627661867 5.426214153 3.335988255 CORE 10 Al Al 0.0000 10
Al 3.810322030 5.423662833 5.462880283 CORE 11 Al Al 0.0000 11
Al 0.869037962 9.653499024 5.662779662 CORE 12 Al Al 0.0000 12
O 3.474267221 3.710826252 0.428638989 CORE 13 O O 0.0000 13
O 2.456897199 1.590648593 1.321798619 CORE 14 O O 0.0000 14
O 2.154650150 6.078485219 1.319012746 CORE 15 O O 0.0000 15
O 0.494055457 7.954003109 1.374484916 CORE 16 O O 0.0000 16
O 9.484136553 5.616226845 1.814508861 CORE 17 O O 0.0000 17
O 4.840208507 2.159044991 1.833761539 CORE 18 O O 0.0000 18
O 9.481891758 2.177214660 2.006490101 CORE 19 O O 0.0000 19
O 4.886472269 5.597814488 2.039071634 CORE 20 O O 0.0000 20
O 5.459324087 7.958909316 2.617504141 CORE 21 O O 0.0000 21
O 7.316275504 10.075766774 3.125458155 CORE 22 O O 0.0000 22
O 7.031213084 6.103903971 3.198571253 CORE 23 O O 0.0000 23
O 8.534932999 3.720771640 3.731915498 CORE 24 O O 0.0000 24
O 9.427612467 9.945674370 4.420941295 CORE 25 O O 0.0000 25
O 4.882274667 6.347504349 4.441286245 CORE 26 O O 0.0000 26
O 9.467485729 6.276780342 4.614934232 CORE 27 O O 0.0000 27

O 4.880836253 9.900246967 4.626185284 CORE 28 O O 0.0000 28
O 2.452384783 10.210713835 5.137472929 CORE 29 O O 0.0000 29
O 2.146147687 5.897305150 5.133964948 CORE 30 O O 0.0000 30
O 4.008505123 3.720088892 5.113403367 CORE 31 O O 0.0000 31
O 0.965851306 7.940684141 6.005379660 CORE 32 O O 0.0000 32
O 0.421011690 5.693118780 6.946366142 CORE 33 O O 0.0000 33
O 4.187599655 10.480959250 6.954662424 CORE 34 O O 0.0000 34
O 0.443446683 10.510423659 7.138521561 CORE 35 O O 0.0000 35
O 4.212323086 5.723265839 7.146850361 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 3.5 for SiO_2

!BIOSYM archive 2
PBC=ON
Energy 0 0.0196 -250.379330 P4/m
!DATE
PBC 8.61851073 7.75614122 8.59216584 90.26574547 90.05028326 89.33105498
Si 6.118635670 1.823866205 0.728945825 CORE 1 Si Si 0.0000 1
Si 6.194810038 4.868470903 0.758726471 CORE 2 Si Si 0.0000 2
Si 3.212961583 1.886381570 1.952131987 CORE 3 Si Si 0.0000 3
Si 3.289601115 4.930696329 1.980802600 CORE 4 Si Si 0.0000 4
Si 7.663090749 7.213739228 2.089490337 CORE 5 Si Si 0.0000 5
Si 1.929841640 7.284162692 3.414018711 CORE 6 Si Si 0.0000 6
Si 6.339139949 7.249921850 4.978562293 CORE 7 Si Si 0.0000 7
Si 0.605805665 7.320250687 6.302843954 CORE 8 Si Si 0.0000 8
Si 4.888519278 1.847554966 6.411548989 CORE 9 Si Si 0.0000 9
Si 4.966309971 4.891389398 6.440300436 CORE 10 Si Si 0.0000 10
Si 1.983229937 1.909171761 7.634226141 CORE 11 Si Si 0.0000 11
Si 2.059913711 4.954037213 7.663280798 CORE 12 Si Si 0.0000 12
O 2.297199826 1.705960952 0.618826501 CORE 13 O O 0.0000 13
O 2.386878446 5.185928846 0.651888957 CORE 14 O O 0.0000 14
O 6.677735381 3.331346646 0.986735045 CORE 15 O O 0.0000 15
O 7.245043535 0.761917079 1.179520011 CORE 16 O O 0.0000 16
O 7.374575176 5.861719563 1.235582784 CORE 17 O O 0.0000 17
O 4.767878151 1.572787531 1.601241459 CORE 18 O O 0.0000 18
O 4.858779015 5.171915735 1.637088837 CORE 19 O O 0.0000 19
O 0.608039816 7.247019679 2.482501466 CORE 20 O O 0.0000 20
O 3.079563247 3.407812393 2.515917558 CORE 21 O O 0.0000 21
O 2.705144751 0.861983645 3.088044328 CORE 22 O O 0.0000 22
O 2.829455156 5.959940489 3.136102801 CORE 23 O O 0.0000 23
O 6.740559244 7.225625043 3.417456512 CORE 24 O O 0.0000 24
O 1.528447006 7.310303081 4.974671414 CORE 25 O O 0.0000 25
O 5.348110283 0.817854693 5.256842997 CORE 26 O O 0.0000 26
O 5.473828640 5.915910597 5.304338492 CORE 27 O O 0.0000 27
O 5.099428778 3.370149890 5.875899283 CORE 28 O O 0.0000 28
O 7.660869766 7.286813584 5.909781578 CORE 29 O O 0.0000 29
O 3.319017079 1.606907481 6.755288087 CORE 30 O O 0.0000 30
O 3.411061624 5.204080050 6.791383517 CORE 31 O O 0.0000 31
O 0.803705122 0.915981996 7.158318386 CORE 32 O O 0.0000 32
O 0.934047321 6.015343963 7.211378206 CORE 33 O O 0.0000 33
O 1.500136743 3.446477425 7.406751526 CORE 34 O O 0.0000 34
O 5.791084958 1.592849795 7.740413291 CORE 35 O O 0.0000 35
O 5.881835805 5.071460090 7.773778578 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 3.5 for [$SiAlO_4H$]

!BIOSYM archive 2
PBC=ON

Energy 0 0.0181 -262.422290 P1
!DATE
PBC 7.48213330 11.00785212 7.87840837 98.91010477 99.36879795 94.76605933
Si 4.113114370 10.563606142 0.805982524 CORE 1 Si Si 0.0000 1
Si -0.814638236 9.701292722 2.131078241 CORE 2 Si Si 0.0000 2
Si 0.913970527 1.665685746 2.816641812 CORE 3 Si Si 0.0000 3
Si 6.075307550 3.580154064 3.884029522 CORE 4 Si Si 0.0000 4
Si 5.244677802 0.062867040 6.333832854 CORE 5 Si Si 0.0000 5
Si -1.507047253 3.139690804 6.906475630 CORE 6 Si Si 0.0000 6
Al 1.587093904 8.765246845 0.113743911 CORE 7 Al Al 0.0000 7
Al 2.315605617 3.456665102 0.502195505 CORE 8 Al Al 0.0000 8
Al 5.090594395 5.260712747 1.494895910 CORE 9 Al Al 0.0000 9
Al 4.008049183 1.104492124 3.493684724 CORE 10 Al Al 0.0000 10
Al -0.835027390 9.013935448 5.127488618 CORE 11 Al Al 0.0000 11
Al 2.284282425 0.553609050 5.520094191 CORE 12 Al Al 0.0000 12
O 5.949050390 4.963966826 0.028637069 CORE 13 O O 0.0000 13
O 1.140898185 4.708719915 0.100998391 CORE 14 O O 0.0000 14
O 2.168841262 7.155069969 0.467669833 CORE 15 O O 0.0000 15
O 5.315263838 9.498986349 1.186807076 CORE 16 O O 0.0000 16
O 0.493898752 9.405793577 1.265042170 CORE 17 O O 0.0000 17
O 1.603958398 2.200466779 1.492612171 CORE 18 O O 0.0000 18
O 4.324559059 6.871494154 1.449826874 CORE 19 O O 0.0000 19
O 3.569565640 4.234001558 1.606013404 CORE 20 O O 0.0000 20
O 4.334742471 0.114290907 2.155428460 CORE 21 O O 0.0000 21
O 0.045914859 0.303762449 2.620156809 CORE 22 O O 0.0000 22
O 5.966451198 4.904192665 2.971670436 CORE 23 O O 0.0000 23
O -0.954298911 8.753959310 3.434966819 CORE 24 O O 0.0000 24
O 4.765160327 2.643917337 3.571785609 CORE 25 O O 0.0000 25
O -0.029434244 2.722468668 3.598743541 CORE 26 O O 0.0000 26
O 2.189086510 1.235743168 3.842538763 CORE 27 O O 0.0000 27
O 4.076789033 0.304579441 5.144101299 CORE 28 O O 0.0000 28
O 6.104231863 3.957244680 5.479070091 CORE 29 O O 0.0000 29
O 0.746785161 9.841444864 5.532072938 CORE 30 O O 0.0000 30
O 6.316070547 -1.006386514 5.837480126 CORE 31 O O 0.0000 31
O -0.509344382 7.476819648 6.091496409 CORE 32 O O 0.0000 32
O 5.907245090 1.512737463 6.596491604 CORE 33 O O 0.0000 33
O 1.835892929 1.537694539 6.778314517 CORE 34 O O 0.0000 34
O 1.730988611 8.454599598 7.540561863 CORE 35 O O 0.0000 35
O 4.372570732 -0.490621421 7.595985088 CORE 36 O O 0.0000 36
H 1.735111657 6.273776879 0.350142651 CORE 37 H H 0.0000 37
H 3.267405828 6.993050492 0.968308846 CORE 38 H H 0.0000 38
H 4.773282158 7.732439887 1.388077675 CORE 39 H H 0.0000 39
H 3.668223072 3.744565367 2.445144562 CORE 40 H H 0.0000 40
H -0.708855470 6.622162507 5.675949564 CORE 41 H H 0.0000 41
H 1.283045667 9.307704591 6.187120506 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 4 for AlPO

!BIOSYM archive 2
PBC=ON
Energy 0 0.0199 -234.468358 R-3
!DATE
PBC 5.15105686 12.43745646 12.43747204 118.12576003 82.06516968 82.06410618
P 3.047441978 -2.511164979 7.518402602 CORE 1 P P 0.0000 1
P 4.764577921 1.607363407 9.083530595 CORE 2 P P 0.0000 2
P 1.330479107 0.903593496 4.734017738 CORE 3 P P 0.0000 3
P 7.254696823 5.255656025 5.933969695 CORE 4 P P 0.0000 4
P 3.820598702 4.551841433 1.584618753 CORE 5 P P 0.0000 5

P 5.537733894 8.670248126 3.149632115 CORE 6 P P 0.0000 6
Al 4.752721425 7.114682794 5.919929440 CORE 7 Al Al 0.0000 7
Al 1.318642897 3.634200285 3.201624518 CORE 8 Al Al 0.0000 8
Al 3.035712655 7.728614536 1.546580297 CORE 9 Al Al 0.0000 9
Al 5.549473741 -1.569438433 9.121481131 CORE 10 Al Al 0.0000 10
Al 7.266543483 2.524983096 7.466435256 CORE 11 Al Al 0.0000 11
Al 3.832464967 -0.955504016 4.748124737 CORE 12 Al Al 0.0000 12
O 5.120946342 7.853634369 4.376560160 CORE 13 O O 0.0000 13
O 3.464247334 -1.694434226 6.291480475 CORE 14 O O 0.0000 14
O 5.062991039 4.331165233 2.444450255 CORE 15 O O 0.0000 15
O 3.522174358 1.828017174 8.223586700 CORE 16 O O 0.0000 16
O 5.860883581 10.113807036 3.557167010 CORE 17 O O 0.0000 17
O 6.780076625 8.035800760 2.528690934 CORE 18 O O 0.0000 18
O 5.239114313 0.048579293 4.973183801 CORE 19 O O 0.0000 19
O 6.111995916 6.138688974 6.452669797 CORE 20 O O 0.0000 20
O 4.190209523 -2.518787372 8.542656539 CORE 21 O O 0.0000 21
O 4.441386149 1.976329832 10.537409935 CORE 22 O O 0.0000 22
O 6.158419152 1.978320319 3.687807557 CORE 23 O O 0.0000 23
O 6.837891001 4.601279716 4.613095558 CORE 24 O O 0.0000 24
O 5.181263499 0.136757443 8.989753880 CORE 25 O O 0.0000 25
O 2.677951108 3.660854940 2.089930060 CORE 26 O O 0.0000 26
O 5.907250297 2.498329242 8.578112001 CORE 27 O O 0.0000 27
O 3.403929711 6.022398412 1.678295661 CORE 28 O O 0.0000 28
O 1.747302457 1.557904197 6.054988839 CORE 29 O O 0.0000 29
O 2.426775619 4.180809416 6.980292014 CORE 30 O O 0.0000 30
O 4.143807975 4.182839306 0.130587901 CORE 31 O O 0.0000 31
O 4.394992301 8.677978899 2.125414174 CORE 32 O O 0.0000 32
O 2.473206518 0.020473246 4.215392482 CORE 33 O O 0.0000 33
O 3.346049805 6.110579238 5.694883181 CORE 34 O O 0.0000 34
O 1.805088084 -1.876603571 8.139380758 CORE 35 O O 0.0000 35
O 2.724311065 -3.954567091 7.110913525 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 4 for SiO_2

!BIOSYM archive 2
PBC=ON
Energy 0 0.0172 -250.271060 C2
!DATE
PBC 8.85418849 8.60328164 8.85453875 91.61672942 111.34756105 91.60375908
Si 7.539588476 7.599410031 0.036921715 CORE 1 Si Si 0.0000 1
Si 5.969187284 4.823694390 0.392908528 CORE 2 Si Si 0.0000 2
Si 3.365996689 5.992641888 1.557258814 CORE 3 Si Si 0.0000 3
Si 7.562840013 3.492497758 2.773303806 CORE 4 Si Si 0.0000 4
Si -1.111944526 0.360201437 2.907180223 CORE 5 Si Si 0.0000 5
Si 4.880753905 7.535887418 3.649215085 CORE 6 Si Si 0.0000 6
Si 1.342247226 4.928704688 3.821423842 CORE 7 Si Si 0.0000 7
Si 5.865269271 4.794516971 4.978851255 CORE 8 Si Si 0.0000 8
Si 0.333343870 7.633288761 5.225028408 CORE 9 Si Si 0.0000 9
Si 3.135073998 3.361858566 5.790752475 CORE 10 Si Si 0.0000 10
Si 3.317783850 0.242330753 5.931572539 CORE 11 Si Si 0.0000 11
Si -1.653176402 6.333776118 7.191251021 CORE 12 Si Si 0.0000 12
O 2.484537723 6.334847599 0.243161052 CORE 13 O O 0.0000 13
O 4.527383479 4.943906483 1.129875496 CORE 14 O O 0.0000 14
O 6.978169103 4.012421913 1.358203118 CORE 15 O O 0.0000 15
O 7.726125958 8.106488708 1.554150890 CORE 16 O O 0.0000 16
O 4.101216212 7.300260876 2.223432905 CORE 17 O O 0.0000 17
O -0.891737786 1.934906360 2.626122270 CORE 18 O O 0.0000 18
O 2.420432571 5.344436072 2.691513081 CORE 19 O O 0.0000 19

O 0.017265662 4.387105619 3.083490182 CORE 20 O O 0.0000 20
O 6.231488324 0.110755173 3.471437453 CORE 21 O O 0.0000 21
O 6.478086797 3.667620498 3.979762837 CORE 22 O O 0.0000 22
O 0.012073091 -0.140477100 3.956130970 CORE 23 O O 0.0000 23
O 5.649716672 6.172890049 4.125025889 CORE 24 O O 0.0000 24
O 1.977293380 3.731764474 4.714477463 CORE 25 O O 0.0000 25
O 3.805698135 7.955446255 4.781860959 CORE 26 O O 0.0000 26
O 0.955281580 6.196206836 4.767766289 CORE 27 O O 0.0000 27
O 4.436770502 4.305109473 5.556597385 CORE 28 O O 0.0000 28
O 3.565846455 1.811406160 5.629331199 CORE 29 O O 0.0000 29
O 1.730629837 -0.081806165 5.934320213 CORE 30 O O 0.0000 30
O -1.953330204 5.037478906 6.229922052 CORE 31 O O 0.0000 31
O -0.873327359 7.437049971 6.293828642 CORE 32 O O 0.0000 32
O 2.541909341 3.624625425 7.275246434 CORE 33 O O 0.0000 33
O 3.911634817 -0.142374410 7.392889791 CORE 34 O O 0.0000 34
O -3.079377073 6.913214018 7.672288168 CORE 35 O O 0.0000 35
O 6.564100330 6.295645689 0.018274658 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 4 for [$SiAlO_4H$]

!BIOSYM archive 2
PBC=ON
Energy 0 0.0180 -262.014289 P1
!DATE
PBC 9.69393557 8.88569797 9.84558754 90.13528348 115.02752654 116.38803813
Si -1.906521700 2.183567183 1.922337051 CORE 1 Si Si 0.0000 1
Si 6.118247048 0.183223413 3.279777373 CORE 2 Si Si 0.0000 2
Si 1.930658497 4.097764221 4.529234430 CORE 3 Si Si 0.0000 3
Si 5.532690220 -1.162789008 5.867604492 CORE 4 Si Si 0.0000 4
Si 3.002589650 2.997925105 7.106138833 CORE 5 Si Si 0.0000 5
Si 3.153067766 -0.108973142 7.564653523 CORE 6 Si Si 0.0000 6
Al 3.497872304 0.011392019 1.305188697 CORE 7 Al Al 0.0000 7
Al -2.108241648 5.384820228 2.440494950 CORE 8 Al Al 0.0000 8
Al 0.976459648 1.719434928 2.833934329 CORE 9 Al Al 0.0000 9
Al 4.401375446 5.841267732 3.692002279 CORE 10 Al Al 0.0000 10
Al 1.260072479 -0.967765063 5.184989786 CORE 11 Al Al 0.0000 11
Al -5.205834744 5.689850762 6.713354592 CORE 12 Al Al 0.0000 12
O 7.091438524 1.792279752 0.475693628 CORE 13 O O 0.0000 13
O -1.586051377 6.706955281 1.474116398 CORE 14 O O 0.0000 14
O 2.514570480 1.491414686 1.847906830 CORE 15 O O 0.0000 15
O -0.494799079 1.386138969 2.040100431 CORE 16 O O 0.0000 16
O -1.703925191 3.778342273 2.055938993 CORE 17 O O 0.0000 17
O 4.938555130 -0.072355813 2.208522286 CORE 18 O O 0.0000 18
O -3.959724988 5.512803953 2.489597472 CORE 19 O O 0.0000 19
O 6.722453248 1.696776029 3.074802136 CORE 20 O O 0.0000 20
O 3.391003743 7.096519516 3.137113670 CORE 21 O O 0.0000 21
O 1.092109026 3.350484804 3.388792719 CORE 22 O O 0.0000 22
O 3.439140930 4.448583819 4.068696979 CORE 23 O O 0.0000 23
O -1.669502129 5.866553017 4.192401584 CORE 24 O O 0.0000 24
O 1.256715545 0.675377240 4.364976660 CORE 25 O O 0.0000 25
O 5.491710275 0.082505142 4.813280786 CORE 26 O O 0.0000 26
O 1.102050807 5.441458073 5.016291516 CORE 27 O O 0.0000 27
O -4.278839528 6.188629035 5.204678341 CORE 28 O O 0.0000 28
O 1.982801604 3.036400929 5.808726764 CORE 29 O O 0.0000 29
O -2.725485669 -1.384735332 6.541819892 CORE 30 O O 0.0000 30
O 1.804664087 -0.648480852 6.796640507 CORE 31 O O 0.0000 31
O -5.443708962 3.990473431 6.930054271 CORE 32 O O 0.0000 32
O 4.415434510 -0.961665046 7.023634299 CORE 33 O O 0.0000 33

O 3.449320069 1.450425318 7.228096235 CORE 34 O O 0.0000 34
O -0.327474831 -1.734086416 8.208375401 CORE 35 O O 0.0000 35
O 2.151653550 3.484841484 8.441188669 CORE 36 O O 0.0000 36
H -2.824366003 6.276815970 0.194120336 CORE 37 H H 0.0000 37
H 5.454010192 5.425074776 1.554228360 CORE 38 H H 0.0000 38
H 2.991588898 2.333075090 1.803920425 CORE 39 H H 0.0000 39
H -0.753776253 5.646873557 4.483820904 CORE 40 H H 0.0000 40
H 1.515154962 1.351795149 5.040628863 CORE 41 H H 0.0000 41
H 0.539785627 -1.317169400 8.008320233 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 4.5 for AlPO

!BIOSYM archive 2
PBC=ON
Energy 0 0.0187 -234.145536 P2_1/m
!DATE
PBC 12.84915310 12.88904848 5.35032906 90.00000000 90.00000000 62.71147678
P 7.768386329 6.634504704 1.337582265 CORE 1 P P 0.0000 1
P 7.452535375 1.529422658 1.337582265 CORE 2 P P 0.0000 2
P 14.732895671 7.222905133 1.337582265 CORE 3 P P 0.0000 3
P 10.990028790 4.820109797 4.012746795 CORE 4 P P 0.0000 4
P 11.305879737 9.925191832 4.012746795 CORE 5 P P 0.0000 5
P 4.025519440 4.231709361 4.012746795 CORE 6 P P 0.0000 6
Al 9.445493800 3.944638483 1.337582265 CORE 7 Al Al 0.0000 7
Al 4.736913244 5.878098280 1.337582265 CORE 8 Al Al 0.0000 8
Al 13.100137413 9.849518717 1.337582265 CORE 9 Al Al 0.0000 9
Al 9.312921314 7.509976011 4.012746795 CORE 10 Al Al 0.0000 10
Al 14.021501870 5.576516215 4.012746795 CORE 11 Al Al 0.0000 11
Al 5.658277701 1.605095777 4.012746795 CORE 12 Al Al 0.0000 12
O 12.124009485 9.579884506 5.260829885 CORE 13 O O 0.0000 13
O 4.648725941 4.870484739 5.259029979 CORE 14 O O 0.0000 14
O 6.634405629 1.874729989 0.089499175 CORE 15 O O 0.0000 15
O 14.109689173 6.584129756 0.091299082 CORE 16 O O 0.0000 16
O 8.328344021 7.322346430 0.091585303 CORE 17 O O 0.0000 17
O 10.430071092 4.132268063 5.258743760 CORE 18 O O 0.0000 18
O 6.245272090 6.767183895 1.337582265 CORE 19 O O 0.0000 19
O 7.815621215 0.036862696 1.337582265 CORE 20 O O 0.0000 20
O 8.746369984 2.341964622 1.337582265 CORE 21 O O 0.0000 21
O 16.254912978 7.027680575 1.337582265 CORE 22 O O 0.0000 22
O 8.149184011 5.139959156 1.337582265 CORE 23 O O 0.0000 23
O 14.442777262 8.726084945 1.337582265 CORE 24 O O 0.0000 24
O 6.634405629 1.874729989 2.585665355 CORE 25 O O 0.0000 25
O 14.109689173 6.584129756 2.583865448 CORE 26 O O 0.0000 26
O 12.124009485 9.579884506 2.764663705 CORE 27 O O 0.0000 27
O 4.648725941 4.870484739 2.766463611 CORE 28 O O 0.0000 28
O 10.430071092 4.132268063 2.766749830 CORE 29 O O 0.0000 29
O 8.328344021 7.322346430 2.583579227 CORE 30 O O 0.0000 30
O 12.513143022 4.687430599 4.012746795 CORE 31 O O 0.0000 31
O 10.942793898 11.417751800 4.012746795 CORE 32 O O 0.0000 32
O 10.012045131 9.112649874 4.012746795 CORE 33 O O 0.0000 33
O 2.503502138 4.426933919 4.012746795 CORE 34 O O 0.0000 34
O 10.609231104 6.314655336 4.012746795 CORE 35 O O 0.0000 35
O 4.315637853 2.728529549 4.012746795 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 4.5 for SiO_2

!BIOSYM archive 2
PBC=ON

Energy 0 0.0193 -249.876679 R-3m

!DATE

PBC 9.35153626 9.34860556 9.34844441 85.77080536 85.74307737 94.25917219

Si 8.113055485 4.957747710 2.732853791 CORE 1 Si Si 0.0000 1

Si 1.045056112 2.841538512 2.734980269 CORE 2 Si Si 0.0000 2

Si 6.453865804 3.168329349 4.667298568 CORE 3 Si Si 0.0000 3

Si 8.736586030 1.053780667 4.671262383 CORE 4 Si Si 0.0000 4

Si 3.328624155 3.006030661 4.844218870 CORE 5 Si Si 0.0000 5

Si 8.112671738 7.245550519 4.845187324 CORE 6 Si Si 0.0000 6

Si 1.670733060 1.220085002 6.782161736 CORE 7 Si Si 0.0000 7

Si 6.453666525 5.460093820 6.783089455 CORE 8 Si Si 0.0000 8

Si 1.044744184 7.412124909 6.955179745 CORE 9 Si Si 0.0000 9

Si 3.328609128 5.296672898 6.958963857 CORE 10 Si Si 0.0000 10

Si 8.736548650 5.624527445 8.890815269 CORE 11 Si Si 0.0000 11

Si 1.670791743 3.507262739 8.893120651 CORE 12 Si Si 0.0000 12

O 7.797189980 5.182557436 1.165438075 CORE 13 O O 0.0000 13

O 1.292321124 2.540476401 1.167718087 CORE 14 O O 0.0000 14

O 0.206758588 4.227429505 2.920703716 CORE 15 O O 0.0000 15

O 6.938477909 4.032350021 3.375637685 CORE 16 O O 0.0000 16

O 0.212396993 1.601137018 3.380825738 CORE 17 O O 0.0000 17

O 8.153108637 6.399048239 3.466898601 CORE 18 O O 0.0000 18

O 2.479441719 2.993102928 3.467389516 CORE 19 O O 0.0000 19

O 4.890919629 2.802004380 4.490426474 CORE 20 O O 0.0000 20

O 7.796917156 8.789978107 4.495426381 CORE 21 O O 0.0000 21

O 7.301225200 1.793742356 4.769106494 CORE 22 O O 0.0000 22

O 0.205997221 7.116297826 5.588878300 CORE 23 O O 0.0000 23

O 3.098386295 4.434548132 5.594879853 CORE 24 O O 0.0000 24

O 2.847890732 1.789084905 5.812568258 CORE 25 O O 0.0000 25

O 6.937930415 6.678903713 5.818903703 CORE 26 O O 0.0000 26

O 6.682648646 4.033123438 6.029715904 CORE 27 O O 0.0000 27

O 9.579181859 1.349483894 6.035337506 CORE 28 O O 0.0000 28

O 2.479061857 6.669880425 6.862193608 CORE 29 O O 0.0000 29

O 1.292667389 8.998307908 7.130404386 CORE 30 O O 0.0000 30

O 4.890804030 5.665886533 7.134314718 CORE 31 O O 0.0000 31

O 7.301050730 5.468051156 8.161330272 CORE 32 O O 0.0000 32

O 1.626708313 2.064690622 8.161553445 CORE 33 O O 0.0000 33

O 0.212089061 6.867887746 8.243335865 CORE 34 O O 0.0000 34

O 2.848412079 4.428240327 8.249220042 CORE 35 O O 0.0000 35

O 9.579582004 4.241749433 8.703342203 CORE 36 O O 0.0000 36

end

end

GM in Table S6 at r_s = 4.5 for [$SiAlO_4H$]

!BIOSYM archive 2

PBC=ON

Energy 0 0.0182 -261.604835 P1

!DATE

PBC 9.15269960 9.09191479 9.43441470 66.95554660 84.10908732 82.75786896

Si 1.376227366 7.001316674 2.040726417 CORE 1 Si Si 0.0000 1

Si 6.131076443 4.294899549 2.805045106 CORE 2 Si Si 0.0000 2

Si 8.813907827 5.404098776 4.080302181 CORE 3 Si Si 0.0000 3

Si 4.390673383 2.678171077 4.767583982 CORE 4 Si Si 0.0000 4

Si 1.353213102 3.005860583 5.196434054 CORE 5 Si Si 0.0000 5

Si 7.856727277 7.991081504 5.278405905 CORE 6 Si Si 0.0000 6

Al 6.865017313 1.531725459 1.339670027 CORE 7 Al Al 0.0000 7

Al 4.296864921 6.465095431 1.463812885 CORE 8 Al Al 0.0000 8

Al 5.753996484 8.921908545 3.158694468 CORE 9 Al Al 0.0000 9

Al 10.257570784 9.534987787 3.768894725 CORE 10 Al Al 0.0000 10

Al 7.008456379 10.165162416 7.126313816 CORE 11 Al Al 0.0000 11

Al 9.972217978 11.822479607 8.014974052 CORE 12 Al Al 0.0000 12
O 9.884067758 7.836554905 0.779328566 CORE 13 O O 0.0000 13
O 6.746180367 9.287099722 1.629844143 CORE 14 O O 0.0000 14
O 2.613918334 6.064877950 1.574972917 CORE 15 O O 0.0000 15
O 6.386586119 3.088072478 1.742112280 CORE 16 O O 0.0000 16
O 5.693011024 5.583501306 1.926380182 CORE 17 O O 0.0000 17
O 8.385498525 1.080427764 2.142081945 CORE 18 O O 0.0000 18
O 4.407960553 8.062092473 2.343984626 CORE 19 O O 0.0000 19
O 9.280927215 6.187626268 2.714654298 CORE 20 O O 0.0000 20
O 1.946133468 8.132383169 3.090278833 CORE 21 O O 0.0000 21
O 7.485724322 4.559131677 3.684116570 CORE 22 O O 0.0000 22
O 5.305884327 10.434042465 3.793467452 CORE 23 O O 0.0000 23
O 4.954827574 3.929337288 3.877756648 CORE 24 O O 0.0000 24
O 1.016344326 1.778992551 4.221348904 CORE 25 O O 0.0000 25
O 6.660681930 7.904709109 4.189365422 CORE 26 O O 0.0000 26
O 0.859532074 4.428794832 4.552965617 CORE 27 O O 0.0000 27
O 8.970168547 9.083286725 4.816729623 CORE 28 O O 0.0000 28
O 8.498791487 6.449660676 5.328344768 CORE 29 O O 0.0000 29
O 2.969038881 3.109058596 5.476492009 CORE 30 O O 0.0000 30
O 6.617908694 11.338259121 5.938570090 CORE 31 O O 0.0000 31
O 9.709398842 2.818375212 6.593255767 CORE 32 O O 0.0000 32
O 7.303493243 8.497551593 6.738860300 CORE 33 O O 0.0000 33
O 8.201622947 4.553139176 8.295607013 CORE 34 O O 0.0000 34
O 8.475164112 10.745472769 8.125266398 CORE 35 O O 0.0000 35
O 5.633919480 10.424793271 8.353439872 CORE 36 O O 0.0000 36
H 7.684296511 6.495504825 0.161640789 CORE 37 H H 0.0000 37
H 6.333625165 8.925750811 0.835012306 CORE 38 H H 0.0000 38
H 9.983438591 9.461672279 1.540638607 CORE 39 H H 0.0000 39
H 3.495541502 8.246175973 2.737330176 CORE 40 H H 0.0000 40
H 8.394673908 5.196540297 7.590146892 CORE 41 H H 0.0000 41
H 4.862560206 10.784498721 7.886287401 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 5 for AlPO

!BIOSYM archive 2
PBC=ON
Energy 0 0.0200 -233.965249 R-3
!DATE
PBC 9.46899444 9.47008214 9.45861105 94.50302200 85.47427984 85.43895964
P 7.986406380 2.016082025 0.710577668 CORE 1 P P 0.0000 1
P 3.920256016 1.749346269 2.697257768 CORE 2 P P 0.0000 2
P 6.353830934 6.976537889 2.786423881 CORE 3 P P 0.0000 3
P 8.571070283 3.661807718 4.888037962 CORE 4 P P 0.0000 4
P 1.534866897 8.887518569 4.977578798 CORE 5 P P 0.0000 5
P 6.939586165 8.625085642 6.964348276 CORE 6 P P 0.0000 6
Al 6.346707632 9.368527461 0.717222400 CORE 7 Al Al 0.0000 7
Al 6.300903732 3.841673652 2.679020298 CORE 8 Al Al 0.0000 8
Al 0.787439731 1.851332216 2.898868117 CORE 9 Al Al 0.0000 9
Al 4.668660135 8.789953740 4.776648216 CORE 10 Al Al 0.0000 10
Al 8.626031270 6.796988172 4.993905076 CORE 11 Al Al 0.0000 11
Al 8.577021713 1.268319192 6.957954160 CORE 12 Al Al 0.0000 12
O 7.156497791 0.726153707 0.843531102 CORE 13 O O 0.0000 13
O 7.222006842 3.197146125 1.329858549 CORE 14 O O 0.0000 14
O 9.326213562 1.821343085 1.420035645 CORE 15 O O 0.0000 15
O 4.363442021 0.927153311 1.476006584 CORE 16 O O 0.0000 16
O 6.440370616 7.816093474 1.512414369 CORE 17 O O 0.0000 17
O 6.000876965 5.540172475 2.399919544 CORE 18 O O 0.0000 18
O 2.461066023 2.163263979 2.507844838 CORE 19 O O 0.0000 19

O 4.770719929 3.012637004 2.824831042 CORE 20 O O 0.0000 20
O 7.714568236 7.014746498 3.505121853 CORE 21 O O 0.0000 21
O 0.628243860 0.293794923 3.700940687 CORE 22 O O 0.0000 22
O 5.255318437 7.522997614 3.712396612 CORE 23 O O 0.0000 23
O 9.670767411 3.121364160 3.960322483 CORE 24 O O 0.0000 24
O 4.073655610 0.910017732 3.978719375 CORE 25 O O 0.0000 25
O 7.210112982 3.620794239 4.169039612 CORE 26 O O 0.0000 26
O 10.158099175 7.621787434 4.840637050 CORE 27 O O 0.0000 27
O 2.995163682 8.477619742 5.167493405 CORE 28 O O 0.0000 28
O 8.919726126 5.098397981 5.278382428 CORE 29 O O 0.0000 29
O 8.487646420 2.819453088 6.160116553 CORE 30 O O 0.0000 30
O 9.801600598 0.260388078 6.202498996 CORE 31 O O 0.0000 31
O 5.598806062 8.814448605 6.255370158 CORE 32 O O 0.0000 32
O 7.710810474 7.449692912 6.342877658 CORE 33 O O 0.0000 33
O 7.009460249 0.479412849 6.834351637 CORE 34 O O 0.0000 34
O 6.671613158 8.314331644 8.436261997 CORE 35 O O 0.0000 35
O 9.001886994 1.518036314 8.632811167 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 5 for SiO_2

!BIOSYM archive 2
PBC=ON
Energy 0 0.0166 -249.879520 R-3m
!DATE
PBC 9.35455180 9.35501242 9.35413722 94.18705706 94.16947887 94.18896414
Si 6.851546059 3.696723086 1.191489221 CORE 1 Si Si 0.0000 1
Si 1.370346089 8.792073793 1.189685196 CORE 2 Si Si 0.0000 2
Si 4.509776004 8.958325423 1.370294429 CORE 3 Si Si 0.0000 3
Si 6.788849045 6.839539377 1.371660891 CORE 4 Si Si 0.0000 4
Si 6.852292498 1.411697801 3.302026917 CORE 5 Si Si 0.0000 5
Si 8.447003335 8.625159700 3.301850573 CORE 6 Si Si 0.0000 6
Si 6.791743635 1.343618965 6.449665627 CORE 7 Si Si 0.0000 7
Si -0.969834094 8.557369655 6.449436330 CORE 8 Si Si 0.0000 8
Si 8.449124850 3.128899760 8.380744369 CORE 9 Si Si 0.0000 9
Si 1.373417244 1.011062355 8.380632501 CORE 10 Si Si 0.0000 10
Si 4.512835524 1.176437966 8.561592210 CORE 11 Si Si 0.0000 11
Si -0.970133303 6.272069139 8.560513549 CORE 12 Si Si 0.0000 12
O 0.894504562 7.569852595 0.224670493 CORE 13 O O 0.0000 13
O 5.666418617 3.133094571 0.227438169 CORE 14 O O 0.0000 14
O 8.291508575 3.544211093 0.441979455 CORE 15 O O 0.0000 15
O 1.796410617 0.887592155 0.442249927 CORE 16 O O 0.0000 16
O 5.349574764 7.576490163 1.289918984 CORE 17 O O 0.0000 17
O 6.555244111 5.248632096 1.526727522 CORE 18 O O 0.0000 18
O 2.940009193 8.609373259 1.523896377 CORE 19 O O 0.0000 19
O 0.531515625 8.765971677 2.573791644 CORE 20 O O 0.0000 20
O 6.887838214 2.857911604 2.575597908 CORE 21 O O 0.0000 21
O 5.666842985 0.495292621 2.664413307 CORE 22 O O 0.0000 22
O 7.618575608 7.376077065 2.665539597 CORE 23 O O 0.0000 23
O 8.292512743 0.677709225 3.089475035 CORE 24 O O 0.0000 24
O 6.557576576 1.622047258 4.875823656 CORE 25 O O 0.0000 25
O -0.674369739 8.346611540 4.875396251 CORE 26 O O 0.0000 26
O 7.627564463 -0.039611484 6.661383270 CORE 27 O O 0.0000 27
O 7.621532858 2.591785454 7.085463628 CORE 28 O O 0.0000 28
O 0.897863794 0.145133869 7.086360040 CORE 29 O O 0.0000 29
O 5.352810040 1.204408620 7.178344727 CORE 30 O O 0.0000 30
O -1.005251995 7.111157529 7.176643929 CORE 31 O O 0.0000 31
O 2.943338033 1.358196133 8.225322262 CORE 32 O O 0.0000 32
O -0.673449181 4.719945660 8.225491936 CORE 33 O O 0.0000 33

O 0.534321362 2.393177816 8.464156602 CORE 34 O O 0.0000 34
O 5.451030956 0.484976841 0.007716013 CORE 35 O O 0.0000 35
O 7.624345838 7.158575713 0.008735459 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 5 for [$SiAlO_4H$]

!BIOSYM archive 2
PBC=ON
Energy 0 0.0188 -260.962325 P1
!DATE
PBC 9.78745758 9.73667913 9.78573003 85.64131141 85.75880875 94.10992480
Si 5.291098300 6.592866040 0.002742870 CORE 1 Si Si 0.0000 1
Si 8.537112187 9.126407819 2.186329023 CORE 2 Si Si 0.0000 2
Si 3.682860254 1.470938111 2.230009990 CORE 3 Si Si 0.0000 3
Si 3.477036304 6.990522535 4.355644987 CORE 4 Si Si 0.0000 4
Si 1.222245428 9.354692401 7.550506416 CORE 5 Si Si 0.0000 5
Si 1.774418065 5.242019183 9.623581716 CORE 6 Si Si 0.0000 6
Al 1.160325278 1.252394045 0.234005484 CORE 7 Al Al 0.0000 7
Al 3.464342930 4.670404170 2.073760778 CORE 8 Al Al 0.0000 8
Al 5.288057775 8.892282876 2.229065870 CORE 9 Al Al 0.0000 9
Al 1.160687138 9.281508507 4.356951197 CORE 10 Al Al 0.0000 10
Al 3.618645640 7.238552672 7.560829981 CORE 11 Al Al 0.0000 11
Al 9.262223722 7.520309734 9.508101929 CORE 12 Al Al 0.0000 12
O 4.893558084 7.840478948 0.920346482 CORE 13 O O 0.0000 13
O 4.933221299 5.192349119 1.029280245 CORE 14 O O 0.0000 14
O 9.651514930 0.463867153 1.051881996 CORE 15 O O 0.0000 15
O 2.074007957 4.845645382 1.062374863 CORE 16 O O 0.0000 16
O 2.678770443 1.085197084 1.046840754 CORE 17 O O 0.0000 17
O 8.885107104 7.548460489 1.455449105 CORE 18 O O 0.0000 18
O 5.011025966 0.597284650 2.291724255 CORE 19 O O 0.0000 19
O 3.934222430 3.041709900 2.430746998 CORE 20 O O 0.0000 20
O 6.976163394 9.117587269 2.519532692 CORE 21 O O 0.0000 21
O -0.313019281 9.123913083 3.482177371 CORE 22 O O 0.0000 22
O 3.447830722 5.647440047 3.492892255 CORE 23 O O 0.0000 23
O 2.776548317 1.081069004 3.705763483 CORE 24 O O 0.0000 24
O 4.876133867 7.892784772 3.794602530 CORE 25 O O 0.0000 25
O 2.238307783 7.961553929 4.074090400 CORE 26 O O 0.0000 26
O 3.811527564 6.743147051 5.906031940 CORE 27 O O 0.0000 27
O 0.957639950 9.753710343 6.014246978 CORE 28 O O 0.0000 28
O 2.633565709 8.636082965 7.803104370 CORE 29 O O 0.0000 29
O 2.601340384 5.746626478 8.148045913 CORE 30 O O 0.0000 30
O 9.801308689 8.632989906 8.303276775 CORE 31 O O 0.0000 31
O 2.039971422 1.241313525 8.272104120 CORE 32 O O 0.0000 32
O 5.087740289 7.217920270 8.442732516 CORE 33 O O 0.0000 33
O 1.571784800 3.667601065 9.385396771 CORE 34 O O 0.0000 34
O 7.573626290 7.193547391 9.459501353 CORE 35 O O 0.0000 35
O 0.414644078 6.076630459 9.668897555 CORE 36 O O 0.0000 36
H 5.646155941 4.539415297 1.005724370 CORE 37 H H 0.0000 37
H 9.416987519 6.990898718 2.041626795 CORE 38 H H 0.0000 38
H 5.637676869 7.793644080 4.381801361 CORE 39 H H 0.0000 39
H 2.855892978 1.798562391 4.347223410 CORE 40 H H 0.0000 40
H 2.456476704 5.134148961 7.414628069 CORE 41 H H 0.0000 41
H 1.969691021 1.917989569 7.585874911 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 5.5 for AlPO

!BIOSYM archive 2
PBC=ON

Energy 0 0.0196 -233.946437 R-3

!DATE

PBC 9.46367740 9.46339346 9.46311034 95.20810929 84.80343596 84.77524030

P 3.299000200 3.169827545 0.701017403 CORE 1 P P 0.0000 1

P 5.829700885 8.368604105 0.732090461 CORE 2 P P 0.0000 2

P 7.956390326 5.028628485 2.866334973 CORE 3 P P 0.0000 3

P 9.624443067 0.804156693 2.895169915 CORE 4 P P 0.0000 4

P 5.570001366 0.573537503 4.930268607 CORE 5 P P 0.0000 5

P 8.208085653 2.458857281 8.043595034 CORE 6 P P 0.0000 6

Al 5.673675682 5.234000082 0.684216385 CORE 7 Al Al 0.0000 7

Al 9.627405604 3.206412852 0.836704352 CORE 8 Al Al 0.0000 8

Al 3.295863636 0.767909218 2.761157607 CORE 9 Al Al 0.0000 9

Al 8.110133014 8.163271995 2.913104193 CORE 10 Al Al 0.0000 10

Al 7.961387935 2.641603645 4.921182135 CORE 11 Al Al 0.0000 11

Al 5.819439953 0.390362019 8.052828767 CORE 12 Al Al 0.0000 12

O 5.429403634 6.936489323 0.376488664 CORE 13 O O 0.0000 13

O 1.836385707 3.548048431 0.464504050 CORE 14 O O 0.0000 14

O 4.117225612 4.453924645 0.842120766 CORE 15 O O 0.0000 15

O 7.208770970 8.379260443 1.416579415 CORE 16 O O 0.0000 16

O 9.491833177 1.626337619 1.600175465 CORE 17 O O 0.0000 17

O 4.771160563 8.958706783 1.675424228 CORE 18 O O 0.0000 18

O 9.018115812 4.438676317 1.926096991 CORE 19 O O 0.0000 19

O 3.431559905 2.346508482 1.995007375 CORE 20 O O 0.0000 20

O 6.579189065 5.016425152 2.178010030 CORE 21 O O 0.0000 21

O 9.665744659 8.945257277 2.757096415 CORE 22 O O 0.0000 22

O 1.622885601 0.424102176 3.130274203 CORE 23 O O 0.0000 23

O 8.354905047 6.461063025 3.222477054 CORE 24 O O 0.0000 24

O 9.128276091 1.627784608 4.092706351 CORE 25 O O 0.0000 25

O 7.876548295 4.210906675 4.155945984 CORE 26 O O 0.0000 26

O 7.211034500 8.865546734 4.244897812 CORE 27 O O 0.0000 27

O 4.217872434 0.777327468 4.246214728 CORE 28 O O 0.0000 28

O 6.373129524 1.885102329 4.855593577 CORE 29 O O 0.0000 29

O 5.323725077 0.188620324 6.389534749 CORE 30 O O 0.0000 30

O 8.456690338 2.843072383 6.584684323 CORE 31 O O 0.0000 31

O 7.408852649 1.144786045 8.117277345 CORE 32 O O 0.0000 32

O 9.559259843 2.259764975 8.731133384 CORE 33 O O 0.0000 33

O 7.423915413 3.589153684 8.726274431 CORE 34 O O 0.0000 34

O 6.763782477 8.245820207 8.819586404 CORE 35 O O 0.0000 35

O 4.654632300 1.407611259 8.880000259 CORE 36 O O 0.0000 36

end

end

GM in Table S6 at r_s = 5.5 for SiO_2

!BIOSYM archive 2

PBC=ON

Energy 0 0.0186 -248.934270 P1

!DATE

PBC 9.61079757 9.60093444 9.47763182 75.08307414 101.80313751 98.34039342

Si 6.692845023 6.980731902 0.202613228 CORE 1 Si Si 0.0000 1

Si 6.744352012 4.095022158 1.131581386 CORE 2 Si Si 0.0000 2

Si 4.658490169 1.964792127 1.145722852 CORE 3 Si Si 0.0000 3

Si 7.843810634 9.420684167 1.511560800 CORE 4 Si Si 0.0000 4

Si 6.123211148 2.568765924 3.618232439 CORE 5 Si Si 0.0000 5

Si 7.024896676 10.080205841 4.407079750 CORE 6 Si Si 0.0000 6

Si 6.101509966 3.359398336 6.600152193 CORE 7 Si Si 0.0000 7

Si -0.661145289 1.939331982 6.843427618 CORE 8 Si Si 0.0000 8

Si 6.840268320 8.671604132 7.043500174 CORE 9 Si Si 0.0000 9

Si 7.192868209 5.838703122 8.100512422 CORE 10 Si Si 0.0000 10

Si -0.159303848 3.844405975 8.987953862 CORE 11 Si Si 0.0000 11

Si 4.702054443 2.233115577 8.998435487 CORE 12 Si Si 0.0000 12
O 8.152741437 3.898638050 0.354409818 CORE 13 O O 0.0000 13
O 5.580203015 3.149273697 0.481347448 CORE 14 O O 0.0000 14
O 5.231406548 0.520029042 0.630209633 CORE 15 O O 0.0000 15
O 3.119965870 2.141137315 0.720594036 CORE 16 O O 0.0000 16
O 7.889702137 0.631529951 0.894849589 CORE 17 O O 0.0000 17
O 0.953632104 0.647727770 0.938622757 CORE 18 O O 0.0000 18
O 6.284878434 5.653165261 1.042348582 CORE 19 O O 0.0000 19
O 7.789079646 7.843829828 1.072308797 CORE 20 O O 0.0000 20
O 6.933420886 3.659926623 2.699989980 CORE 21 O O 0.0000 21
O 4.804325576 2.093774992 2.775383973 CORE 22 O O 0.0000 22
O -1.742583591 9.544243373 3.132633741 CORE 23 O O 0.0000 23
O 7.028854109 1.246725241 3.897509200 CORE 24 O O 0.0000 24
O 5.710180026 3.261183768 5.028731526 CORE 25 O O 0.0000 25
O -0.328638682 1.708017493 5.251249657 CORE 26 O O 0.0000 26
O 6.683315360 8.831338131 5.417131880 CORE 27 O O 0.0000 27
O 7.377425484 2.399738491 6.952413216 CORE 28 O O 0.0000 28
O 6.464747514 4.901189204 6.978980743 CORE 29 O O 0.0000 29
O -2.046933416 7.270930283 7.412363529 CORE 30 O O 0.0000 30
O 4.840699225 2.838238330 7.491343514 CORE 31 O O 0.0000 31
O -1.901034693 9.966465632 7.553274674 CORE 32 O O 0.0000 32
O 0.246305514 3.042066871 7.605809464 CORE 33 O O 0.0000 33
O 5.377734897 8.719725592 7.776696866 CORE 34 O O 0.0000 34
O -1.049313331 5.145711543 8.617886388 CORE 35 O O 0.0000 35
O 3.434576703 10.101893904 8.983693525 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 5.5 for [$SiAlO_4H$]

!BIOSYM archive 2
PBC=ON
Energy 0 0.0156 -260.436460 P1
!DATE
PBC 9.71060826 9.63952645 9.84684184 85.59135311 84.82764195 92.86673729
Si 8.783622863 9.208849131 2.079585232 CORE 1 Si Si 0.0000 1
Si 3.708381515 1.652308072 2.179520051 CORE 2 Si Si 0.0000 2
Si 3.706381834 7.132129203 4.274701250 CORE 3 Si Si 0.0000 3
Si 1.548925943 9.518260673 7.375115398 CORE 4 Si Si 0.0000 4
Si 2.247431100 5.486853430 9.528853095 CORE 5 Si Si 0.0000 5
Si 6.235587049 7.608389331 9.614564441 CORE 6 Si Si 0.0000 6
Al 1.209326070 1.441324862 0.025659512 CORE 7 Al Al 0.0000 7
Al 3.447013780 4.915315103 1.963920102 CORE 8 Al Al 0.0000 8
Al 5.490405939 9.015950744 2.110810308 CORE 9 Al Al 0.0000 9
Al 1.457159440 9.494787703 4.168978014 CORE 10 Al Al 0.0000 10
Al 3.894605529 7.353158230 7.481712684 CORE 11 Al Al 0.0000 11
Al 9.480985514 7.811208300 9.425561047 CORE 12 Al Al 0.0000 12
O 2.906880498 1.098136923 0.648416368 CORE 13 O O 0.0000 13
O 4.947275627 8.029157927 0.794349289 CORE 14 O O 0.0000 14
O 4.837115219 5.389039909 0.754744262 CORE 15 O O 0.0000 15
O 9.750718441 0.654538887 0.978446037 CORE 16 O O 0.0000 16
O 1.922822903 5.235594662 1.159267296 CORE 17 O O 0.0000 17
O 9.166162855 7.646413136 1.284466778 CORE 18 O O 0.0000 18
O 3.829081444 3.229058364 1.966395161 CORE 19 O O 0.0000 19
O 7.200475180 9.166651029 2.221466490 CORE 20 O O 0.0000 20
O 5.110263998 0.888981484 2.126178650 CORE 21 O O 0.0000 21
O 2.678972503 1.214979725 3.307159373 CORE 22 O O 0.0000 22
O 3.713303611 5.777160868 3.414406241 CORE 23 O O 0.0000 23
O -0.095933628 9.155546792 3.421094164 CORE 24 O O 0.0000 24
O 5.109165075 8.053965618 3.663487335 CORE 25 O O 0.0000 25

O 2.443735964 8.060329452 3.967321810 CORE 26 O O 0.0000 26
O 4.115252564 6.959020495 5.802808139 CORE 27 O O 0.0000 27
O 1.245217647 9.897246278 5.864902307 CORE 28 O O 0.0000 28
O 2.950744058 8.835690095 7.715698414 CORE 29 O O 0.0000 29
O 2.155476539 1.529474059 8.107626622 CORE 30 O O 0.0000 30
O 5.463828179 7.555067454 8.231647309 CORE 31 O O 0.0000 31
O 10.041203497 8.852916853 8.200375174 CORE 32 O O 0.0000 32
O 3.017669389 6.026308751 8.260663395 CORE 33 O O 0.0000 33
O 0.593966667 6.159581360 9.456756936 CORE 34 O O 0.0000 34
O 7.832900198 7.376048565 9.495545934 CORE 35 O O 0.0000 35
O 1.882628966 3.919217887 9.507902593 CORE 36 O O 0.0000 36
H 3.479162410 0.507295142 0.132877206 CORE 37 H H 0.0000 37
H 5.317114568 4.589546479 0.497230871 CORE 38 H H 0.0000 38
H 0.045184490 7.084265341 1.812953014 CORE 39 H H 0.0000 39
H 5.785486451 8.101003331 4.353978957 CORE 40 H H 0.0000 40
H 2.199030614 2.194693842 7.404355477 CORE 41 H H 0.0000 41
H 9.664990274 5.434776291 9.428408407 CORE 42 H H 0.0000 42
end
end

GM in Table S6 at r_s = 6 for AlPO

!BIOSYM archive 2
PBC=ON
Energy 0 0.0223 -226.463767 P1
!DATE
PBC 9.84608346 9.72782226 7.75839768 94.09699209 95.06147270 74.66497536
P 2.121438358 5.271651315 1.469247618 CORE 1 P P 0.0000 1
P 6.093656679 2.174456320 3.262766065 CORE 2 P P 0.0000 2
P 7.199452185 4.724575606 2.745367255 CORE 3 P P 0.0000 3
P 5.274224290 5.647434497 6.090573685 CORE 4 P P 0.0000 4
P 9.646544794 4.179714867 7.089236965 CORE 5 P P 0.0000 5
P 3.639854635 1.305965398 7.109732847 CORE 6 P P 0.0000 6
Al 10.063993662 7.390217362 0.510062411 CORE 7 Al Al 0.0000 7
Al 6.514451004 0.327838474 0.893274772 CORE 8 Al Al 0.0000 8
Al 4.275840046 4.563704129 3.499037684 CORE 9 Al Al 0.0000 9
Al 7.246371472 3.507207241 5.541496036 CORE 10 Al Al 0.0000 10
Al 6.179059782 7.639283716 7.126382535 CORE 11 Al Al 0.0000 11
Al 2.506622211 3.417804680 7.002375914 CORE 12 Al Al 0.0000 12
O 8.288747271 8.090744366 0.451063954 CORE 13 O O 0.0000 13
O 3.408812885 2.399939367 0.438125658 CORE 14 O O 0.0000 14
O 5.101102575 1.171832537 7.554987947 CORE 15 O O 0.0000 15
O 10.839274298 4.237097875 0.877658257 CORE 16 O O 0.0000 16
O 3.211370859 5.238074062 0.375717112 CORE 17 O O 0.0000 17
O 10.627846011 9.025823830 0.567236004 CORE 18 O O 0.0000 18
O 11.232638922 6.577673160 1.644665938 CORE 19 O O 0.0000 19
O 6.031859077 0.834320447 2.549582556 CORE 20 O O 0.0000 20
O 2.674127313 4.739095211 2.774642614 CORE 21 O O 0.0000 21
O 6.983629421 3.112403071 2.311966417 CORE 22 O O 0.0000 22
O 8.111825652 5.373303502 1.796774564 CORE 23 O O 0.0000 23
O 5.731986341 5.265431649 2.775133094 CORE 24 O O 0.0000 24
O 4.723859894 2.841247731 3.429642010 CORE 25 O O 0.0000 25
O 6.778505227 2.052027323 4.636374991 CORE 26 O O 0.0000 26
O 7.719916594 4.572554107 4.203836273 CORE 27 O O 0.0000 27
O 4.105511752 5.336828216 5.109773230 CORE 28 O O 0.0000 28
O 6.324720614 6.684497124 5.569062558 CORE 29 O O 0.0000 29
O 5.921524481 4.282837173 6.399752395 CORE 30 O O 0.0000 30
O 8.468015074 3.286406668 6.782035485 CORE 31 O O 0.0000 31
O 0.981237701 3.770852966 6.190136710 CORE 32 O O 0.0000 32
O 3.525663282 2.354621568 5.958392329 CORE 33 O O 0.0000 33

O 4.828436167 6.400763914 7.379481829 CORE 34 O O 0.0000 34
O 3.083182730 -0.090509204 6.765394918 CORE 35 O O 0.0000 35
O 9.350544322 5.671833751 7.003406002 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 6 for SiO_2

!BIOSYM archive 2
PBC=ON
Energy 0 0.0187 -246.346128 Imcm
!DATE
PBC 10.50835871 12.16180885 12.16190514 96.58685114 64.45689745 115.54318287
Si 3.641919597 2.606126338 0.987342406 CORE 1 Si Si 0.0000 1
Si 6.544843587 2.614907548 0.989366599 CORE 2 Si Si 0.0000 2
Si 1.290952852 4.046928902 2.301168592 CORE 3 Si Si 0.0000 3
Si 8.895795782 4.049613440 2.309823993 CORE 4 Si Si 0.0000 4
Si -0.155760638 6.608532411 2.635572524 CORE 5 Si Si 0.0000 5
Si -0.152296665 8.942846922 2.930151281 CORE 6 Si Si 0.0000 6
Si 6.547539737 0.529075790 3.255681546 CORE 7 Si Si 0.0000 7
Si 3.644643168 0.531272094 3.263802119 CORE 8 Si Si 0.0000 8
Si 8.898487508 1.964110436 4.575874951 CORE 9 Si Si 0.0000 9
Si 11.801992760 1.972468762 4.577311007 CORE 10 Si Si 0.0000 10
Si 10.345894792 2.521108112 7.097975374 CORE 11 Si Si 0.0000 11
Si 10.342469702 3.018188172 9.397768246 CORE 12 Si Si 0.0000 12
O 2.463129504 3.692287857 1.236961872 CORE 13 O O 0.0000 13
O 7.717819621 3.705675203 1.249227796 CORE 14 O O 0.0000 14
O 5.091076991 3.218799646 1.460901153 CORE 15 O O 0.0000 15
O -0.161082516 7.923695083 1.609540416 CORE 16 O O 0.0000 16
O -0.163123692 3.523839418 1.741681708 CORE 17 O O 0.0000 17
O 6.854892847 1.243915101 1.820359480 CORE 18 O O 0.0000 18
O 3.334680321 1.238786935 1.825163968 CORE 19 O O 0.0000 19
O 1.178508394 5.669055492 2.498491676 CORE 20 O O 0.0000 20
O 9.015200114 5.670494406 2.515063063 CORE 21 O O 0.0000 21
O 1.184662989 9.881178869 3.050405004 CORE 22 O O 0.0000 22
O -1.486976661 9.882108482 3.066528428 CORE 23 O O 0.0000 23
O 1.601751645 3.339485985 3.739615711 CORE 24 O O 0.0000 24
O 8.587835188 3.335200324 3.745088143 CORE 25 O O 0.0000 25
O 5.098053805 1.054141623 3.824282165 CORE 26 O O 0.0000 26
O -0.146962693 7.627693656 3.956140558 CORE 27 O O 0.0000 27
O 10.352295783 1.360665238 4.103470377 CORE 28 O O 0.0000 28
O 7.726102583 0.873187216 4.316078963 CORE 29 O O 0.0000 29
O 2.471361120 0.885388878 4.327248694 CORE 30 O O 0.0000 30
O 9.011292992 2.302786493 6.174345263 CORE 31 O O 0.0000 31
O 11.682969879 2.318982642 6.173788331 CORE 32 O O 0.0000 32
O 10.337175616 3.925599159 7.998139108 CORE 33 O O 0.0000 33
O 10.351330984 1.613691970 8.497706544 CORE 34 O O 0.0000 34
O 9.005164756 3.219607921 10.321800013 CORE 35 O O 0.0000 35
O 11.676797750 3.236174493 10.321775184 CORE 36 O O 0.0000 36
end
end

GM in Table S6 at r_s = 6 for $[SiAlO_4H]$

!BIOSYM archive 2
PBC=ON
Energy 0 0.0195 -257.852563 P1
!DATE
PBC 11.84170195 11.05201134 10.42549716 76.32327342 86.20064015 70.38058647
Si 7.282362987 1.608661769 0.725737376 CORE 1 Si Si 0.0000 1
Si 1.842491107 1.339215197 1.118395832 CORE 2 Si Si 0.0000 2
Si 4.700715072 1.177998204 1.912215330 CORE 3 Si Si 0.0000 3

Si 11.436961430 3.264546463 2.059512343 CORE 4 Si Si 0.0000 4
Si 10.744200958 10.860381258 3.456054088 CORE 5 Si Si 0.0000 5
Si 9.315210466 9.452970858 9.593010325 CORE 6 Si Si 0.0000 6
Al 9.036054422 4.080355898 0.318401958 CORE 7 Al Al 0.0000 7
Al 6.975798111 9.309612080 0.372359584 CORE 8 Al Al 0.0000 8
Al 10.158362872 9.218113464 1.126977370 CORE 9 Al Al 0.0000 9
Al 8.661430132 3.139054374 3.298480273 CORE 10 Al Al 0.0000 10
Al 7.225095282 2.158467591 5.762186811 CORE 11 Al Al 0.0000 11
Al 9.176893782 11.754284343 7.670967830 CORE 12 Al Al 0.0000 12
O 7.242978989 7.633535849 0.198513349 CORE 13 O O 0.0000 13
O 7.281370023 0.075320318 0.182295941 CORE 14 O O 0.0000 14
O 9.883439881 7.736953244 0.323049007 CORE 15 O O 0.0000 15
O 10.693562436 3.710324875 0.686383131 CORE 16 O O 0.0000 16
O 5.585803495 10.133325956 0.971366280 CORE 17 O O 0.0000 17
O 5.691155927 2.044990253 0.937416357 CORE 18 O O 0.0000 18
O 8.423515946 10.016775625 1.269631987 CORE 19 O O 0.0000 19
O 12.367767047 1.929632556 1.786179334 CORE 20 O O 0.0000 20
O 8.260264516 4.369087729 2.018189713 CORE 21 O O 0.0000 21
O 3.204182688 1.752858426 2.003043490 CORE 22 O O 0.0000 22
O 7.838245090 1.600003562 2.414888780 CORE 23 O O 0.0000 23
O 12.485036988 4.424255212 2.573526064 CORE 24 O O 0.0000 24
O 10.796179718 9.417698443 2.759310681 CORE 25 O O 0.0000 25
O 10.352144853 2.872987728 3.204828372 CORE 26 O O 0.0000 26
O 5.443949111 1.027005286 3.379026962 CORE 27 O O 0.0000 27
O 7.867970493 3.400471881 4.806133103 CORE 28 O O 0.0000 28
O 11.314525736 11.052498939 4.935520829 CORE 29 O O 0.0000 29
O 5.364283729 1.940053775 5.985692617 CORE 30 O O 0.0000 30
O 7.123848773 2.133386265 7.579392037 CORE 31 O O 0.0000 31
O 9.315674857 10.121809934 8.092544771 CORE 32 O O 0.0000 32
O 8.009649245 12.467888743 8.813520116 CORE 33 O O 0.0000 33
O 9.384142609 7.860227155 9.533410803 CORE 34 O O 0.0000 34
O 2.796925614 4.308528889 9.712032306 CORE 35 O O 0.0000 35
O 8.824391694 5.004352498 10.004165998 CORE 36 O O 0.0000 36
H 7.977775733 5.268635624 2.220023319 CORE 37 H H 0.0000 37
H 12.246623088 5.330869268 2.360993410 CORE 38 H H 0.0000 38
H 4.848299350 1.644456271 5.221319198 CORE 39 H H 0.0000 39
H 7.744666596 2.243823252 8.318344418 CORE 40 H H 0.0000 40
H 3.849083619 2.916668256 8.713078480 CORE 41 H H 0.0000 41
H 2.162388704 4.939985304 9.356186147 CORE 42 H H 0.0000 42
end
end

The structure of $Si_6Al_6O_{24}Na_6(H_2O)_6$

!BIOSYM archive 2
PBC=ON
Energy 0 0.0261 -332.656975 P1
!DATE
PBC 9.32668567 9.51214518 9.67455313 88.61408154 85.52856948 94.49244790
Si 4.667621465 5.995760912 0.135386891 CORE 1 Si Si 0.0000 1
Si 7.942034386 8.434340094 2.277331787 CORE 2 Si Si 0.0000 2
Si 3.295922786 1.011016857 2.551828715 CORE 3 Si Si 0.0000 3
Si 3.086644295 6.342549233 4.439490674 CORE 4 Si Si 0.0000 4
Si 0.952006696 8.362564361 7.626601652 CORE 5 Si Si 0.0000 5
Si 1.449907298 4.262468621 9.549187227 CORE 6 Si Si 0.0000 6
Al 0.865108724 0.861444233 0.415466394 CORE 7 Al Al 0.0000 7
Al 3.156851132 4.102803450 2.004471282 CORE 8 Al Al 0.0000 8
Al 4.636947996 8.132130482 2.424836226 CORE 9 Al Al 0.0000 9
Al 0.828816525 8.639729198 4.547481852 CORE 10 Al Al 0.0000 10
Al 3.173680951 6.094309194 7.498196746 CORE 11 Al Al 0.0000 11

```
Al      8.723743471     6.604476675     9.631042437 CORE    12 Al Al    0.0000    12
Na      3.056399634     3.301532300     4.995609109 CORE    13 Na Na    0.0000    13
Na      9.296619183     4.413968451     6.812958219 CORE    14 Na Na    0.0000    14
Na      6.426596359     8.021429000     4.914793325 CORE    15 Na Na    0.0000    15
Na      3.348049797     8.879071516     9.437116451 CORE    16 Na Na    0.0000    16
Na      6.537302974     3.493637760     0.501401779 CORE    17 Na Na    0.0000    17
Na      0.485547786     5.729834418     2.818113419 CORE    18 Na Na    0.0000    18
O       4.043024896     7.251905249     0.995953212 CORE    19 O  O     0.0000    19
O       4.450005349     4.568470112     0.914528134 CORE    20 O  O     0.0000    20
O       8.935213801     0.400292828     1.557898083 CORE    21 O  O     0.0000    21
O       1.580278345     4.228544668     1.237309672 CORE    22 O  O     0.0000    22
O       2.457544038     0.792242747     1.163847553 CORE    23 O  O     0.0000    23
O       8.580938495     7.209642961     1.378764249 CORE    24 O  O     0.0000    24
O       4.742582644     0.277955022     2.352596113 CORE    25 O  O     0.0000    25
O       3.569476133     2.599204215     2.802637467 CORE    26 O  O     0.0000    26
O       6.362762194     8.225781808     2.522375869 CORE    27 O  O     0.0000    27
O       8.597616893     8.367001661     3.773242146 CORE    28 O  O     0.0000    28
O       2.876018063     5.126454657     3.387116439 CORE    29 O  O     0.0000    29
O       2.497535476     0.460609724     3.856426312 CORE    30 O  O     0.0000    30
O       4.269615678     7.362517251     3.981422893 CORE    31 O  O     0.0000    31
O       1.626856495     7.075313087     4.504865842 CORE    32 O  O     0.0000    32
O       8.318838136     4.412252058     4.342500896 CORE    33 O  O     0.0000    33
O       7.057232575     2.267383334     2.468066967 CORE    34 O  O     0.0000    34
O       3.462674304     5.586444707     5.842728193 CORE    35 O  O     0.0000    35
O       0.443991875     9.072485781     6.231141949 CORE    36 O  O     0.0000    36
O       7.045453931     9.663337489     6.809197261 CORE    37 O  O     0.0000    37
O       7.061159378     6.251549498     6.411759905 CORE    38 O  O     0.0000    38
O       7.370480748     3.012231539     7.677450167 CORE    39 O  O     0.0000    39
O       2.444641121     7.703981305     7.546731133 CORE    40 O  O     0.0000    40
O       2.080735541     4.900980156     8.185552444 CORE    41 O  O     0.0000    41
O       9.159067951     7.224202445     8.023826995 CORE    42 O  O     0.0000    42
O       1.051297809     9.502561716     8.753908347 CORE    43 O  O     0.0000    43
O       4.733289389     6.250548989     8.295447433 CORE    44 O  O     0.0000    44
O       1.225787980     2.674421570     9.271705313 CORE    45 O  O     0.0000    45
O       7.007615829     6.448077873     9.563453683 CORE    46 O  O     0.0000    46
O       8.542394915     4.643948979     0.127531438 CORE    47 O  O     0.0000    47
O       1.459168075     2.443381834     6.475399823 CORE    48 O  O     0.0000    48
H       7.758286128     1.622322269     2.201915992 CORE    49 H  H     0.0000    49
H       7.596345742     4.962987349     4.687582867 CORE    50 H  H     0.0000    50
H       7.891639091     3.677643031     3.858094100 CORE    51 H  H     0.0000    51
H       6.266124665     1.711386871     2.612930101 CORE    52 H  H     0.0000    52
H       8.005232935     9.541243646     6.596684526 CORE    53 H  H     0.0000    53
H       7.756902168     6.668809751     6.974906962 CORE    54 H  H     0.0000    54
H       6.554016520     3.288756874     7.237806780 CORE    55 H  H     0.0000    55
H       7.512942773     2.082347468     7.399297774 CORE    56 H  H     0.0000    56
H       6.928600373     9.146965896     7.621434554 CORE    57 H  H     0.0000    57
H       6.287831462     6.158315078     7.009249689 CORE    58 H  H     0.0000    58
H       1.345103226     1.488091242     6.285001608 CORE    59 H  H     0.0000    59
H       1.542070794     2.469141937     7.457498203 CORE    60 H  H     0.0000    60
end
end
```