Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

Understanding Formation Thermodynamics of Structurally Diverse Zeolite Oligomers with First Principles Calculations

Sungil Hong[1], Adam J. Mallette[2], James J. Neeway[3], Radha Kishan Motkuri[3], Jeffrey D. Rimer[2], and Giannis Mpourmpakis[1,*]

[1]Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, 15261, USA.

[2]Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, 77204, USA

[3]Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, WA, 99352, USA

Corresponding author's e-mail: gmpourmp@pitt.edu

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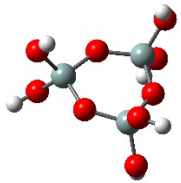
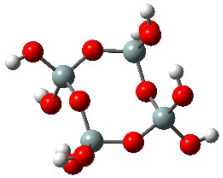
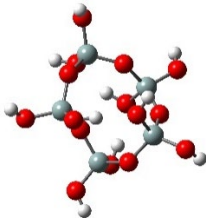
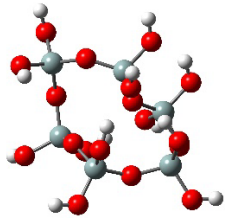
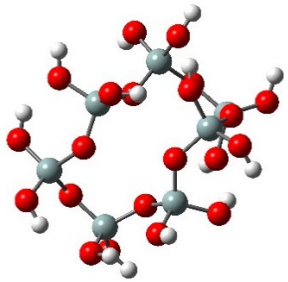
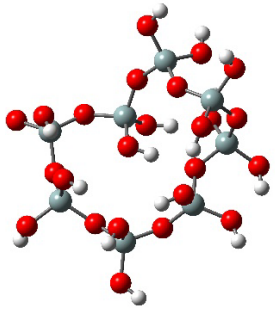
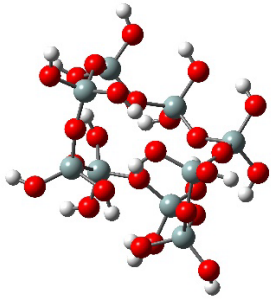
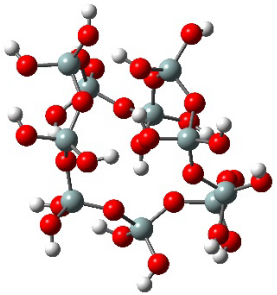
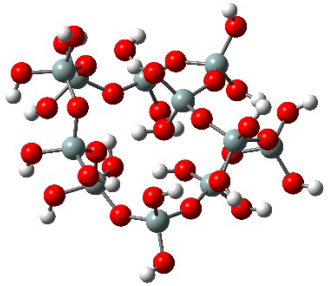
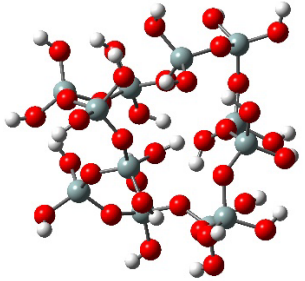
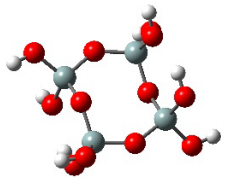
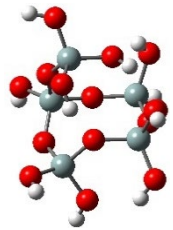
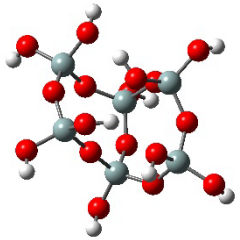
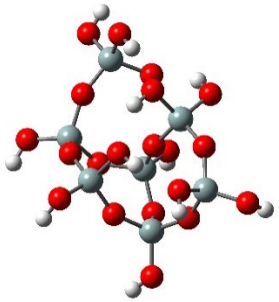
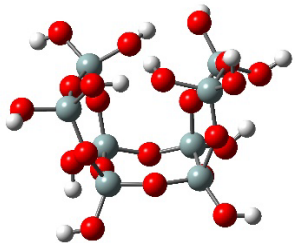
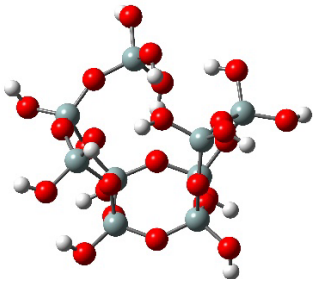
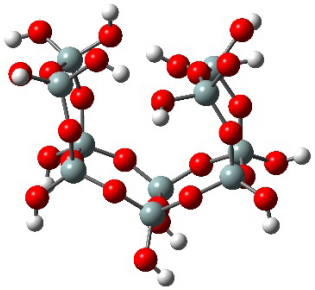
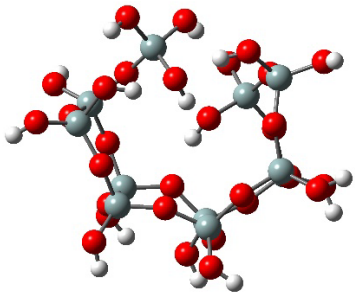
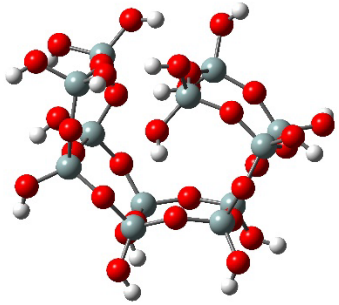
Table S1. Full list of pure-silicate monocycles, multicycles and cages with optimized molecular structures (grey ball = Si, red ball = O, and white ball = H).

Mono-cycles	**Name**	3MR	4MR	5MR	6MR
	Structure	 $Si_3O_9H_6$	 $Si_4O_{12}H_8$	 $Si_5O_{15}H_{10}$	 $Si_6O_{18}H_{12}$
	Name	7MR	8MR	9MR	
	Structure	 $Si_7O_{21}H_{14}$	 $Si_8O_{24}H_{16}$	 $Si_9O_{27}H_{18}$	
	Name	10MR	11MR	12MR	
	Structure	 $Si_{10}O_{30}H_{20}$	 $Si_{11}O_{33}H_{22}$	 $Si_{12}O_{36}H_{24}$	

Multi-cycles	**Name**	Mono-ring	Branched mono-ring	Di-ring
	Structure	 $Si_4O_{12}H_8$	 $Si_5O_{15}H_{10}$	 $Si_6O_{17}H_{10}$
	Name	Branched di-ring	Tri-ring	Branched tri-ring
	Structure	 $Si_7O_{20}H_{12}$	 $Si_8O_{22}H_{12}$	 $Si_9O_{25}H_{14}$
	Name	Tetra-ring	Branched tetra-ring	Penta-ring
	Structure	 $Si_{10}O_{27}H_{14}$	 $Si_{11}O_{30}H_{16}$	 $Si_{12}O_{32}H_{16}$

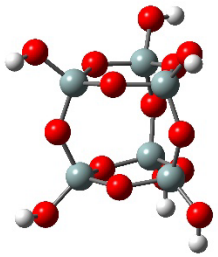
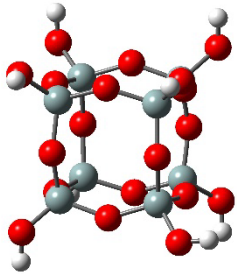
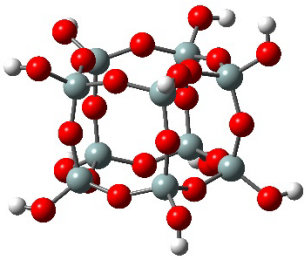
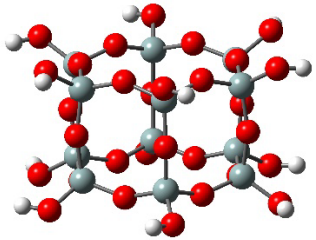
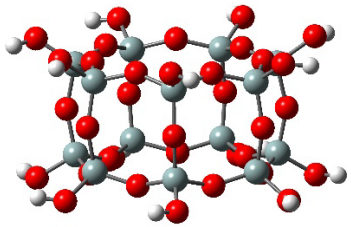
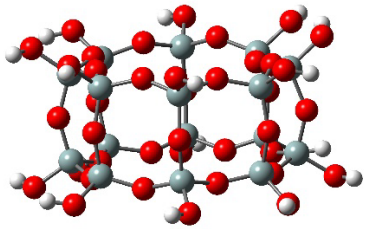
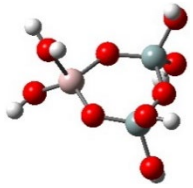
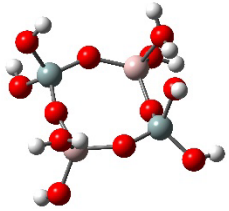
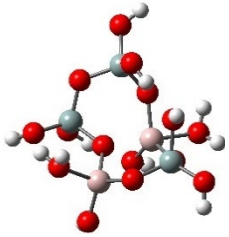
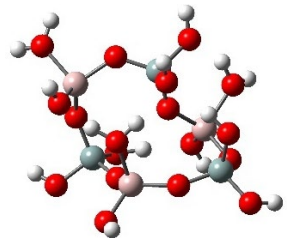
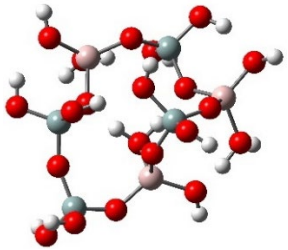
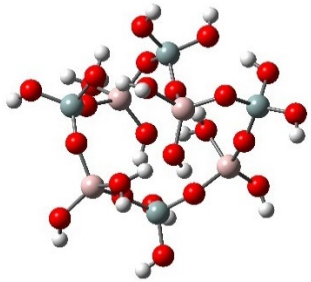
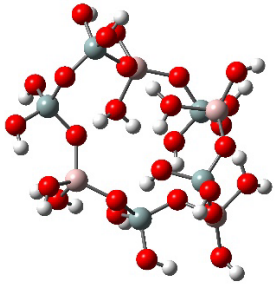
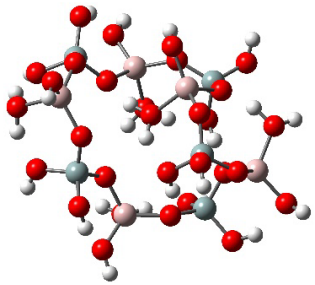
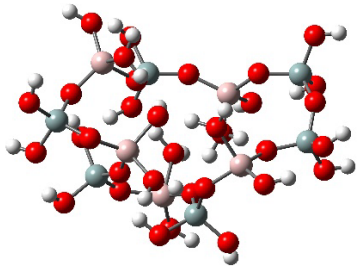
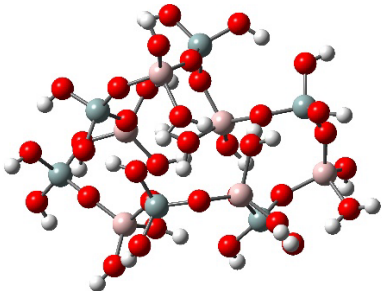
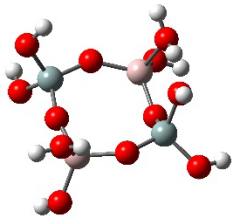
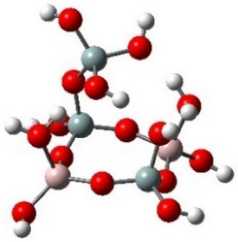
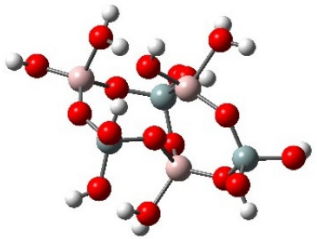
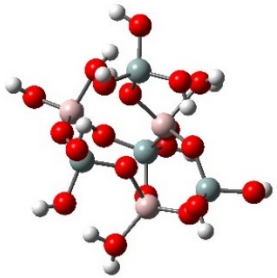
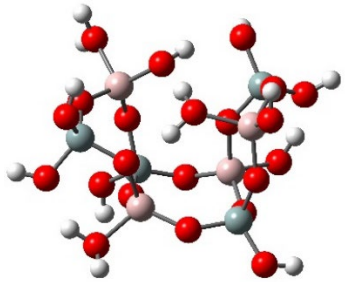
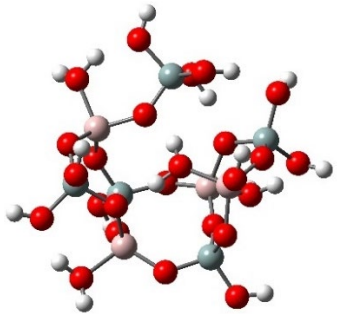
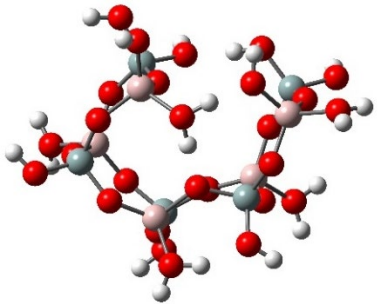
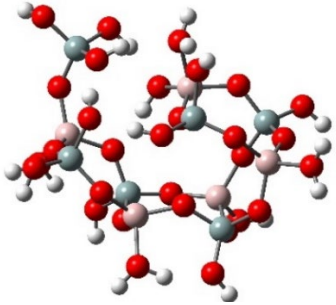
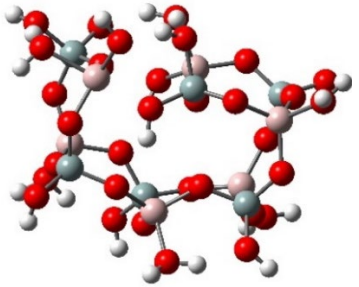
Cages	**Name**	Trigonal prism	Tetragonal prism	Pentagonal prism
	Structure	 $Si_6O_{15}H_6$	 $Si_8O_{20}H_8$	 $Si_{10}O_{25}H_{10}$
	Name	Hexagonal prism	Heptagonal prism	Octagonal prism
	Structure	 $Si_{12}O_{30}H_{12}$	 $Si_{14}O_{35}H_{14}$	 $Si_{16}O_{40}H_{16}$

Table S2. Full list of aluminosilicate monocycles, multicycles, and cages with optimized molecular structures (grey ball = Si, pink ball = Al, red ball = O, and white ball = H).

Mono-cycles	**Name**	3MR	4MR	5MR	6MR
	Structure	 $Si_2Al_1O_9H_7$	 $Si_2Al_2O_{12}H_{10}$	 $Si_3Al_2O_{15}H_{12}$	 $Si_3Al_3O_{18}H_{15}$
	Name	7MR	8MR	9MR	
	Structure	 $Si_4Al_3O_{21}H_{17}$	 $Si_4Al_4O_{24}H_{20}$	 $Si_5Al_4O_{27}H_{22}$	
	Name	10MR	11MR	12MR	
	Structure	 $Si_5Al_5O_{30}H_{25}$	 $Si_6Al_5O_{33}H_{27}$	 $Si_6Al_6O_{36}H_{30}$	

Multi-cycles	**Name**	Mono-ring	Branched mono-ring	Di-ring
	Structure	 $Si_2Al_2O_{12}H_{10}$	 $Si_3Al_2O_{15}H_{12}$	 $Si_3Al_3O_{17}H_{13}$
	Name	Branched di-ring	Tri-ring	Branched tri-ring
	Structure	 $Si_4Al_3O_{20}H_{15}$	 $Si_4Al_4O_{22}H_{16}$	 $Si_5Al_4O_{25}H_{18}$
	Name	Tetra-ring	Branched tetra-ring	Penta-ring
	Structure	 $Si_5Al_5O_{27}H_{19}$	 $Si_6Al_5O_{30}H_{21}$	 $Si_6Al_6O_{32}H_{22}$

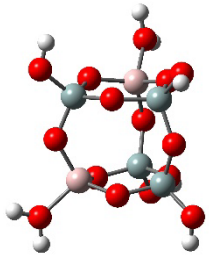
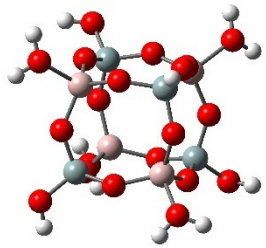
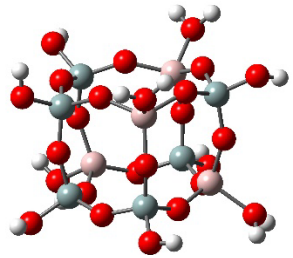
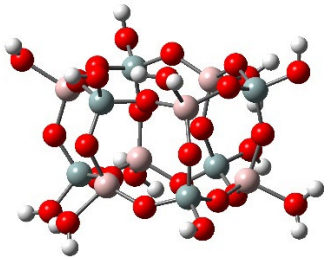
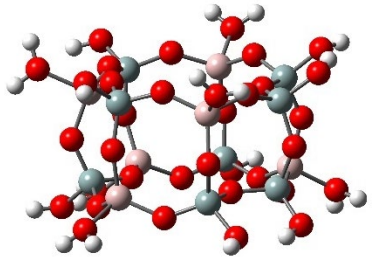
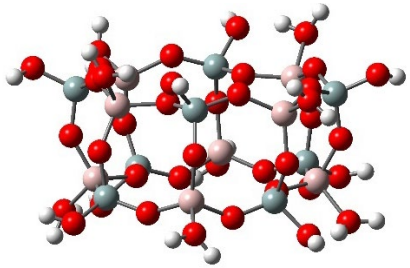
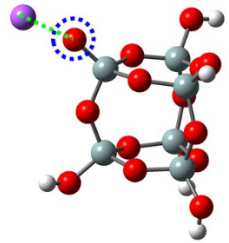
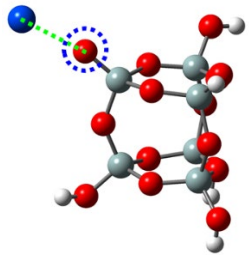
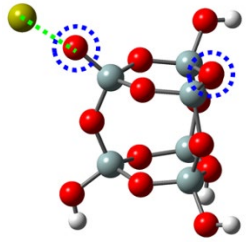
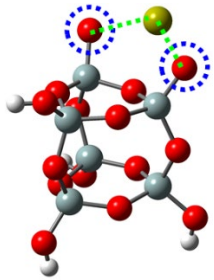
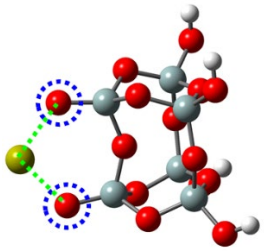
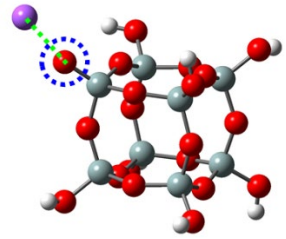
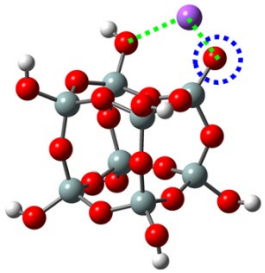
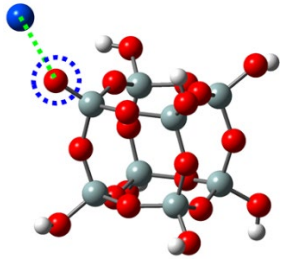
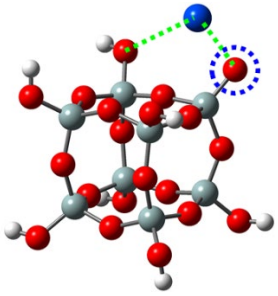
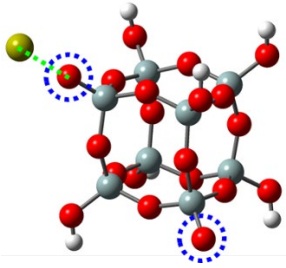
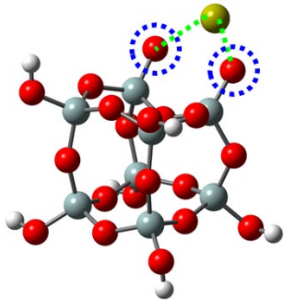
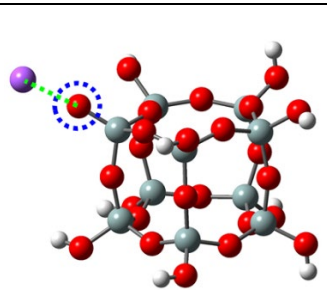
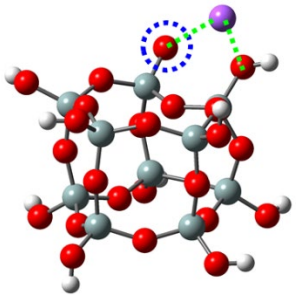
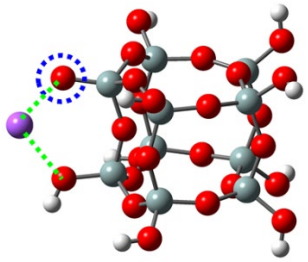
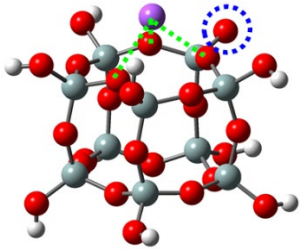
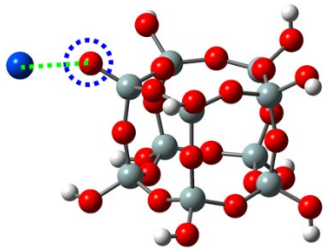
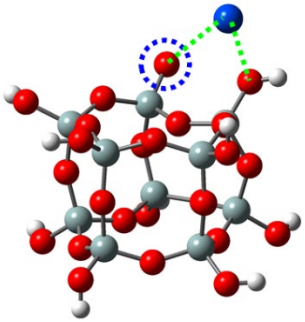
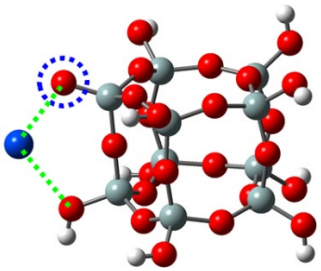
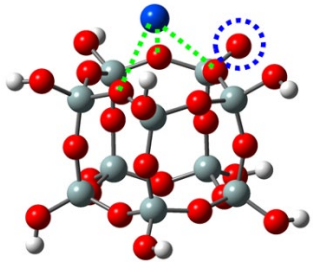
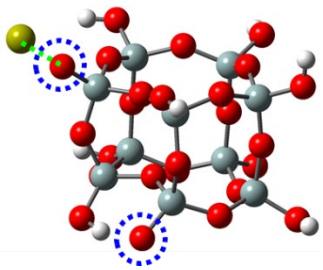
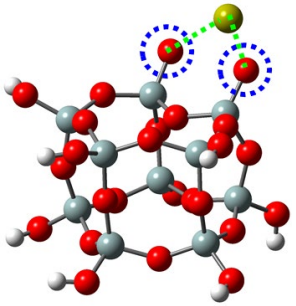
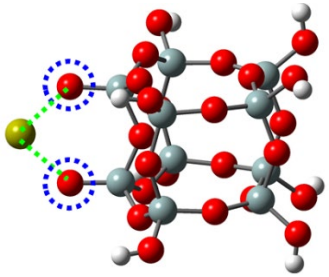
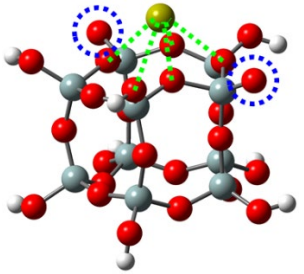
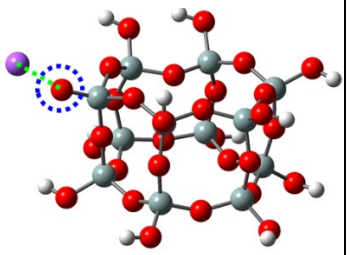
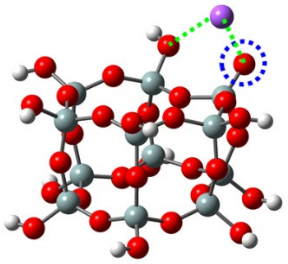
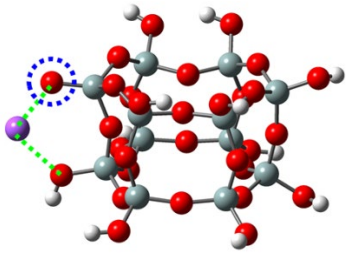
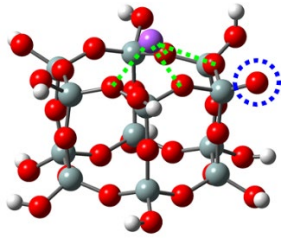
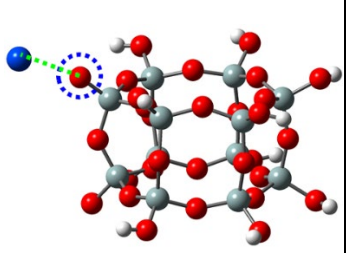
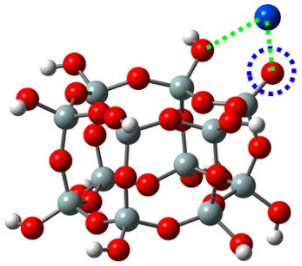
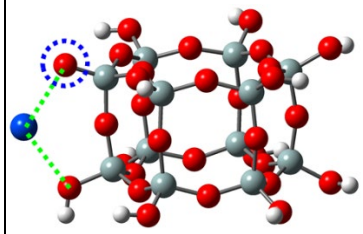
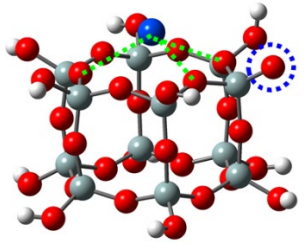
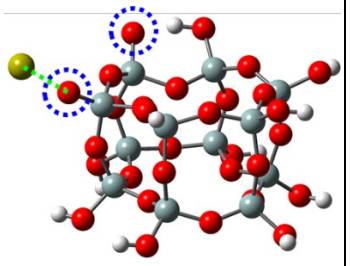
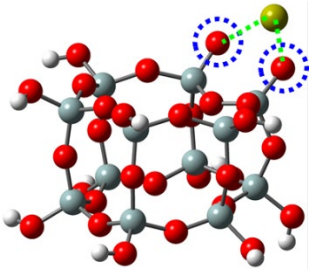
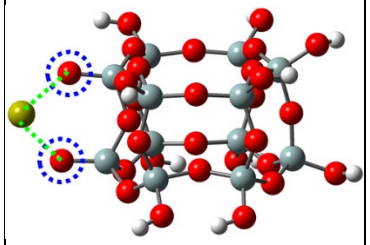
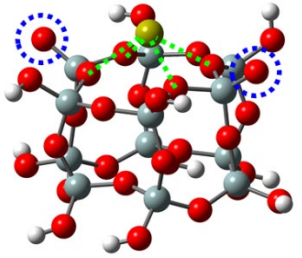
Cages	**Name**	Trigonal prism	Tetragonal prism	Pentagonal prism
	Structure	 $Si_4Al_2O_{15}H_8$	 $Si_4Al_4O_{20}H_{12}$	 $Si_6Al_4O_{25}H_{14}$
	Name	Hexagonal prism	Heptagonal prism	Octagonal prism
	Structure	 $Si_6Al_6O_{30}H_{18}$	 $Si_8Al_6O_{35}H_{20}$	 $Si_8Al_8O_{40}H_{24}$

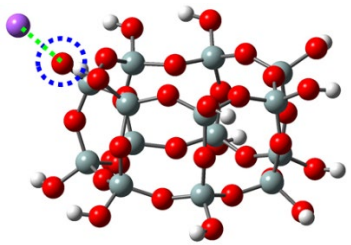
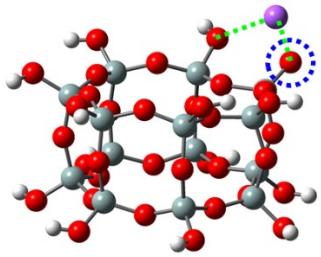
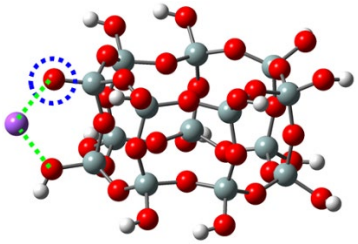
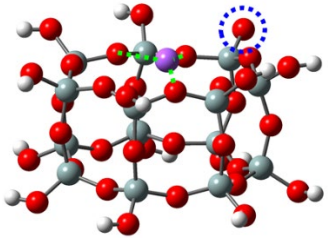
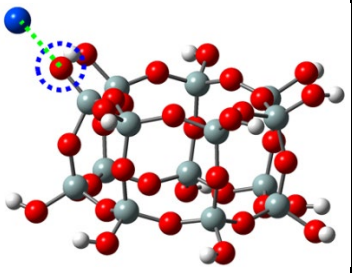
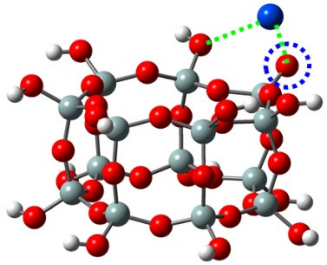
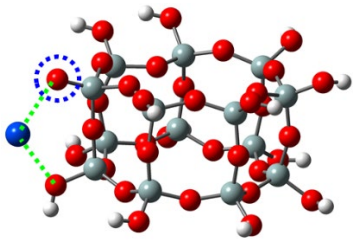
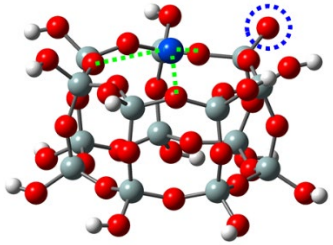
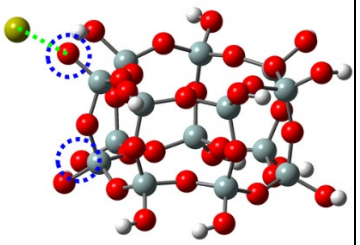
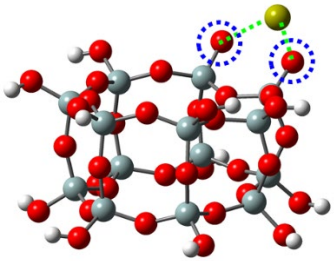
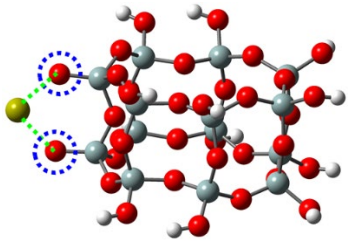
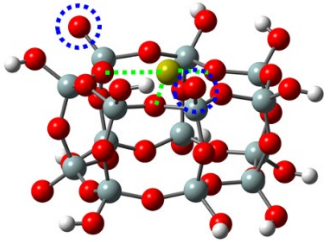
Table S3. Optimized molecular structures of pure-silicate cages with an external cation (grey ball = Si, red = O, white = H, purple = Na, blue = K, and yellow = Ca). The oxygen sites from which a proton is removed to maintain overall charge neutrality are highlighted with blue dotted circles. The green dotted lines connect the cations with the oxygen atoms that they electrostatically interact with. Blank cells indicate that the cation located at the corresponding position moved to a different position during optimization.

Trigonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^+		•	•	•	•
K^+		•	•	•	•
Ca^{2+}				•	•

Tetragonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^+			(Same with top edge)	•	•
K^+			(Same with top edge)	•	•
Ca^{2+}			(Same with top edge)	•	•

Pentagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}					•
K^{+}					•
Ca^{2+}					•

Hexagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}					•
K^{+}					•
Ca^{2+}					•

Heptagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}					•
K^{+}					•
Ca^{2+}					•

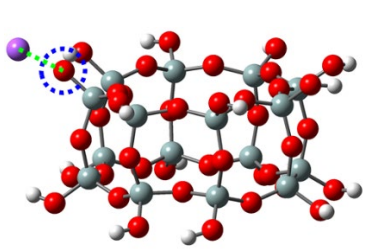
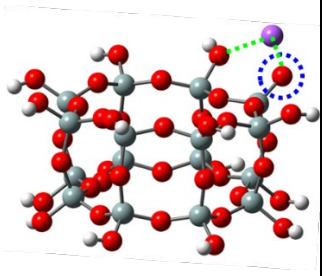
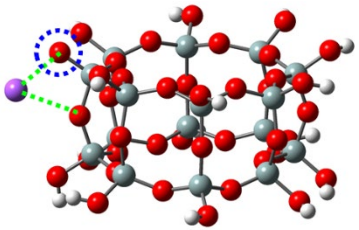
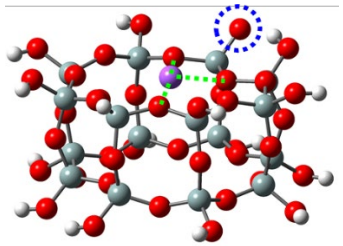
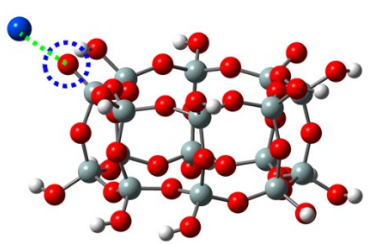
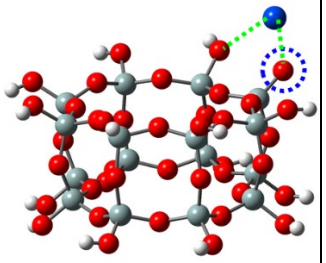
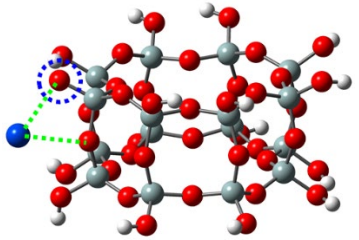
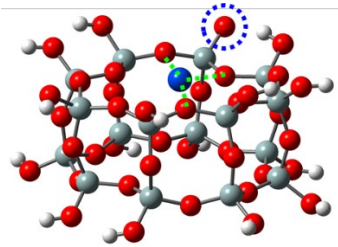
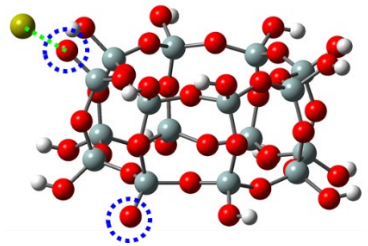
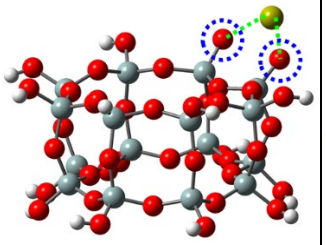
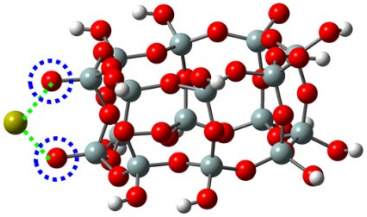
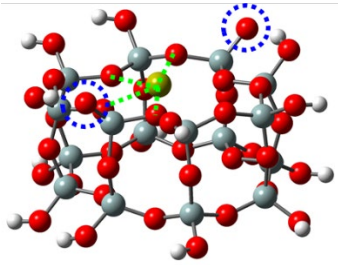
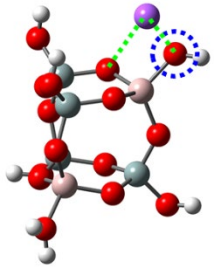
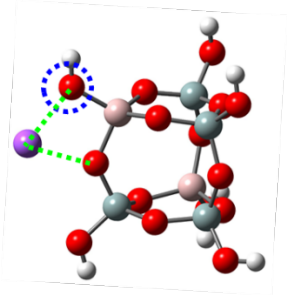
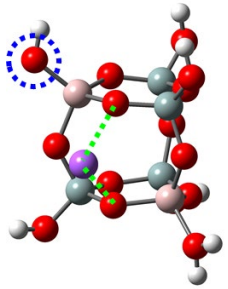
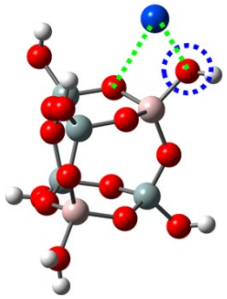
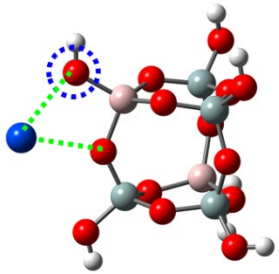
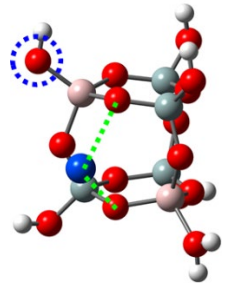
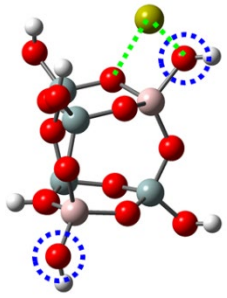
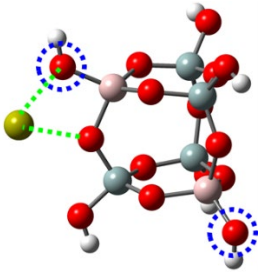
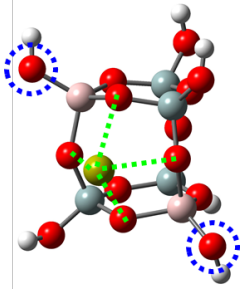
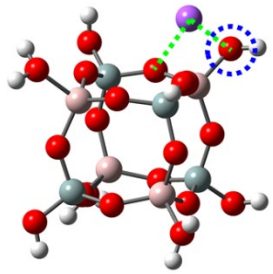
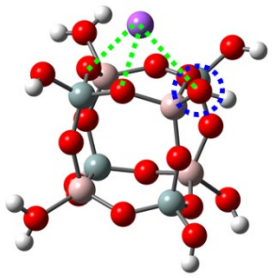
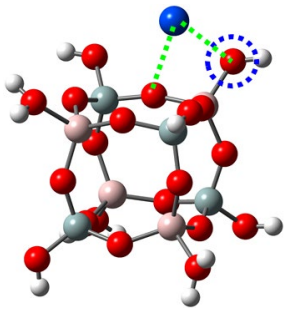
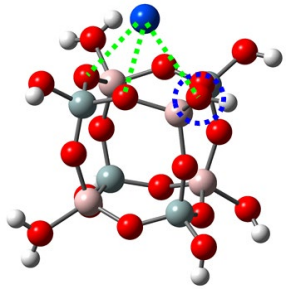
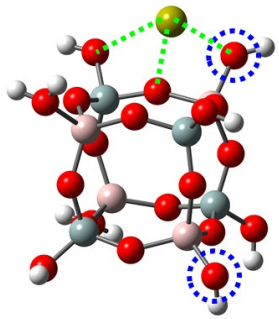
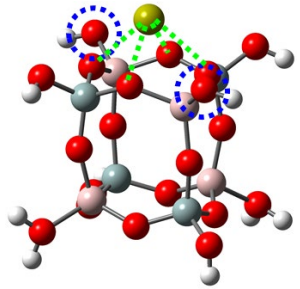
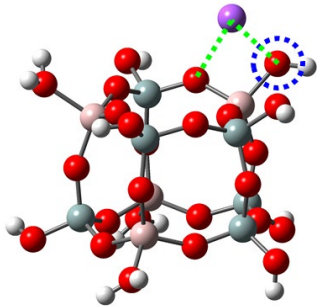
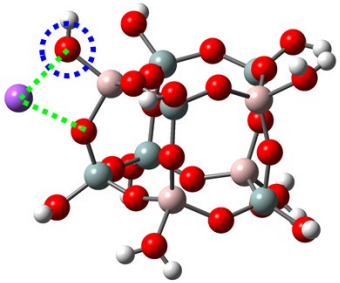
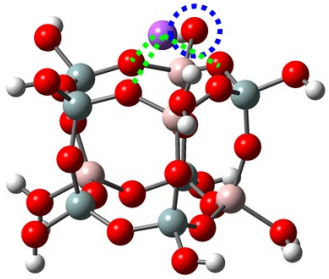
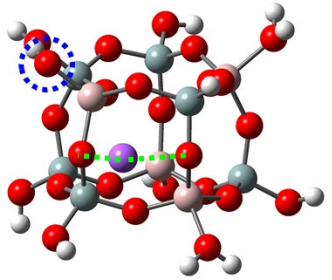
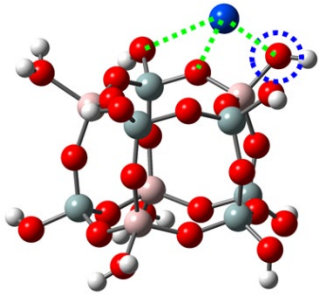
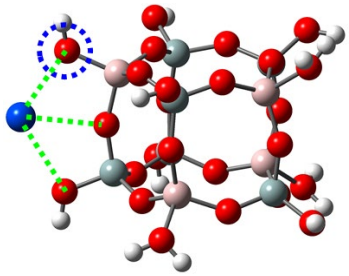
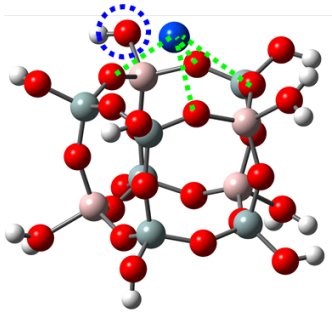
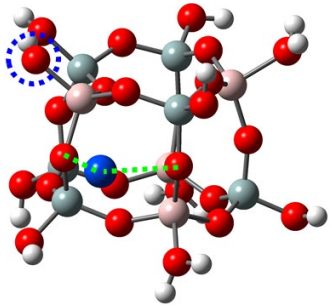
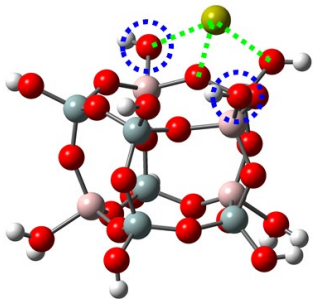
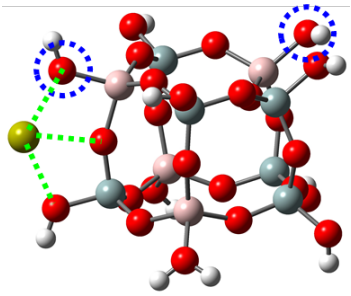
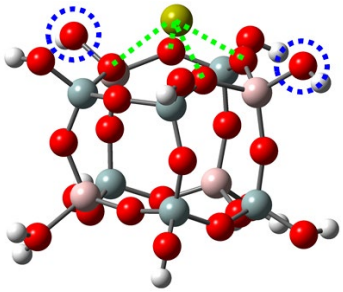
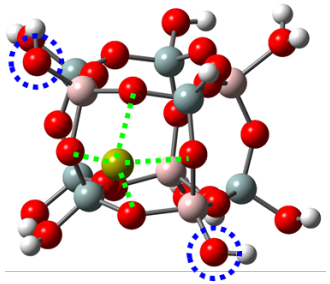
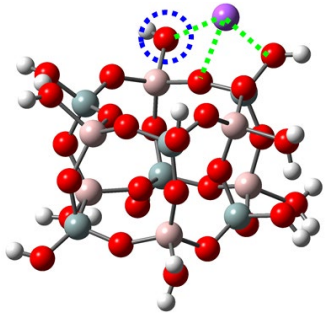
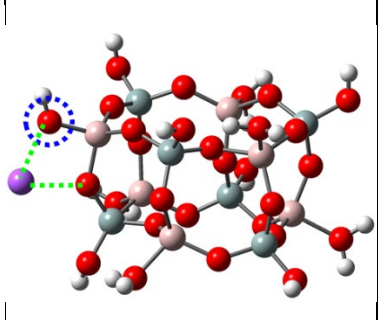
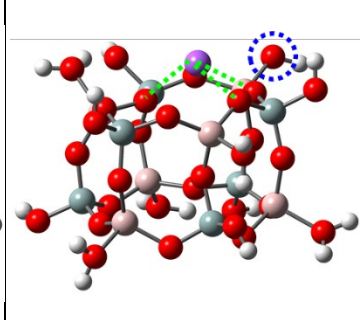
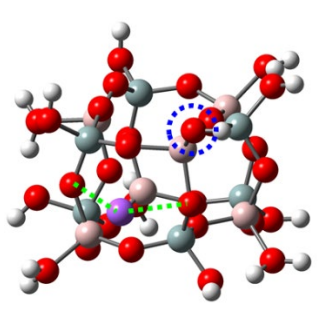
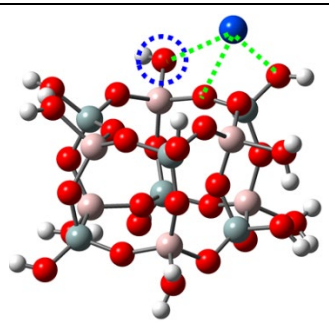
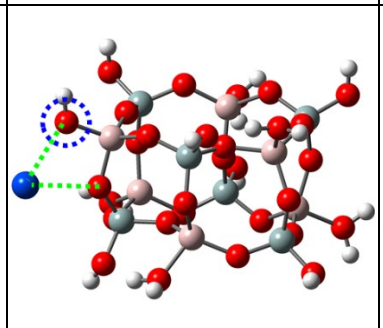
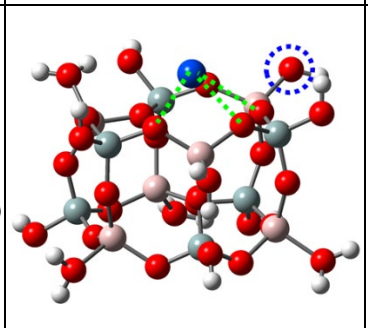
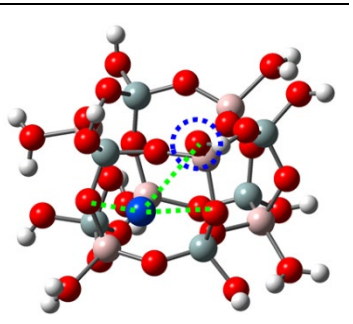
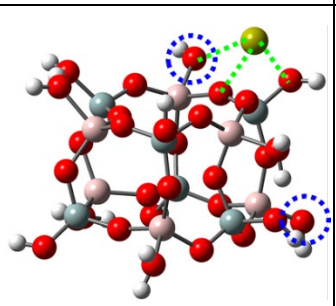
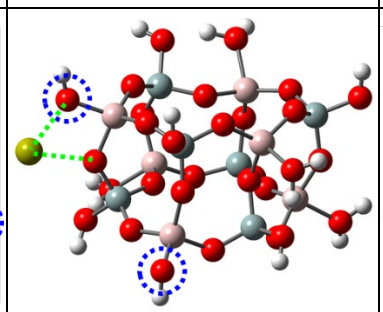
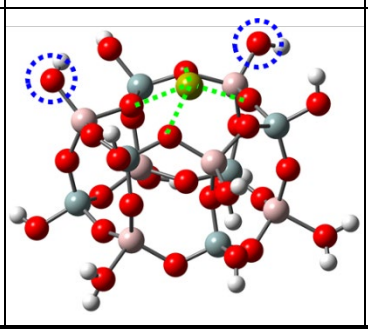
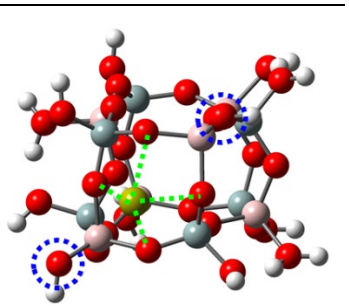
Octagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}					•
K^{+}					•
Ca^{2+}					•

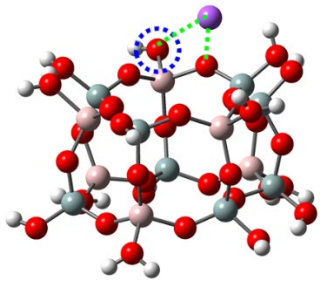
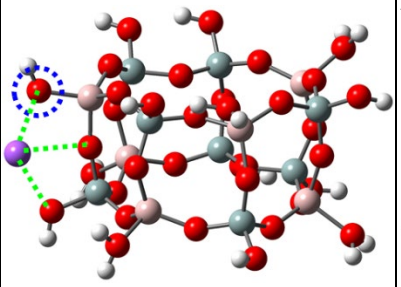
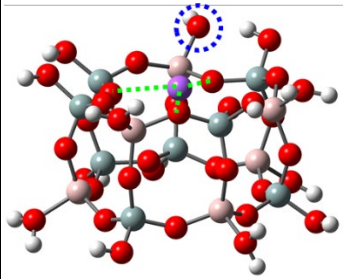
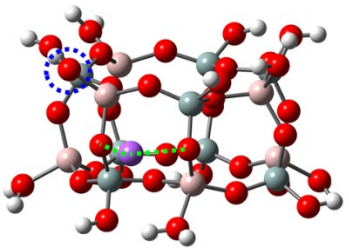
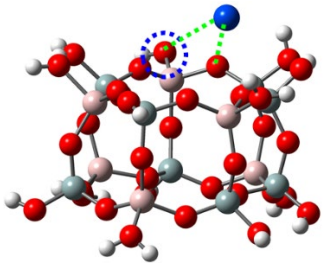
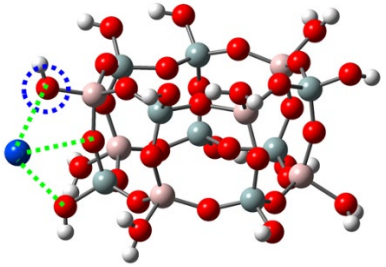
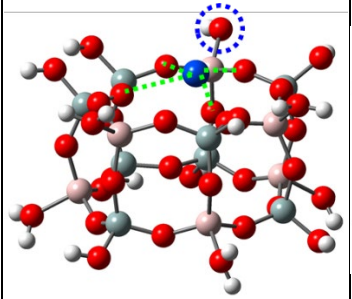
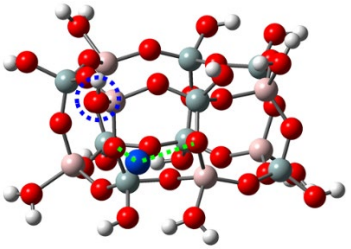
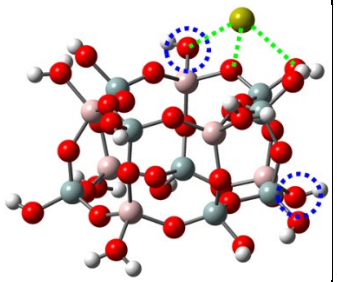
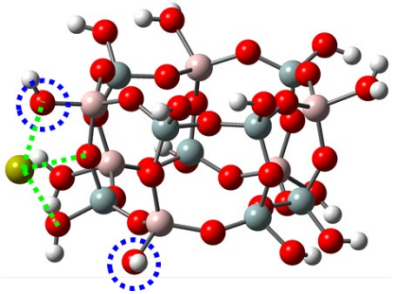
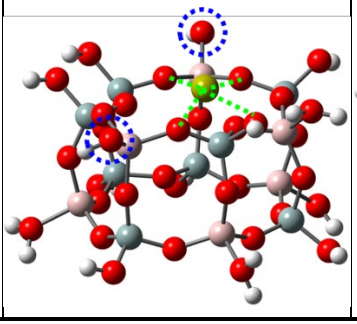
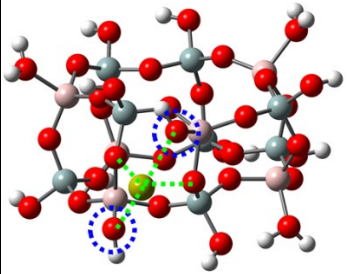
Table S4. Optimized molecular structures of aluminosilicate cages with an external cation (grey ball = Si, pink w= Al, red = O, white = H, purple = Na, blue = K, and yellow = Ca). The oxygen sites on which a proton is removed to maintain overall charge neutrality are highlighted with blue dotted circles. The green dotted lines connect the cations with the oxygen atoms that they electrostatically interact with. Blank cells indicate that the cation located at the corresponding positions moved to a different position during optimization.

Trigonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^+	•			•	
K^+	•			•	
Ca^{2+}	•			•	

Tetragonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}	•		(Same with top edge)		(Same with top surface)
K^{+}	•		(Same with top edge)		(Same with top surface)
Ca^{2+}	•		(Same with top edge)		(Same with top surface)

Pentagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}	•				
K^{+}	•				
Ca^{2+}	•				

Hexagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}	•				
K^{+}	•				
Ca^{2+}	•				

Heptagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^+	•				
K^+	•				
Ca^{2+}	•				

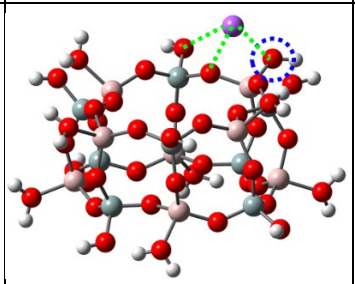
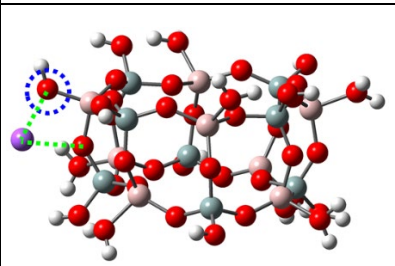
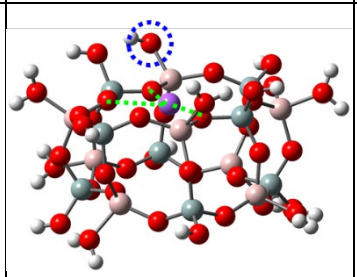
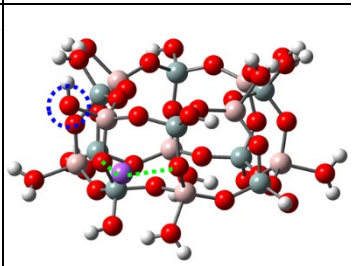
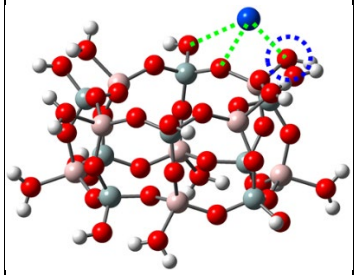
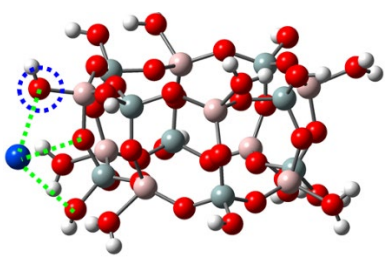
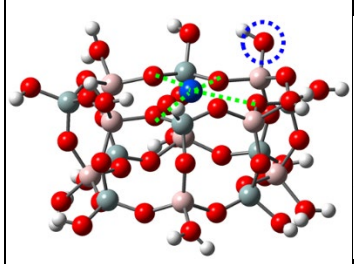
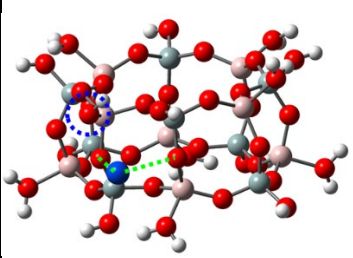
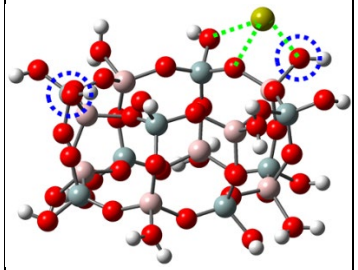
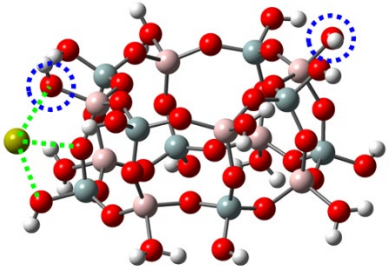
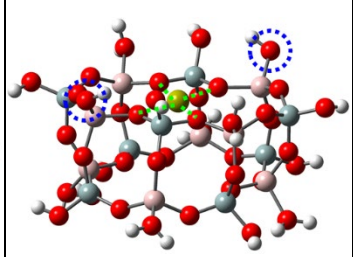
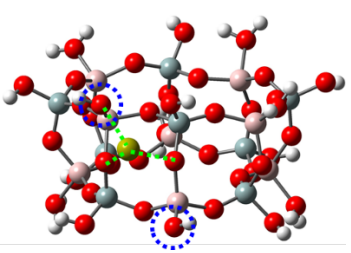
Octagonal prisms	Vertex	Top Edge	Lateral Edge	Top Surface	Lateral Surface
Na^{+}	•				
K^{+}	•				
Ca^{2+}	•				

Table S5. Optimized molecular structures of pure-silicate cages with an internal cation (grey ball = Si, red = O, white = H, purple = Na, blue = K, and yellow = Ca). The oxygen sites from which a proton is removed to maintain overall charge neutrality are highlighted with blue dotted circles.

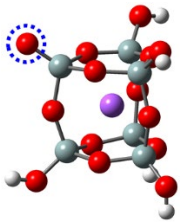
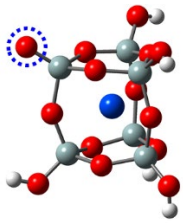
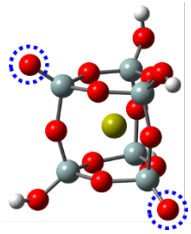
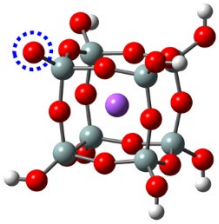
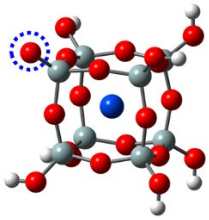
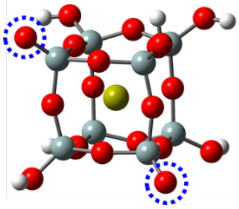
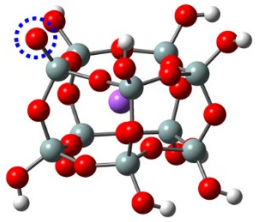
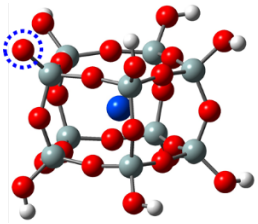
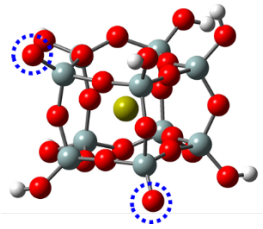
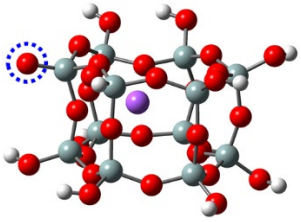
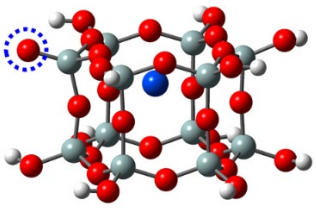
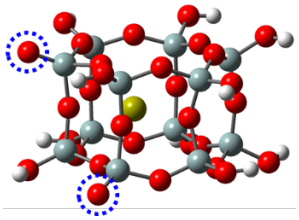
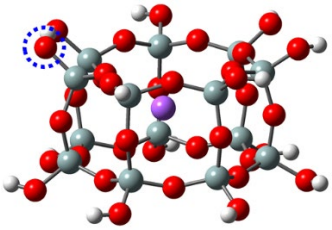
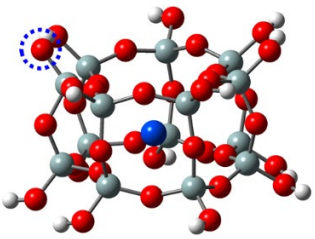
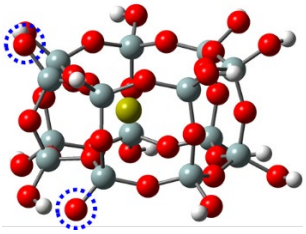
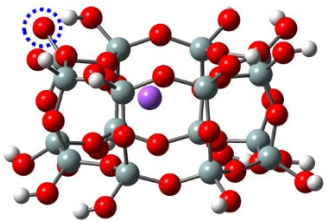
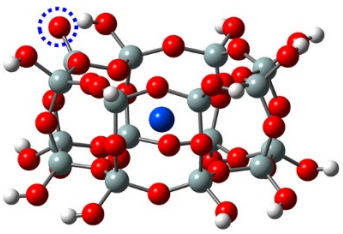
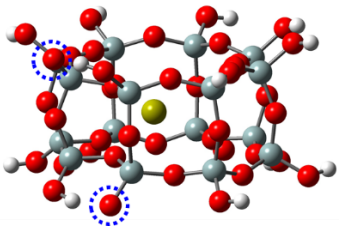
	Na^+	K^+	Ca^{2+}
Trigonal prisms			
Tetragonal prisms			
Pentagonal prisms			
Hexagonal prisms			
Heptagonal prisms			
Octagonal prisms			

Table S6. Optimized molecular structures of aluminosilicate cages with an internal cation (grey ball = Si, pink = Al, red = O, white = H, purple = Na, blue = K, and yellow = Ca). The oxygen sites from which a proton is removed to maintain overall charge neutrality are highlighted with blue dotted circles.

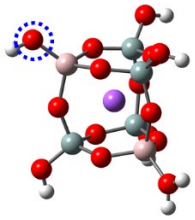
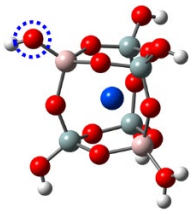
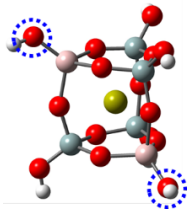
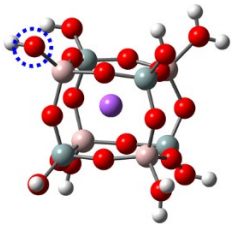
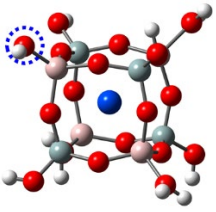
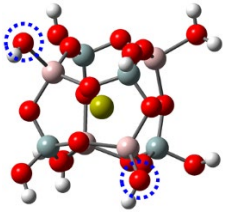
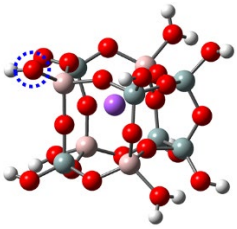
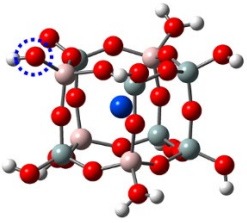
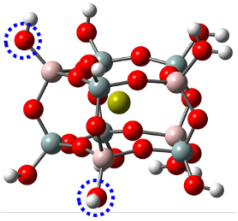
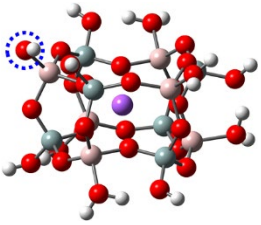
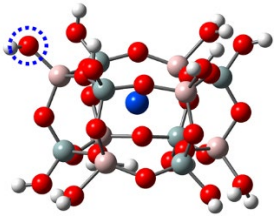
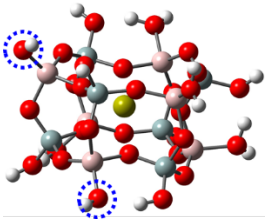
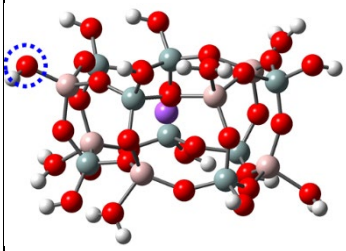
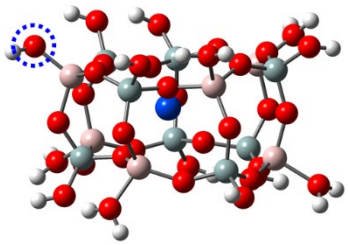
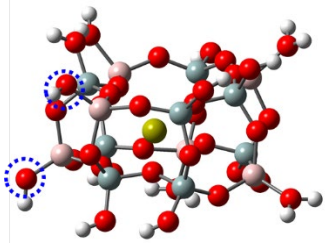
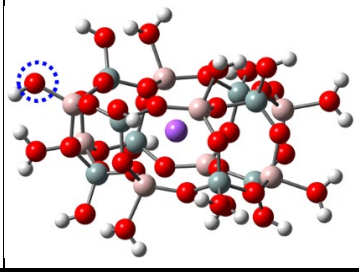
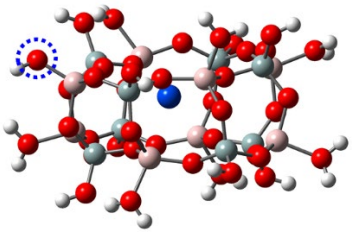
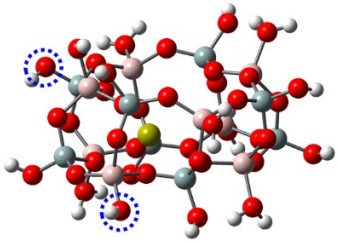
	Na^+	K^+	Ca^{2+}
Trigonal prisms			
Tetragonal prisms			
Pentagonal prisms			
Hexagonal prisms			
Heptagonal prisms			
Octagonal prisms			

Table S7. Formation electronic energy, enthalpy, entropy, and Gibbs free energy of pure-silicate species, determined at 100 °C. All values are normalized by the number of tetrahedral atoms in each species, in order to remove the effects arising from structure size.

Pure-silicates		Electronic energy (kJ/mol)	Enthalpy (kJ/mol)	Entropy (J/mol·K)	Gibbs free energy (kJ/mol)
Monocycles	3MR	-5.91	-7.05	28.29	-17.61
	4MR	-19.20	-19.27	5.86	-21.46
	5MR	-25.63	-25.30	-4.64	-23.57
	6MR	-26.50	-26.02	-10.68	-22.03
	7MR	-27.66	-26.84	-15.74	-20.97
	8MR	-28.30	-27.53	-20.45	-19.90
	9MR	-37.45	-36.39	-27.66	-26.07
	10MR	-31.75	-30.58	-27.89	-20.17
	11MR	-37.50	-36.11	-32.97	-23.80
	12MR	-38.05	-36.63	-34.53	-23.75
Multicycles	Mono-ring	-19.20	-19.27	5.86	-21.46
	Branched mono-ring	-26.41	-26.07	-5.74	-23.92
	Di-ring	-22.60	-22.98	12.03	-27.47
	Branched di-ring	-29.09	-29.02	-0.88	-28.70
	Tri-ring	-24.76	-25.41	14.36	-30.76
	Branched tri-ring	-26.36	-26.67	6.98	-29.27
	Tetra-ring	-22.58	-23.35	19.75	-30.72
	Branched tetra-ring	-26.48	-26.85	9.57	-30.42
	Penta-ring	-24.83	-25.63	17.37	-32.11
Cages	Trigonal prism	-4.27	-6.84	53.80	-26.91
	Tetragonal prism	-16.25	-18.52	49.63	-37.04
	Pentagonal prism	-18.37	-20.27	45.01	-37.06
	Hexagonal prism	-18.66	-20.53	46.28	-37.80
	Heptagonal prism	-18.38	-20.19	44.79	-36.91
	Octagonal prism	-18.30	-19.99	40.22	-35.00

Table S8. Formation electronic energy, enthalpy, entropy, and Gibbs free energy of aluminosilicate species, determined at 100 °C. All values are normalized by the number of tetrahedral atoms in each species, in order to remove the effects arising from structure size.

Aluminosilicates		Electronic energy (kJ/mol)	Enthalpy (kJ/mol)	Entropy (J/mol·K)	Gibbs free energy (kJ/mol)
Monocycles	3MR	-17.82	-18.42	24.00	-27.38
	4MR	-37.25	-37.13	11.41	-41.39
	5MR	-47.75	-47.16	-15.89	-41.23
	6MR	-55.26	-54.56	-22.14	-46.30
	7MR	-59.56	-59.63	-27.86	-49.24
	8MR	-63.01	-63.15	-33.84	-50.52
	9MR	-62.47	-62.28	-38.71	-47.83
	10MR	-64.07	-63.50	-39.51	-48.76
	11MR	-66.15	-65.73	-41.69	-50.17
	12MR	-76.37	-76.18	-51.12	-57.10
Multicycles	Mono-ring	-37.25	-37.13	11.41	-41.39
	Branched mono-ring	-48.36	-47.77	-15.14	-42.12
	Di-ring	-53.31	-53.86	-3.27	-52.64
	Branched di-ring	-51.96	-52.19	-9.63	-48.60
	Tri-ring	-51.53	-51.96	2.12	-52.76
	Branched tri-ring	-54.86	-54.93	-4.27	-53.34
	Tetra-ring	-49.95	-50.35	10.20	-54.16
	Branched tetra-ring	-52.44	-52.28	-2.18	-51.47
	Penta-ring	-59.20	-59.30	-1.60	-58.70
Cages	Trigonal prism	-19.07	-21.06	51.57	-40.30
	Tetragonal prism	-34.09	-35.36	47.04	-52.92
	Pentagonal prism	-35.56	-36.78	43.90	-53.16
	Hexagonal prism	-43.72	-44.91	30.83	-56.41
	Heptagonal prism	-40.13	-41.08	33.38	-53.54
	Octagonal prism	-44.89	-45.91	28.27	-56.46

Structural Information

(1) Pure-silicates (Monocycles, Multicycles, and Cages without a cation): **1-25**
(2) Aluminosilicates (Monocycles, Multicycles, and Cages without a cation): **26-50**
(3) Pure-silicates with an external cation (The most stable position only): **51-68**
(4) Aluminosilicates with an external cation (The most stable position only): **69-86**
(5) Pure-silicates with an internal cation: **87-104**
(6) Aluminosilicates with an internal cation: **105-122**

(1) Pure-silicates (Monocycles, Multicycles, and Cages without a cation)

1_Si_Mono_3MR

Atom	x	y	z
Si	-5.348125	0.310340	0.277011
O	-6.957983	0.289668	0.504987
H	-7.528899	0.126584	-0.249181
O	-4.756465	0.491286	1.780296
H	-3.817172	0.656895	1.887874
O	-4.876025	1.531930	-0.716616
Si	-4.011502	1.603337	-2.107464
O	-4.788232	2.407930	-3.291086
H	-5.514877	1.972903	-3.744009
O	-2.642868	2.411458	-1.761340
H	-2.056622	2.648066	-2.484109
O	-3.734108	0.047495	-2.558788
O	-4.810642	-1.068635	-0.439201
O	-2.771957	-2.333168	-1.644944
H	-2.185068	-2.124664	-0.913927
Si	-4.087021	-1.401008	-1.877254
O	-5.073839	-2.167478	-2.919367
H	-5.321160	-3.075869	-2.729959

2_Si_Mono_4MR

Atom	x	y	z
Si	1.468593	-1.572503	-0.129037
O	1.410290	-0.017034	-0.660388
Si	1.546966	1.480266	-0.024861
O	0.065833	2.174163	-0.030723
O	-0.062829	-2.119034	-0.002364
Si	-1.560025	-1.485772	0.125907
Si	-1.449654	1.568480	0.023053
O	-1.415491	0.065019	0.658069
O	-2.321412	-2.428179	1.212797
H	-3.258136	-2.277119	1.360356
O	-2.353822	-1.477816	-1.300816
H	-2.391622	-0.612684	-1.734084
O	2.258539	-1.609349	1.299638
H	2.340443	-0.748757	1.736042
O	2.178059	-2.556974	-1.213485
H	3.120235	-2.451282	-1.366152
O	2.113031	1.209403	1.490327

H	2.276494	1.943352	2.088086
O	2.599827	2.426456	-0.821870
H	2.315034	2.858558	-1.631017
O	-2.294924	2.619496	0.929759
H	-3.227134	2.446990	1.084944
O	-2.067529	1.328292	-1.481763
H	-2.134212	2.058787	-2.102473

3_Si_Mono_5MR

Atom	x	y	z
O	-2.850210	-0.819298	0.035851
O	-2.445724	1.824480	-0.044723
O	0.044806	2.407162	-0.827483
O	0.490338	0.132228	0.379753
O	-0.601994	-2.143747	-0.392425
Si	-3.022500	0.579181	0.845224
Si	-1.994279	-1.647499	-1.079344
Si	0.361101	-1.457096	0.754072
Si	1.041034	1.102320	-0.820363
Si	-1.226932	2.910750	0.058465
O	-2.134091	0.486070	2.230878
H	-1.615594	1.285153	2.423837
O	-4.619735	0.711634	1.117594
H	-4.941119	1.450536	1.640138
O	-1.547745	-0.666681	-2.322116
H	-2.229731	-0.259530	-2.864696
O	-2.862882	-2.878062	-1.683235
H	-3.331070	-3.459947	-1.079190
O	1.840607	-2.129802	0.695414
H	1.919698	-3.086471	0.670377
O	-0.287824	-1.600959	2.236394
H	-1.003309	-0.972496	2.432984
O	1.023911	0.346928	-2.261180
H	0.162813	-0.024228	-2.517203
O	2.566941	1.525587	-0.442993
H	3.050315	2.092489	-1.048842
O	-0.902938	2.940715	1.669458
H	-0.202535	3.501115	2.013512
O	-1.686820	4.387041	-0.438805
H	-1.585441	4.615853	-1.366032

4_Si_Mono_6MR

Atom	x	y	z
Si	-1.121606	2.390914	0.003211
O	-1.936760	3.765158	0.339929
O	-1.849586	1.770230	-1.316944
H	-1.562166	0.906713	-1.623566
O	0.450410	2.683768	-0.319131
H	1.001651	2.913663	0.441654
O	-1.194831	1.379349	1.282658
Si	-1.734741	5.320125	0.782204
Si	-2.182154	0.710533	2.398405

O	-2.563227	6.242822	-0.268819
H	-2.680402	7.174510	-0.068167
O	-0.156919	5.737527	0.765751
H	0.493538	5.166126	1.197891
O	-2.360783	5.516618	2.294440
O	-3.485594	1.606309	2.754671
H	-3.413213	2.358979	3.364633
O	-1.275370	0.465039	3.739973
O	-2.679615	-0.701823	1.744710
H	-3.324116	-1.218115	2.234755
Si	-1.949281	4.758426	3.676474
Si	0.290885	0.337138	4.159572
O	1.027229	1.780504	3.878256
O	0.282621	-0.051111	5.737836
H	1.118857	-0.265743	6.158020
O	1.095279	-0.810001	3.323628
H	1.486943	-0.564531	2.481536
O	-0.841146	3.612876	3.276035
O	-1.338815	5.809633	4.754823
H	-0.468100	5.587381	5.113112
O	-3.218419	3.902500	4.263854
H	-3.998044	4.352856	4.600744
Si	0.739585	3.332183	3.546075
O	1.146603	4.334422	4.771175
H	1.950843	4.210152	5.281923
O	1.468522	3.761818	2.122002
H	2.425715	3.874831	2.102610

5_Si_Mono_7MR

Atom	x	y	z
Si	-3.215863	1.313590	-0.108052
O	-1.787366	1.212608	0.696254
O	-4.468223	0.968573	0.880245
H	-4.619107	0.021647	1.001392
O	-3.149976	0.175093	-1.293243
O	-3.407489	2.800564	-0.733391
H	-2.703741	3.425592	-0.504616
Si	-2.875164	-1.415378	-1.043060
O	-3.803752	-1.846576	0.246190
H	-3.338286	-2.324995	0.949482
O	-3.279284	-2.148377	-2.436003
H	-3.126032	-3.092469	-2.522376
O	-1.306757	-1.680400	-0.654676
Si	-0.435401	-2.217190	0.611314
Si	-0.456950	2.130871	0.882950
O	-1.566063	-2.727427	1.686500
H	-1.312615	-2.998548	2.572381
O	0.543376	-3.457978	0.197713
H	1.048872	-3.279633	-0.610221
O	0.485872	-1.025297	1.258060
O	0.707013	1.637072	-0.156970
O	0.090191	2.119582	2.408983
H	0.844877	1.533650	2.590351
O	-0.995412	3.633282	0.471463

H	-0.427765	4.398751	0.589548
Si	2.084109	-0.904870	1.613800
Si	2.097584	1.988932	-0.918672
O	2.543374	-2.031652	2.694566
H	2.408609	-2.956786	2.470083
O	2.348398	0.554923	2.301700
H	2.838063	1.202741	1.761527
O	3.157902	2.282289	0.307190
H	4.040256	2.607686	0.106677
O	2.035956	3.296864	-1.876025
H	1.619730	3.233773	-2.739684
O	2.541720	0.667563	-1.772583
Si	2.852845	-0.892787	-1.391760
O	1.625880	-1.892145	-1.820128
H	1.255259	-1.852783	-2.706265
O	4.209175	-1.400888	-2.124755
H	4.989878	-0.841263	-2.103980
O	2.946184	-1.027892	0.230712

6_Si_Mono_8MR

Atom	x	y	z
Si	0.347880	2.171177	0.033016
O	0.739537	2.712404	1.521016
H	0.240062	3.485678	1.821538
O	1.739485	1.767736	-0.709341
H	1.699965	1.148520	-1.442003
O	-0.610455	0.845582	0.092204
O	-0.454189	3.355836	-0.776248
Si	-2.119506	0.614669	0.661944
Si	-1.105239	4.791494	-0.371613
O	-2.955925	-0.218551	-0.462300
H	-3.860784	-0.439869	-0.196333
O	-2.025964	-0.240896	2.056965
O	-2.717507	2.107483	0.962412
H	-3.668639	2.166269	1.135607
O	-0.944613	4.968848	1.252603
H	-1.689554	5.361667	1.724173
O	-0.285489	6.015213	-1.073708
H	-0.231029	6.044365	-2.032263
O	-2.682838	4.846383	-0.809529
Si	-4.026090	5.547067	-0.227823
Si	-2.799406	-0.581967	3.439034
O	-3.946368	-1.749274	3.188549
H	-3.675876	-2.672119	3.167516
O	-1.652499	-1.040147	4.495691
H	-1.913662	-1.285928	5.386914
O	-3.656581	0.719387	3.919290
O	-3.672094	6.147648	1.278772
H	-3.573303	7.097801	1.397181
O	-4.501623	6.672967	-1.290783
H	-5.384352	7.047330	-1.227417
O	-5.183189	4.427297	0.043128
Si	-5.133485	1.111513	4.526709
Si	-5.951031	3.734104	1.296715

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   O -6.240799  0.641489  3.404749
   O -5.484940  0.267240  5.872048
   H -5.054080  0.509142  6.695332
   O -5.195384  2.701746  4.834178
   H -5.221122  3.358671  4.118878
   O -5.464171  2.172083  1.404383
   O -5.524195  4.498563  2.683574
   H -4.882550  5.220169  2.581132
   O -7.562829  3.602396  1.099569
   H -8.131423  4.376576  1.068862
  Si -6.201672  0.737431  1.775300
   O -5.245901 -0.444078  1.172335
   H -4.975975 -1.146171  1.794007
   O -7.680224  0.690023  1.111229
   H -8.117638  1.548092  1.024731
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7_Si_Mono_9MR
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Atom         x         y         z
  Si -1.339257  3.953330 -2.565505
   O -2.689726  3.694388 -3.449534
   H -3.346140  4.423810 -3.394523
   O -0.081558  3.977502 -3.596213
   H  0.807749  3.939807 -3.235461
   O -1.113409  2.794639 -1.447805
   O -1.512570  5.401154 -1.816645
  Si -1.676855  2.107815 -0.077234
  Si -2.097033  6.183151 -0.529455
   O -3.306075  2.300854 -0.053140
   O -1.306116  0.522131 -0.051582
   H -2.065683 -0.070346 -0.142695
   O -1.010213  2.808239  1.235655
   H -1.305690  3.716043  1.381000
   O -0.887407  7.080987  0.076191
   H -1.018511  7.563560  0.896388
   O -3.387225  7.064581 -1.067891
   H -3.931905  7.486896 -0.390642
   O -2.653498  5.099315  0.580135
  Si -4.658712  1.413367 -0.166180
  Si -4.186665  4.915147  1.158916
   O -5.525669  1.785901 -1.504285
   O -5.566689  1.693691  1.171186
   H -6.422525  2.123473  1.004083
   O -4.134507 -0.140623 -0.242824
   H -4.724936 -0.763593 -0.688234
   O -5.199646  4.389141 -0.018071
   O -4.635349  6.438150  1.578419
   H -5.589708  6.596621  1.541803
   O -4.182843  3.886480  2.414769
   H -4.554850  3.010436  2.225052
  Si -6.547554  0.963073 -2.477407
  Si -6.768274  4.586772 -0.429115
   O -6.201273  1.181352 -4.041205
   O -8.025475  1.575700 -2.098558
   H -8.783356  1.433590 -2.672296
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   O -6.352721 -0.599740 -2.031112
   H -6.768059 -1.315586 -2.519044
   O -6.885247  4.819670 -2.030982
   O -7.642931  3.278615  0.011427
   H -7.966848  2.706203 -0.710081
   O -7.215164  5.897750  0.449653
   H -8.134660  6.174831  0.478807
  Si -5.610645  2.376769 -5.008636
  Si -6.062191  5.143653 -3.403673
   O -5.928434  3.789441 -4.275646
   O -6.422481  2.373049 -6.420847
   H -6.313776  1.623233 -7.010531
   O -4.022904  2.163689 -5.263151
   H -3.406402  2.582167 -4.634166
   O -4.525214  5.616742 -3.099861
   H -4.282883  6.285784 -2.432828
   O -6.808377  6.326830 -4.235855
   H -7.743649  6.233893 -4.434089
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8_Si_Mono_10MR
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Atom         x         y         z
   O  0.066333  5.591176 -1.381017
   H  0.086263  5.135157 -0.528990
   O -1.188546  6.059571 -3.684717
   H -0.503528  5.786376 -4.299513
   O -1.566679  3.709039 -2.373240
   O -2.625297  5.969987 -1.526571
  Si -1.008742  2.306297 -1.763410
  Si -3.110750  5.920623  0.040380
   O -0.129918  1.451420 -2.832787
   H -0.545225  0.639376 -3.158234
   O -0.124996  2.738933 -0.462202
   H  0.393617  2.075663 -0.000049
   O -2.354577  1.445560 -1.355776
   O -1.792098  5.360695  0.828409
   H -1.872573  5.065279  1.738854
   O -3.606132  7.403172  0.501049
   H -4.446400  7.430964  0.978086
   O -4.350166  4.871748  0.210544
   O -2.016713 -0.620683 -2.850048
   H -2.085838 -1.534421 -3.140297
   O -2.922863 -0.984609 -0.277668
   O -4.498845  0.014626 -2.095777
   O -6.601617  3.536663  0.662409
   H -7.451431  3.347112  0.226996
   O -6.213321  6.199667  1.320043
   H -7.098754  6.549877  1.450100
   O -6.615281  5.429996 -1.202098
  Si -5.945577  0.258536 -1.319326
  Si -7.610842  4.700921 -2.287610
   O -6.654975 -1.189147 -1.055092
   H -7.238419 -1.486384 -1.766140
   O -5.702219  0.966585  0.111854
   H -5.816432  1.926924  0.215210
```

```
   O -6.875530  1.120110 -2.354783
   O -8.602114  5.768803 -3.011204
   H -8.252372  6.309163 -3.724314
   O -8.506109  3.659266 -1.396664
   H -8.932492  2.948349 -1.904522
   O -6.673027  3.953398 -3.395864
   O -9.168814  1.831689 -3.362193
   H -9.783816  2.022675 -4.075788
   O -8.256609 -0.751243 -3.459177
   H -8.713547 -1.221960 -4.161157
   O -7.125899  1.173759 -4.997735
   O -4.825678  2.464125 -4.544380
   O -4.156586  4.862342 -3.764700
   H -3.915175  5.473342 -3.056673
   O -4.777280  3.017233 -1.868692
   H -3.867563  2.822809 -1.604301
  Si -5.513062  1.224120 -5.347234
   O -5.309828  1.498033 -6.935848
   H -5.732533  0.908019 -7.564440
   O -4.812159 -0.184806 -4.915786
   H -4.605545 -0.289900 -3.975460
   H -2.108406 -1.078595  0.223458
  Si -7.886988  0.840257 -3.597177
  Si -5.075668  3.571657 -3.380228
  Si -5.971462  4.990347  0.236196
  Si -2.941534 -0.060584 -1.614824
  Si -1.290596  5.320274 -2.244498
-------------------------------------

9_Si_Mono_11MR
-------------------------------------
Atom         x         y         z
   O -5.499399 -0.144976  1.601870
   H -5.573454 -0.763298  0.862322
   O -3.939446  0.777282  3.587391
   H -4.306594  0.282405  4.324129
   O -3.109131 -1.266480  2.022126
   O -3.209266  1.223378  1.132337
  Si -2.864988 -2.270981  0.761002
  Si -3.416867  1.650451 -0.438598
   O -2.045786 -3.599630  1.192058
   H -1.087230 -3.574653  1.008989
   O -4.348088 -2.597879  0.149168
   H -4.369174 -2.748188 -0.806045
   O -1.984364 -1.439989 -0.372397
   O -4.210116  0.390871 -1.111446
   H -4.719205  0.520534 -1.915847
   O -4.204164  3.063726 -0.595017
   H -3.693014  3.774690 -1.010812
   O -1.926289  1.785717 -1.119009
   O  0.549809 -3.210257  0.320010
   H  1.295275 -3.078590  0.938675
   O  1.566858 -4.552152 -1.832718
   O  2.036933 -2.020546 -1.588588
   O -0.020221  2.640816 -2.792514
   H  0.744207  2.042434 -2.722980
```

```
   O -1.902833  4.257790 -1.766999
   H -1.557451  5.133207 -1.960268
   O  0.056132  3.326606 -0.182175
  Si  2.586885 -0.525743 -1.921550
  Si  1.584411  3.254650  0.407535
   O  3.911131 -0.598339 -2.876458
   H  4.746727 -0.693457 -2.400071
   O  1.462512  0.327853 -2.742042
   H  0.550250 -0.018249 -2.731250
   O  3.031663  0.182287 -0.510265
   O  1.922933  4.575573  1.304223
   H  1.537526  4.632316  2.182186
   O  2.588620  3.215091 -0.870694
   H  3.476491  2.894916 -0.649249
   O  1.661683  1.922404  1.353818
   O  4.663443  1.955876  0.473195
   H  5.375095  2.308450  1.013855
   O  5.543580 -0.438110 -0.498368
   H  6.409756 -0.628657 -0.129692
   O  4.173291 -0.328807  1.832181
   O  1.550165 -0.511522  2.310173
   O -0.639764  0.907116  2.360280
   H -1.415159  1.260583  1.901268
   O  0.281590  0.098640 -0.022826
   H -0.597578 -0.312363 -0.050321
  Si  2.988025 -1.228550  2.520472
   O  3.348041 -1.494791  4.081541
   H  3.697120 -0.772493  4.609778
   O  2.814104 -2.688568  1.782942
   H  3.525346 -3.334301  1.828766
   H  1.081226 -5.366908 -1.681694
  Si  4.390159  0.345153  0.363198
  Si  0.701574  0.603904  1.480039
  Si -0.877523  3.011516 -1.471340
  Si  0.933271 -3.159038 -1.275601
  Si -3.970518  0.126485  2.104172
   O -3.092452 -2.453705 -2.487754
   H -3.137127 -2.883684 -3.346238
   O -1.225555 -0.402207 -2.686973
   O -0.464677 -2.829898 -2.068193
   H -1.619684  0.418021 -2.341183
  Si -1.703775 -1.784851 -1.954709
-------------------------------------

10_Si_Mono_12MR
-------------------------------------
Atom         x         y         z
   O  4.791194 -1.446301  2.332465
   H  5.070938 -0.645376  1.867800
   O  2.745405 -2.564685  3.634505
   H  2.992731 -2.248167  4.506831
   O  2.415604 -0.229286  2.273156
   O  2.665926 -2.579411  1.049806
  Si  2.759440  1.238628  1.636210
  Si  3.054399 -2.378059 -0.532558
   O  2.272998  2.426248  2.626468
```

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 H  1.311995  2.583840  2.589807
 O  4.376786  1.331075  1.387158
 H  4.636709  1.472847  0.464864
 O  1.945981  1.341692  0.201973
 O  3.889656 -0.975251 -0.485740
 H  4.355674 -0.580363 -1.229961
 O  3.861551 -3.660271 -1.121809
 H  3.411017 -4.133563 -1.836117
 O  1.717043 -2.140196 -1.447436
 O -0.386682  2.439500  1.947263
 H -1.134407  2.112133  2.483587
 O -2.286960  3.798579  0.567899
 O -0.875854  2.034266 -0.711628
 O  0.000657 -2.081889 -3.487814
 H -0.731361 -1.479670 -3.268795
 O  1.542921 -4.220798 -2.896489
 H  1.148194 -4.942571 -3.392355
 O -0.553813 -3.575457 -1.326149
Si -1.953625  1.182131 -1.603261
Si -2.115615 -3.269109 -0.921473
 O -3.019075  2.160319 -2.370650
 H -3.863960  2.282774 -1.917782
 O -1.105849  0.360144 -2.725329
 H -0.139289  0.492060 -2.669603
 O -2.818516  0.209926 -0.612126
 O -2.939272 -4.657966 -0.684070
 H -2.787395 -5.135928  0.135133
 O -2.770677 -2.473171 -2.181695
 H -3.609994 -2.036929 -1.969715
 O -2.094724 -2.403692  0.462133
 O -4.885391 -1.366341 -0.728925
 H -5.658062 -1.820810 -0.383504
 O -5.126787  1.346694 -0.490811
 H -6.034583  1.503441 -0.219203
 O -4.259991 -0.151157  1.592169
 O -1.727421 -0.603361  2.337819
 O  0.034922 -2.507485  2.082311
 H  0.822008 -2.836406  1.627760
 O -0.153678 -0.657676  0.104806
 H  0.432966  0.079396  0.327501
Si -3.148153  0.043356  2.777639
 O -3.734161 -0.550956  4.171060
 H -4.191929 -1.395384  4.162629
 O -2.766123  1.623512  3.015910
 H -3.440628  2.251690  3.288099
 H -2.495749  4.420562  1.269492
Si -4.314371  0.000810 -0.029765
Si -0.950229 -1.520289  1.235902
Si  0.613343 -3.009064 -2.306585
Si -0.807234  3.109114  0.512571
Si  3.175704 -1.681156  2.343731
 O  3.964619  1.577326 -1.450171
 H  4.399175  2.122914 -2.112934
 O  1.586863  0.496472 -2.292904
 O  0.394409  4.151236  0.131195
 H  1.669051 -0.432018 -2.001235
```

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  Si  2.316922  1.628230 -1.367735
   O  2.293170  5.540250 -1.168941
   H  2.069554  6.428888 -0.880744
   O -0.111951  4.905740 -2.315832
   H  0.075435  5.015710 -3.251556
  Si  1.095380  4.447435 -1.317891
   O  1.808276  3.081439 -1.865203
-------------------------------------

11_Si_Multi_Mono-ring
-------------------------------------
Atom         x         y         z
  Si  1.468593 -1.572503 -0.129037
   O  1.410290 -0.017034 -0.660388
  Si  1.546966  1.480266 -0.024861
   O  0.065833  2.174163 -0.030723
   O -0.062829 -2.119034 -0.002364
  Si -1.560025 -1.485772  0.125907
  Si -1.449654  1.568480  0.023053
   O -1.415491  0.065019  0.658069
   O -2.321412 -2.428179  1.212797
   H -3.258136 -2.277119  1.360356
   O -2.353822 -1.477816 -1.300816
   H -2.391622 -0.612684 -1.734084
   O  2.258539 -1.609349  1.299638
   H  2.340443 -0.748757  1.736042
   O  2.178059 -2.556974 -1.213485
   H  3.120235 -2.451282 -1.366152
   O  2.113031  1.209403  1.490327
   H  2.276494  1.943352  2.088086
   O  2.599827  2.426456 -0.821870
   H  2.315034  2.858558 -1.631017
   O -2.294924  2.619496  0.929759
   H -3.227134  2.446990  1.084944
   O -2.067529  1.328292 -1.481763
   H -2.134212  2.058787 -2.102473
-------------------------------------

12_Si_Multi_Branched_Mono-ring
-------------------------------------
Atom         x         y         z
  Si  1.836065 -1.257707 -0.042316
   O  2.118889  0.246773 -0.618895
  Si  1.938614  1.860078 -0.565978
   O  0.460402  2.235887 -1.183964
   O  0.272769 -1.345614  0.430433
  Si -0.976159 -0.568091  1.110620
  Si -1.022071  1.915897 -0.590917
   O -0.812779  1.050889  0.799017
   O -0.860935 -0.791320  2.727889
   H -1.633764 -0.641123  3.279540
   O -2.410561 -1.096345  0.557904
   H -2.667996 -0.724875 -0.296603
   O  2.866326 -1.613611  1.169205
   O  1.994274 -2.364358 -1.225655
   H  2.868189 -2.508535 -1.596508
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   O  2.020198  2.385478  0.970735
   O  3.103756  2.630733 -1.390800
   H  3.206192  2.447771 -2.328048
   O -1.724352  3.350572 -0.302543
   H -2.631435  3.370740  0.014462
   O -1.897585  0.888391 -1.517091
   H -2.121401  1.104662 -2.426361
   H  2.778964 -0.999537  1.913463
  Si  1.631733  2.025686  2.517975
   O  1.650656  0.383630  2.652653
   H  0.903951 -0.038369  3.105819
   O  2.765783  2.619453  3.523436
   H  3.025523  3.539100  3.430169
   O  0.175023  2.639247  2.932249
   H -0.558401  2.318840  2.393023
-------------------------------------

13_Si_Multi_Di-ring
-------------------------------------
Atom         x         y         z
  Si -0.834771  2.206380 -0.733935
   O  0.062049  1.610665  0.488727
  Si  0.938900  0.978154  1.694490
   O  0.240269 -0.431387  2.132816
   O -2.187064  1.298119 -0.843066
  Si -2.889148 -0.090026 -0.382126
  Si -0.844903 -1.479217  1.502307
   O -2.142418 -0.663585  0.952605
   O -2.690456 -1.099169 -1.664768
   H -3.144058 -1.946560 -1.676972
   O -4.481419  0.076894 -0.101735
   H -4.766653  0.442461  0.739576
   O  0.037961  2.221783 -2.106468
   H  0.693189  1.510157 -2.175702
   O -1.373430  3.714400 -0.423394
   H -0.735112  4.430379 -0.466639
   O  1.001420  1.900745  3.027019
   H  1.474840  2.735698  2.989856
   O  2.442219  0.704064  1.107366
   O -0.140700 -2.267330  0.254075
   O -1.379345 -2.515410  2.629322
   H -0.743309 -3.065647  3.093068
  Si  2.978141  0.089879 -0.315274
   O  2.180016 -1.301808 -0.599903
  Si  0.740987 -1.900160 -1.076781
   O  4.586641 -0.126363 -0.248348
   H  4.972942 -0.500499  0.547480
   O  0.910267 -3.223916 -2.004403
   H  1.140454 -4.058874 -1.589493
   O  0.027585 -0.702983 -1.931480
   H -0.894947 -0.856303 -2.194700
   O  2.621145  1.068252 -1.580071
   H  3.035849  1.935289 -1.614368
-------------------------------------
```

14_Si_Multi_Branched_Di-ring

Atom	x	y	z
Si	-0.074362	1.985828	-0.282918
O	0.108095	0.570210	0.521763
Si	0.337384	-0.342568	1.850443
O	-1.136762	-0.899986	2.285742
O	-1.675052	2.241169	-0.459140
Si	-3.113309	1.488707	-0.326957
Si	-2.353324	-1.127642	1.196523
O	-3.006070	0.306415	0.792556
O	-3.409630	0.860587	-1.817596
H	-4.286102	0.519290	-2.017478
O	-4.315674	2.515784	0.037379
H	-4.412217	2.826928	0.940947
O	0.678605	1.822814	-1.734253
H	0.318297	1.072938	-2.239617
O	0.564124	3.244434	0.517946
H	1.478596	3.075262	0.794150
O	1.067691	0.574255	2.980461
H	1.225461	0.233141	3.865455
O	1.290151	-1.584756	1.383553
O	-1.693249	-1.820968	-0.126552
O	-3.541115	-2.022051	1.840373
H	-3.331240	-2.889772	2.194951
Si	1.963753	-1.831330	-0.098164
O	0.757037	-1.942126	-1.188597
Si	-0.827317	-1.755436	-1.510916
O	2.879473	-3.171755	-0.098671
H	2.444154	-4.025338	-0.031558
O	-1.353014	-2.898336	-2.543618
H	-1.473455	-3.795148	-2.221343
O	-0.980937	-0.297960	-2.244823
H	-1.879636	0.036470	-2.416227
O	2.937490	-0.589511	-0.452155
Si	3.611210	0.880591	-0.256813
O	3.457316	1.790683	-1.595369
H	2.536837	1.952328	-1.861385
O	2.848608	1.708913	0.953139
H	2.706987	1.316615	1.825236
O	5.186989	0.609130	0.062049
H	5.743233	1.367641	0.256616

15_Si_Multi_Tri-ring

Atom	x	y	z
Si	1.174560	2.482735	0.136686
O	1.732667	1.754808	-1.208644
Si	1.624351	0.580765	-2.327531
O	2.649143	-0.643702	-1.925870
O	1.694208	1.640915	1.440851
Si	1.854726	0.082880	1.904299
Si	2.852602	-1.467948	-0.535990
O	1.815079	-0.834667	0.549814
O	3.223756	-0.162819	2.742692

```
   H  3.977548 -0.460356  2.216499
   O  1.672187  4.026512  0.216324
   H  2.615420  4.207617  0.222083
   O  0.108171 -0.040278 -2.399755
   H -0.002166 -0.940851 -2.027124
   O  4.318484 -1.289140  0.158132
   H  5.131023 -1.497140 -0.310770
  Si -0.993458 -0.627073  2.427733
   O  0.572757 -0.339804  2.815099
   O -1.577874  0.689500  1.678230
  Si -1.857971  1.914825  0.645947
   O -0.446948  2.518358  0.112655
   O -2.627458  3.146138  1.379461
   H -3.523059  2.999122  1.693626
   O -1.841176 -1.004888  3.759668
   H -1.866923 -0.375767  4.485004
  Si -1.517884 -2.371398 -0.072939
   O -1.085856 -1.911169  1.432030
   O -2.543944 -1.279213 -0.684379
  Si -3.130450  0.023175 -1.464733
   O -2.722752  1.358071 -0.610348
   O -4.748108 -0.170665 -1.504955
   H -5.274610  0.520034 -1.914566
   O -2.565080  0.147266 -2.985895
   H -1.601155  0.254970 -3.042085
   O -2.148248 -3.871006 -0.023268
   H -2.761256 -4.088137  0.683543
   O -0.253479 -2.399305 -1.119896
   H  0.539756 -2.936592 -0.961270
   O  2.447261 -3.022644 -0.861456
   H  2.809331 -3.724477 -0.312490
   O  2.060931  1.267986 -3.733330
   H  1.995654  0.748076 -4.538353
-------------------------------------

16_Si_Multi_Branched_Tri-ring
-------------------------------------
Atom         x         y         z
  Si  1.183242 -0.327396  2.320634
   O  2.166174  0.691839  1.538639
  Si  2.826553  1.678245  0.431478
   O  3.189131  0.828042 -0.920006
   O  1.417262 -1.848517  1.771090
  Si  1.517357 -2.545278  0.292064
  Si  2.843003 -0.584657 -1.637582
   O  1.668146 -1.333693 -0.795561
   O  2.762572 -3.580875  0.193617
   H  3.506289 -3.271486 -0.341973
   O  1.375679 -0.260229  3.929862
   H  2.221597 -0.507298  4.312491
   O  4.082325 -1.651452 -1.623013
   H  4.962619 -1.406170 -1.919925
  Si -1.403683 -2.763975 -0.277418
   O  0.115652 -3.314934 -0.013364
   O -1.838872 -1.867326  1.011439
  Si -1.853626 -0.570808  1.989778
```

```
   O -0.363085  0.131109  2.001832
   O -2.176520 -0.984151  3.525984
   H -2.997040 -1.440966  3.728032
   O -2.420136 -4.002946 -0.527409
   H -2.460894 -4.708719  0.122834
  Si -1.687192 -0.354202 -2.238417
   O -1.432659 -1.839645 -1.612235
   O -2.560648  0.528356 -1.199504
  Si -3.470497  1.132896  0.001622
   O -2.898879  0.527697  1.419010
   O -4.998155  0.646702 -0.290155
   H -5.691338  0.962095  0.294978
   O -3.414929  2.756735  0.085299
   H -2.575157  3.056621  0.469693
   O -2.406380 -0.498072 -3.693475
   H -3.159869 -1.088250 -3.775008
   O -0.303693  0.492492 -2.450084
   H  0.477619  0.125473 -2.896670
   O  2.282469 -0.238157 -3.139558
   H  2.481627 -0.842834 -3.860447
   O  4.174616  2.285851  1.104260
   H  4.702159  2.909482  0.599071
  Si  0.270156  3.406540 -0.254276
   O -0.203006  3.129566 -1.779580
   H -0.246427  2.202279 -2.077543
   O  0.220485  5.030387 -0.111782
   H  0.432193  5.412032  0.743041
   O -0.751706  2.736321  0.852275
   H -0.523014  1.909171  1.303666
   O  1.778562  2.846085  0.035845
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17_Si_Multi_Tetra-ring
-------------------------------------
Atom         x         y         z
  Si  0.986394 -2.251063  1.649097
   O  2.063864 -1.109420  2.083920
  Si  3.238073 -0.106249  1.563600
   O  3.594803 -0.481067  0.019017
   O  1.099803 -2.503702  0.048527
  Si  1.004118 -2.330015 -1.563768
  Si  3.244136 -0.182637 -1.547369
   O  2.074092 -1.198812 -2.038955
   O  1.274960 -3.745029 -2.323141
   H  2.130182 -4.167132 -2.208265
   O  1.232921 -3.628803  2.481703
   H  2.089081 -4.058555  2.412545
   O  4.554206 -0.193004  2.512702
   H  5.013504 -1.033426  2.585028
   O  2.720556  1.430831  1.662006
   O  2.756313  1.361768 -1.681675
   O  4.530028 -0.474151 -2.498739
   H  5.307515  0.080931 -2.400885
  Si  1.495766  2.492190  1.509812
   O  1.042466  2.597303 -0.044273
  Si  1.507521  2.413028 -1.600658
```

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   O  0.153076  1.980484  2.308756
   H  0.242385  1.698051  3.223936
   O  2.015930  3.891864 -2.074783
   H  2.294085  4.002037 -2.987316
   O  0.302656  1.803646 -2.497507
   H -0.616357  2.045584 -2.281689
   O  1.926253  3.928147  2.144004
   H  2.766597  4.315948  1.886930
  Si -2.050256 -1.673294 -1.589234
   O -0.487221 -1.861191 -1.996447
   O -2.206753 -1.835491  0.018544
  Si -2.070180 -1.609406  1.622347
   O -0.503039 -1.743336  2.041178
   O -2.991137 -2.676967  2.439341
   H -2.794360 -3.612521  2.346414
   O -2.995459 -2.737241 -2.381268
   H -2.813756 -3.674495 -2.275277
  Si -3.345617  1.138191 -1.587406
   O -2.543202 -0.196780 -2.054994
   O -3.823452  0.975062 -0.043273
  Si -3.405493  1.192730  1.522440
   O -2.599849 -0.134462  2.037058
   O -4.828801  1.371888  2.298034
   H -4.804245  1.576713  3.235880
   O -2.461139  2.499529  1.711473
   H -1.514881  2.346612  1.888394
   O -4.617979  1.456841 -2.550467
   H -5.425627  0.950432 -2.433227
   O -2.262208  2.361013 -1.770370
   H -2.510115  3.249810 -1.499519
-------------------------------------

18_Si_Multi_Branched_Tetra-ring
-------------------------------------
Atom         x         y         z
  Si  1.083687  2.632641 -1.376605
   O  2.424810  1.884912 -1.896708
  Si  3.533222  0.758897 -1.469325
   O  3.544570  0.663133  0.151399
   O  1.244120  3.030787  0.189531
  Si  0.867959  2.540171  1.707926
  Si  3.104726  0.366140  1.693145
   O  1.836126  1.295202  2.096907
   O  1.010271  3.776280  2.752469
   H  1.861086  4.213281  2.842382
   O  0.659374  3.900629 -2.305351
   H  1.165202  4.717762 -2.305295
   O  4.985491  1.082624 -2.105129
   H  5.414249  1.918635 -1.904915
   O  3.079419 -0.692328 -2.078027
   O  2.671088 -1.192183  1.831908
   O  4.304409  0.757239  2.719897
   H  5.142728  0.294433  2.643758
  Si  1.953986 -1.740445 -1.531875
   O  2.545869 -2.677009 -0.348222
  Si  2.699956 -2.732289  1.282520
```

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   O  0.713978 -0.903325 -0.852254
   H  0.304018 -0.142680 -1.301358
   O  4.123379 -3.467698  1.562483
   H  4.387016 -3.624245  2.472493
   O  1.497410 -3.572585  1.982240
   H  0.603639 -3.219642  1.844540
   O  1.343568 -2.656193 -2.738886
   H  1.917449 -3.028274 -3.414642
  Si -2.250402  2.164384  1.388612
   O -0.671798  2.039902  1.763410
   O -2.382286  2.318364 -0.233511
  Si -1.813131  1.836275 -1.680431
   O -0.182898  1.590659 -1.535782
   O -2.095315  2.940023 -2.835249
   H -1.387877  3.586045 -2.963827
   O -2.971619  3.411285  2.141215
   H -2.668874  4.303241  1.952915
  Si -3.919771 -0.472816  1.494959
   O -3.005180  0.819525  1.888447
   O -4.027200 -0.529342 -0.135093
  Si -3.290606 -0.889585 -1.539430
   O -2.481444  0.419864 -2.089092
   O -4.460353 -1.321529 -2.579845
   H -4.213347 -1.601026 -3.465018
   O -2.201767 -2.076304 -1.311118
   O -5.401807 -0.422264  2.156100
   H -6.069644  0.137847  1.753290
   O -3.224209 -1.826541  2.096153
   H -2.253958 -1.839117  2.095085
  Si -1.503124 -3.143703 -0.290502
   O -2.569947 -4.131686  0.440857
   H -3.117728 -3.706964  1.113964
   O -0.465913 -4.086643 -1.106761
   H  0.018059 -3.728199 -1.865705
   O -0.765038 -2.278115  0.930405
   H -0.249901 -1.529922  0.577257
-------------------------------------

19_Si_Multi_Penta-ring
-------------------------------------
Atom         x         y         z
  Si  0.045043  3.089355  1.007475
   O -1.090875  2.177854  1.742431
  Si -2.658280  1.717429  1.704100
   O -3.126860  1.600010  0.154244
   O -0.153914  3.004180 -0.601813
  Si -0.388789  2.426148 -2.102513
  Si -3.187801  1.215571 -1.424508
   O -1.783857  1.596807 -2.146393
   O -0.363729  3.619359 -3.206774
   H -1.053206  4.287464 -3.182365
   O  0.021854  4.631570  1.523129
   H -0.756578  5.169855  1.360034
   O -3.611789  2.735208  2.539869
   H -3.695882  3.644397  2.242006
   O -2.772116  0.280722  2.450123
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   O -3.444199 -0.384127 -1.572505
   O -4.340091  2.069687 -2.192376
   H -5.254247  1.951256 -1.922485
  Si -2.916426 -1.318565  2.155418
   O -3.824896 -1.506708  0.810725
  Si -3.634179 -1.796865 -0.781103
   O -4.979284 -2.572163 -1.260526
   H -5.067296 -2.820995 -2.183898
   O -3.565787 -2.088264  3.428786
   H -4.451157 -1.848799  3.713680
  Si  2.249932  0.817862 -2.023032
   O  0.831575  1.426308 -2.509248
   O  2.769876  1.584233 -0.696879
  Si  2.935543  2.002559  0.867192
   O  1.489984  2.485950  1.441140
   O  4.052272  3.174131  1.037473
   H  3.854490  4.049530  0.695367
   O  3.398453  0.838361 -3.183887
   H  3.786501  1.671727 -3.464012
  Si  3.092312 -1.892465 -1.102865
   O  2.037159 -0.780066 -1.724174
   O  3.198983 -1.672422  0.508795
  Si  3.895530 -0.832809  1.714774
   O  3.489915  0.741673  1.720676
   O  5.512249 -0.989888  1.584463
   H  6.069766 -0.262307  1.870877
   O  3.301427 -1.561607  3.061509
   H  3.523201 -1.215893  3.930257
   O  4.540825 -1.630259 -1.807723
   H  4.556479 -0.995646 -2.534529
   O  2.599511 -3.401994 -1.443418
   H  1.889969 -3.768124 -0.904289
  Si -0.734378 -2.883693 -1.379450
  Si  0.106985 -1.891223  1.430445
   O  0.196452 -2.542370 -0.069881
   O  0.620610 -0.336967  1.293247
   H  0.336095  0.313744  1.945980
   O  0.953815 -2.786937  2.481426
   H  1.827130 -2.458595  2.756860
   O -0.330943 -1.906918 -2.612828
   H  0.499100 -1.423748 -2.477887
   O -0.434716 -4.425222 -1.831605
   H -0.779668 -5.134657 -1.283425
   O -2.309510 -2.711581 -1.008884
   O -1.452592 -1.956741  1.905224
-------------------------------------

20_Si_Cage_Trigonal_prism
-------------------------------------
Atom         x         y         z
  Si -1.493631 -0.133059  1.739497
   O -1.681490  1.241244  0.857184
  Si -1.517295  1.562911 -0.748178
   O -0.014979  2.139206 -1.021662
   O  0.022364 -0.181275  2.342028
  Si  1.531378 -0.140272  1.713991
```

Si	1.496568	1.576717	-0.749223
O	1.677525	1.249794	0.847493
O	2.655413	-0.304750	2.860554
H	2.566868	0.171467	3.690130
O	-2.494584	-0.227342	3.002858
H	-3.444167	-0.212856	2.857633
O	-2.545967	2.686471	-1.284029
H	-3.491580	2.539778	-1.199139
O	-1.682111	0.109584	-1.498142
O	1.642303	0.130472	-1.518407
O	2.615851	2.656319	-1.183779
H	2.533399	3.119639	-2.021284
Si	-1.515108	-1.436975	-0.964516
O	-0.004049	-1.940383	-1.336779
Si	1.508961	-1.421597	-0.994658
O	-2.633555	-2.443727	-1.549661
H	-2.545772	-2.791522	-2.440807
O	2.626530	-2.411200	-1.609564
H	2.525498	-2.753539	-2.501418
O	1.707760	-1.361327	0.633044
O	-1.678067	-1.365725	0.666125

21_Si_Cage_Tetragonal_prism

Atom	x	y	z
Si	2.678469	0.262476	0.256043
O	1.931711	0.948801	1.534264
Si	0.553561	1.636964	2.059899
O	-0.123395	2.498525	0.850059
O	2.166009	1.018855	-1.096656
Si	1.024249	1.028005	-2.263093
Si	-1.089103	2.421685	-0.462557
O	-0.216575	1.958625	-1.755836
O	1.619127	1.550946	-3.677768
H	2.034270	2.416301	-3.715450
O	4.291432	0.324551	0.407084
H	4.722629	1.181777	0.448764
O	-1.714530	3.873040	-0.826114
H	-2.278222	4.311409	-0.183887
Si	-0.562286	-1.645589	-2.050442
O	0.491948	-0.488694	-2.511742
O	0.120596	-2.495077	-0.835931
Si	1.111025	-2.411810	0.458337
O	2.278870	-1.312804	0.179389
O	1.861337	-3.823359	0.729747
H	1.331920	-4.610029	0.882453
O	-0.974706	-2.605893	-3.290111
H	-0.283504	-3.082663	-3.756723
Si	-2.680039	-0.250127	-0.252828
O	-1.936571	-0.949093	-1.526446
O	-2.188922	-1.018545	1.101231
Si	-1.036614	-1.043282	2.251141
O	0.224723	-1.947487	1.747054
O	-1.726294	-1.667609	3.579488
H	-1.193020	-1.786151	4.369381

O	-0.500036	0.475257	2.509449
O	-4.292768	-0.289391	-0.414291
H	-4.732972	-1.140932	-0.474842
O	-2.255809	1.317951	-0.171675
O	0.961276	2.589112	3.307772
H	0.269850	3.072059	3.767564

22_Si_Cage_Pentagonal_prism

Atom	x	y	z
Si	-0.137443	2.497956	-1.635821
O	1.227096	1.736886	-2.099778
Si	2.566836	0.967979	-1.581236
O	2.814538	1.369656	-0.020933
O	-0.115444	2.673313	-0.022710
Si	-0.145980	2.509530	1.591255
Si	2.570260	1.011092	1.549785
O	1.181720	1.686448	2.055938
O	-0.229128	3.950948	2.342487
H	0.517087	4.550181	2.260944
O	-0.282476	3.929602	-2.395750
H	0.438705	4.559917	-2.324122
O	3.849233	1.353157	-2.502250
H	4.093715	2.278086	-2.585546
O	2.386592	-0.636372	-1.719797
O	2.496819	-0.606310	1.710782
O	3.749409	1.630384	2.481885
H	4.648260	1.318005	2.351726
Si	1.647229	-2.071374	-1.551423
O	1.734041	-2.522473	0.013861
Si	1.690659	-2.008899	1.556489
O	2.391536	-3.183709	2.434827
H	2.430592	-3.081018	3.389074
O	2.318515	-3.194334	-2.515466
H	3.252076	-3.393340	-2.407981
Si	-2.689872	0.715182	1.587887
O	-1.475532	1.698279	2.047183
O	-2.880898	0.847538	-0.019872
Si	-2.660531	0.665917	-1.619737
O	-1.429490	1.624351	-2.084750
O	-4.011096	1.009496	-2.455964
H	-4.353069	1.906378	-2.423772
O	-4.057058	1.070619	2.391037
H	-4.397047	1.967509	2.342582
Si	-1.402717	-2.105830	1.638733
O	-2.339272	-0.821572	1.983027
O	-1.531970	-2.451309	0.054383
Si	-1.456436	-2.200101	-1.546052
O	-2.319141	-0.885126	-1.959938
O	-2.075402	-3.531312	-2.245377
H	-2.111529	-3.570713	-3.204421
O	0.089399	-1.939055	-1.994447
O	-1.826939	-3.381030	2.552749
H	-2.725707	-3.714063	2.488922
O	0.142309	-1.748233	2.000654

23_Si_Cage_Hexagonal_prism

Atom	x	y	z
O	0.734071	-3.268266	-0.002346
O	3.213917	-1.001345	-0.010413
O	-0.734315	3.267021	0.000446
O	-2.487191	-2.293056	0.013006
O	2.486744	2.292255	0.012993
O	-3.213162	1.001399	-0.007586
O	-0.798487	-2.492018	2.038476
O	2.617927	0.564450	2.038777
O	1.751932	-1.874062	-2.035371
O	-1.790284	1.949299	2.037771
O	-2.624685	-0.624415	-2.036330
O	0.803727	2.552757	-2.033943
O	1.791566	-1.950602	2.034523
O	2.623888	0.625881	-2.037840
O	0.800050	2.490814	2.040043
O	-0.804854	-2.551073	-2.034861
O	-1.753129	1.875457	-2.033548
O	-2.616267	-0.565951	2.039838
Si	0.664400	-3.041214	1.604338
Si	2.994503	-0.954441	1.597673
Si	2.982615	-0.897485	-1.614444
Si	-0.663229	3.039842	1.607031
Si	-2.315727	-2.158810	-1.595874
Si	2.314718	2.159844	-1.595924
Si	-0.691587	3.024812	-1.604940
Si	-2.319817	-2.102878	1.616969
Si	-2.983414	0.898654	-1.611870
Si	-2.993191	0.953299	1.600386
Si	0.690643	-3.023879	-1.607424
Si	2.320961	2.101583	1.617010
O	3.401810	3.005946	2.433014
H	3.346246	3.961493	2.352401
O	4.319048	-1.475756	2.388193
H	5.132177	-0.973308	2.294036
O	-0.873572	4.441013	2.409328
H	-1.717739	4.891211	2.324280
O	0.875325	-4.442529	2.406205
H	1.719360	-4.892820	2.320332
O	-4.317502	1.473781	2.391832
H	-5.130546	0.971181	2.297753
O	-3.399961	-3.007623	2.433488
H	-3.344909	-3.963110	2.351828
O	1.128488	-4.366939	-2.417009
H	0.591993	-5.156737	-2.313085
O	-3.295413	-3.193614	-2.383649
H	-4.244260	-3.064180	-2.309832
O	-4.339207	1.281318	-2.428088
H	-4.669015	2.181273	-2.366406
O	-1.129961	4.368863	-2.412628
H	-0.593134	5.158392	-2.308357
O	3.294076	3.195393	-2.383144

H	4.242951	3.065975	-2.309629
O	4.337602	-1.279881	-2.432134
H	4.667436	-2.179866	-2.371032

24_Si_Cage_Heptagonal_prism

Atom	x	y	z
O	1.009789	-3.515133	0.152666
O	4.038356	-2.005778	0.213244
O	2.470830	3.932347	0.196779
O	-2.063552	-2.157904	0.085947
O	4.728455	1.317526	0.250074
O	-2.933112	1.179824	0.021294
O	-0.394967	-2.389752	2.128367
O	3.941189	-0.291278	2.231181
O	2.368037	-2.323390	-1.816053
O	-1.652631	2.305430	2.078923
O	-2.014059	-0.417767	-1.913115
O	3.286669	2.335702	-1.755702
O	2.239665	-2.305547	2.162225
O	3.949008	-0.213610	-1.765802
O	3.098274	2.204747	2.137709
O	-0.267069	-2.389132	-1.875366
O	-1.443696	2.156379	-1.936132
O	-2.002533	-0.304520	2.008208
Si	0.951827	-3.208864	1.748430
Si	3.755320	-1.849232	1.806726
Si	3.841993	-1.786431	-1.385807
Si	2.324485	3.584520	1.779228
Si	-1.791608	-1.975608	-1.507254
Si	4.447145	1.278116	-1.351529
Si	2.409293	3.657987	-1.405345
Si	-1.874549	-1.887691	1.678570
Si	-2.584390	1.057988	-1.562728
Si	-2.671434	1.128881	1.625455
Si	1.066147	-3.215264	-1.444494
Si	4.358887	1.222197	1.831420
O	5.650005	1.596304	2.749278
H	6.016157	2.481966	2.683287
O	4.741535	-2.817728	2.667048
H	5.689527	-2.676733	2.604323
O	3.010693	4.749038	2.687936
H	2.692495	5.650569	2.594875
O	0.898854	-4.597135	2.598396
H	1.634287	-5.209705	2.515935
O	-4.055933	1.386195	2.443040
H	-4.795134	0.793057	2.286951
O	-3.042126	-2.633529	2.533554
H	-3.130351	-3.586926	2.456749
O	1.204479	-4.603326	-2.285420
H	0.499321	-5.251865	-2.213938
O	-2.757385	-2.961013	-2.371710
H	-3.708340	-2.845324	-2.301455
O	-3.923270	1.255777	-2.468009
H	-4.380483	2.099555	-2.429622

O	2.933268	4.958829	-2.232723
H	3.835664	5.256521	-2.092101
O	5.777069	1.716676	-2.181511
H	6.577293	1.196530	-2.074048
O	5.018064	-2.540066	-2.222019
H	5.120055	-3.489195	-2.115474
O	-0.871240	3.832861	0.062100
O	0.879379	3.400800	-1.879167
O	0.749591	3.395857	2.138040
Si	-0.788302	3.620277	1.671105
Si	-0.702620	3.540509	-1.528033
O	-1.317889	4.942173	2.460489
H	-2.224572	5.226108	2.319272
O	-1.406440	4.714636	-2.410173
H	-1.093753	5.616574	-2.303820

25_Si_Cage_Octagonal_prism

Atom	x	y	z
O	1.006337	-3.448859	0.118165
O	4.103661	-2.006772	0.160255
O	3.740026	4.359227	0.357007
O	-2.116706	-2.288194	0.119685
O	5.294697	1.035791	0.325312
O	-3.547084	0.787793	0.040157
O	-0.360988	-2.292773	2.102158
O	4.150237	-0.377282	2.252870
O	2.259451	-1.986413	-1.737748
O	-2.383316	2.257009	1.948793
O	-2.275514	-0.563564	-1.886223
O	3.968339	2.479559	-1.498079
O	2.271417	-2.217115	2.094415
O	4.130356	-0.133664	-1.747870
O	3.437825	2.159486	1.845030
O	-0.344054	-2.352596	-1.880051
O	-2.132620	2.062609	-1.799692
O	-2.149771	-0.363172	1.973004
Si	0.976037	-3.125520	1.713710
Si	3.826366	-1.894656	1.759691
Si	3.828557	-1.692605	-1.412872
Si	3.403103	3.790486	1.844521
Si	-1.895051	-2.092096	-1.480526
Si	4.932290	1.195738	-1.258317
Si	3.675076	4.060113	-1.248015
Si	-1.895859	-1.943770	1.694858
Si	-3.103683	0.782004	-1.527745
Si	-3.155026	0.869805	1.619993
Si	1.062758	-3.050100	-1.458747
Si	4.686885	1.094425	1.840100
O	5.821630	1.571054	2.903397
H	5.776513	2.503435	3.156353
O	4.717270	-2.985915	2.574551
H	5.670341	-2.982302	2.454232
O	4.578663	4.207020	2.903269
H	4.826759	5.127140	3.025615

```
   O  0.932257 -4.506825  2.573971
   H  1.661928 -5.125482  2.484789
   O -4.498708  0.847682  2.538083
   H -5.104768  0.107304  2.451566
   O -2.969328 -2.753023  2.613466
   H -2.997561 -3.711506  2.555610
   O  1.390099 -4.360507 -2.367591
   H  0.830866 -5.136354 -2.278920
   O -2.776414 -3.174840 -2.317642
   H -3.728449 -3.186270 -2.189843
   O -4.417320  0.796965 -2.488468
   H -5.038077  1.525689 -2.406526
   O  4.715288  5.019654 -2.049655
   H  5.652027  4.957482 -1.845650
   O  6.281267  1.455611 -2.130143
   H  6.994139  0.813222 -2.089049
   O  4.824553 -2.573190 -2.352249
   H  4.833499 -3.527811 -2.244202
   O -2.331720  4.042566 -0.012324
   O  2.192750  4.404249 -1.810776
   O  1.935726  4.311186  2.292839
  Si -2.177956  3.832150  1.595464
  Si -1.969773  3.659185 -1.553180
   O -3.232620  4.779961  2.394899
   H -4.168892  4.690302  2.199348
   O -2.996481  4.398562 -2.577846
   H -3.084286  5.354344 -2.535507
   O  0.740474  5.395177  0.166901
   O -0.419062  4.059945 -1.841028
   O -0.695642  4.269372  2.088541
  Si  0.766733  5.091301 -1.430165
  Si  0.637590  5.143477  1.769070
   O  0.648078  6.550444  2.585695
   H -0.058523  7.180431  2.421753
   O  0.509962  6.454562 -2.281886
   H  1.086974  7.207451 -2.130600
-------------------------------------
```

(2) Aluminosilicates (Monocycles, Multicycles, and Cages without a cation)

```
26_SiAl_Mono_3MR
-------------------------------------
Atom         x         y         z
  Si -5.312712  0.338378  0.288078
   O -6.942379  0.364731  0.459253
   H -7.469033  0.180395 -0.321342
   O -4.797723  0.296115  1.843159
   H -3.898233  0.584521  2.010861
   O -4.714313  1.605319 -0.523020
   O -4.872731  2.293788 -3.359493
   H -5.382824  1.688763 -3.912871
   O -2.455558  2.772330 -1.882595
   H -1.794233  2.815469 -2.573729
   O -3.532629  0.025855 -2.543429
   O -4.869310 -1.037681 -0.509215
```

```
   O -2.875438 -2.448489 -1.590104
   H -2.363398 -2.311540 -0.789788
  Si -4.064668 -1.363316 -1.911486
   O -5.052128 -2.067302 -3.013856
   H -5.408627 -2.930767 -2.792880
  Al -3.753122  1.655328 -1.972510
   H -5.243007  3.182468 -3.428068
-------------------------------------

27_SiAl_Mono_4MR
-------------------------------------
Atom         x         y         z
   O -6.827363  1.845965  0.058893
   O -8.209360 -0.240841  1.041619
   O -5.426788 -1.169218  1.147067
   O -4.375842  0.453557 -0.754541
  Si -8.251253  1.309014  0.581935
  Si -4.455852 -1.028351 -0.133337
   O -4.250963  3.216756  0.178598
   H -4.601896  3.744468  0.895896
   O -5.332894  2.395056 -2.338627
   H -5.489109  3.277153 -2.696512
   O -8.682066  2.310276  1.822619
   H -9.511451  2.099330  2.257035
   O -9.426777  1.489635 -0.569748
   H -9.541156  0.741947 -1.160231
   O -7.316544 -2.759114  0.002802
   H -6.589197 -2.673127 -0.672208
   O -7.528965 -2.290739  2.900179
   H -6.946005 -2.951265  3.275315
   O -2.913956 -1.491818  0.196075
   H -2.807203 -2.324698  0.661587
   O -5.147075 -2.090525 -1.238395
   H -4.822216 -2.115232 -2.141845
  Al -5.210562  1.952907 -0.494164
  Al -7.110448 -1.516768  1.419632
   H -4.818140  1.878000 -2.970822
   H -8.160391 -2.934166 -0.427898
-------------------------------------

28_SiAl_Mono_5MR
-------------------------------------
Atom         x         y         z
   O -3.089453 -0.093985 -0.216671
   O -2.712767  2.039029  1.281203
   O -0.597439  1.038422 -0.423726
   O  1.596859 -0.267310  0.232696
   O -0.531965 -1.702095 -0.379784
  Si -3.354133  0.540066  1.245011
  Si  0.654145 -1.558285  0.704986
  Si  1.035625  0.929497 -0.719499
   O -2.606383 -0.454033  2.350450
   H -2.833161 -0.314045  3.274520
   O -4.935278  0.556967  1.681830
   H -5.487426  1.242644  1.298830
   O -1.286137 -0.000174 -2.751396
```

H	-1.629984	-0.517289	-3.481967
O	-2.690434	-2.152481	-1.810726
H	-3.590573	-2.163865	-1.460593
O	1.706840	-2.811759	0.732752
H	1.405995	-3.623291	1.147700
O	0.063647	-1.324061	2.211887
H	-0.864503	-1.036221	2.270930
O	1.270787	0.696789	-2.307873
H	0.420333	0.460466	-2.747819
O	1.696969	2.363270	-0.230245
H	2.293729	2.828349	-0.823890
O	-0.243606	3.364511	1.201801
H	0.687430	3.243728	0.904007
O	-1.920350	3.569954	-1.140617
H	-1.631229	3.402409	-2.038149
Al	-1.508502	2.490610	0.126114
Al	-1.667768	-0.576413	-1.127211
H	-0.301507	3.329161	2.164698
H	-2.263299	-2.973468	-1.532052

29_SiAl_Mono_6MR

Atom	x	y	z
O	-2.466808	4.458475	0.259116
O	-3.399971	1.987694	-0.970631
O	-0.834138	2.219777	0.342193
H	-0.156697	2.881377	0.581079
O	-3.329262	2.122202	1.844700
Si	-2.092354	5.906343	0.855853
Si	-3.344476	1.125503	3.109771
O	-2.804948	7.059658	-0.082806
H	-3.008823	7.885519	0.360967
O	-0.462110	6.167217	0.767472
H	0.106854	5.435727	1.045307
O	-2.608873	6.094238	2.394319
O	-3.960871	1.850887	4.445010
H	-3.791843	2.804314	4.573324
O	-1.882175	0.486463	3.448475
O	-4.362906	-0.128691	2.736289
H	-4.255823	-0.917658	3.271615
O	0.724909	1.860950	3.508284
O	0.625513	-0.819928	4.087201
H	1.311079	-0.572418	4.722117
O	-0.006976	0.060049	1.352523
H	0.835765	-0.257274	1.019298
O	-1.136808	3.787947	3.220632
O	-1.013303	5.950144	4.851534
H	-0.114018	5.546965	4.914194
O	-3.528947	4.523754	4.721900
H	-4.374167	4.975401	4.688972
Si	0.422062	3.417074	3.238774
O	1.101174	4.409274	4.379951
H	1.982754	4.252812	4.728084
O	0.956537	3.848736	1.707593
H	1.890689	3.750299	1.495587

Al	-2.223468	5.050895	3.711848
Al	-2.630515	2.741420	0.391120
Al	-0.226582	0.478837	3.045469
H	-1.240225	6.414161	5.665000
H	-3.157055	2.281423	-1.849247
H	0.274095	-1.691055	4.312284
H	-0.491769	1.295306	0.612407

30_SiAl_Mono_7MR

Atom	x	y	z
O	-3.412635	-1.362063	1.009247
O	-0.634670	2.506566	2.164931
O	0.247411	3.614458	-0.331284
O	1.233518	1.152103	-0.610793
O	-0.981792	-0.203655	-0.115556
Si	-4.642508	-0.313602	0.969151
Si	0.656858	-0.213673	0.058561
Si	1.573586	2.754214	-0.662015
O	-5.837326	-0.690905	2.012367
H	-6.054591	0.025667	2.638243
O	-4.147181	1.224214	1.243570
O	-1.004488	-2.956918	0.011188
H	-1.288662	-3.859292	0.157405
O	-3.017196	-1.536277	-1.651644
H	-2.644164	-1.353864	-2.521642
O	1.289070	-1.466488	-0.786760
H	0.784227	-2.280632	-0.631651
O	1.064972	-0.341670	1.632067
H	0.377343	-0.120770	2.288343
O	2.189122	3.096122	-2.143745
H	1.729757	2.735338	-2.905565
O	2.722516	3.148428	0.438891
H	3.564653	2.691363	0.376137
O	-2.253237	4.584951	1.012932
H	-2.288030	5.370897	0.461380
O	-2.138130	2.050722	-0.210787
H	-1.657695	1.158182	-0.285820
Al	-1.098147	3.285027	0.695879
Al	-2.057399	-1.595635	-0.039717
H	-3.923474	-1.139742	-1.558141
Si	-1.265624	1.882303	3.512998
Al	-4.303286	2.203416	2.710368
O	-5.148910	-0.438873	-0.618362
H	-5.855525	0.126788	-0.940820
O	-2.847316	2.192439	3.634765
O	-0.936577	0.258704	3.395599
H	-1.214033	-0.323289	4.107335
O	-0.488180	2.381956	4.873655
H	-0.758969	3.226075	5.241752
O	-5.790794	1.689701	3.430400
H	-6.047334	1.901509	4.328336
O	-4.359114	3.930620	2.080755
H	-5.136931	4.261372	1.617918
H	-3.467239	4.304790	1.619043

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   H -3.004515  1.820650  0.229607
-------------------------------------

31_SiAl_Mono_8MR
-------------------------------------
Atom         x         y         z
  Si -0.330681  1.891928 -0.593040
   O  0.733865  1.226600  0.463937
   H  0.366491  0.746888  1.222248
   O  0.593437  2.175040 -1.922666
   H  0.203718  2.726196 -2.604537
   O -1.572889  0.868420 -0.905417
   O -1.008808  3.254337 -0.022804
   O -4.207218 -0.231700 -0.041549
   H -4.775048 -0.380144  0.821959
   O -2.554453  1.094118  1.750634
   O -3.966744  2.533128 -0.425623
   H -3.634093  3.411511 -0.156270
   O -1.470681  3.404413  2.645780
   H -1.731439  2.517705  2.304609
   O -0.421340  5.794619  1.458368
   H -0.512887  6.608300  0.961704
   O -3.157529  4.848264  0.824900
  Si -4.457689  5.372008  1.647678
  Si -2.083679  0.052541  2.917063
   O -2.838392 -1.413083  2.781703
   H -2.473161 -2.067865  2.179501
   O -0.456972 -0.104633  2.691513
   H  0.068936 -0.587853  3.334764
   O -2.487867  0.679665  4.343666
   O -4.044763  5.690232  3.233110
   H -3.520668  6.477521  3.403308
   O -4.919644  6.771937  0.909196
   H -5.737892  7.170563  1.215255
   O -5.623093  4.278067  1.730792
   O -5.305644  1.318044  4.130818
   O -4.062027  1.663900  6.564938
   H -3.441171  1.898674  7.266152
   O -3.174098  3.415912  4.466490
   H -3.718462  4.200003  4.288207
   O -6.792511  1.642978  1.909566
   O -8.444717  3.876651  1.062526
   H -8.565476  4.787530  1.332033
   O -6.364124  2.770044 -0.579108
   H -6.685932  3.284872 -1.325102
  Si -6.228520  0.624637  3.001734
   O -5.335708 -0.513768  2.140788
   H -4.694268 -1.069373  2.616688
   O -7.410053 -0.275102  3.708291
   H -7.931500  0.153776  4.390761
  Al -1.469562  4.467255  1.129198
  Al -6.853651  3.200730  1.150755
  Al -3.767100  1.796922  4.718488
  Al -2.996982  1.144187  0.045826
   H -4.660882 -0.542956 -0.831870
   H -5.290221  2.636979 -0.616468
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   H -4.787167  1.141862  6.931759
   H -2.108126  3.531397  3.451900
-------------------------------------

32_SiAl_Mono_9MR
-------------------------------------
Atom         x         y         z
   O -1.260668  4.016405 -0.896126
  Si -1.488138  2.619701 -0.079548
  Si -2.098939  5.417847 -1.023782
   O -0.204412  1.634470 -0.265483
   H -0.335688  0.918699 -0.914237
   O -1.678169  3.101853  1.476940
   H -1.899062  2.435496  2.132504
   O -2.858439  1.852891 -0.576949
   O -1.915548  6.392303  0.274085
   H -2.675610  6.376000  0.884617
   O -1.505263  6.121571 -2.371390
   H -1.772987  7.026719 -2.548021
   O -3.688213  5.032502 -1.170046
   O -1.466412 -0.153853 -1.903724
   H -1.268089 -0.953681 -2.391537
   O -3.472872 -0.848997  0.141644
   H -4.454757 -0.957361  0.260656
   O -4.459982  0.014973 -2.261629
   O -4.944220  3.057971  0.444060
   H -5.804955  2.627084  0.205847
   O -4.409121  5.844219  1.362985
   H -4.836921  5.897350  2.217672
   O -6.523822  5.044690 -0.670382
  Si -5.978353 -0.500770 -1.992544
  Si -7.669969  4.029162 -1.186737
   O -6.296880 -1.869383 -2.833349
   H -7.199243 -1.928353 -3.188380
   O -5.987981 -0.773265 -0.347425
   H -6.789371 -1.082872  0.084022
   O -7.087712  0.621188 -2.382868
   O -9.167316  4.430345 -0.662533
   H -9.497875  5.305901 -0.877764
   O -7.346203  2.535683 -0.553129
   H -7.357817  1.781483 -1.186050
   O -7.638687  3.924906 -2.830908
   O -9.015488  2.085854 -3.789416
   H -8.527628  2.928453 -3.415818
   O -8.828539 -0.928972 -3.929038
   H -9.229774 -1.285535 -4.722538
   O -6.879272  0.847591 -5.225217
   O -6.411445  3.500673 -5.332963
   O -6.557153  6.284671 -4.255465
   H -7.407239  6.724514 -4.236527
   O -4.758867  4.271701 -3.319165
   H -4.286700  4.623333 -2.494641
  Si -5.800964  2.016560 -5.519527
   O -5.207402  1.919665 -7.046508
   H -4.883023  1.063260 -7.334614
   O -4.545557  1.888826 -4.414673
```

H	-4.520690	1.136911	-3.798974
Al	-6.441608	4.593605	-3.980955
Al	-4.955314	4.873356	0.045093
Al	-3.028789	0.255735	-1.300741
Al	-7.975952	0.572498	-3.914450
H	-4.418389	3.383819	-3.593050
H	-4.177015	2.525120	0.078875
H	-3.009257	-0.874454	0.986701
H	-9.957853	2.100708	-3.590177

33_SiAl_Mono_10MR

Atom	x	y	z
O	0.186184	5.086727	-1.311256
H	-0.213761	5.524561	-0.525411
O	-0.300832	5.950797	-4.132821
H	0.257579	5.457992	-4.734254
O	-1.453616	3.502545	-2.929204
O	-2.249043	6.194963	-2.061305
Si	-1.277703	2.129654	-2.109069
Si	-2.923750	6.224527	-0.605233
O	-0.638693	0.952265	-3.060651
H	-0.831134	0.060000	-2.726525
O	-0.177071	2.541550	-0.910073
H	0.077207	1.895583	-0.246895
O	-2.657424	1.605875	-1.426392
O	-1.643402	5.951756	0.428827
H	-1.787572	5.898292	1.376680
O	-3.639442	7.666287	-0.298045
H	-4.320297	7.619208	0.393785
O	-4.041998	5.032914	-0.434000
O	-1.831423	-1.043897	-1.499882
H	-1.891827	-1.999221	-1.535057
O	-3.822639	-0.160168	0.561300
H	-4.813828	-0.220379	0.637250
O	-4.680986	-0.429383	-2.012913
O	-5.941622	3.478630	1.089436
H	-6.569590	2.899969	0.559578
O	-5.514816	6.467156	1.428835
H	-6.267323	6.811962	1.910891
O	-6.905317	5.119310	-0.841696
Si	-6.263902	-0.558764	-1.692827
Si	-7.898462	4.007743	-1.461912
O	-6.894280	-2.001153	-2.133707
H	-7.582996	-1.932531	-2.819882
O	-6.324015	-0.374869	-0.035494
H	-7.139183	-0.550281	0.442785
O	-7.108341	0.633954	-2.413120
O	-9.486129	4.355087	-1.306525
H	-9.803465	5.191893	-1.655822
O	-7.645695	2.593415	-0.632350
H	-7.500496	1.811490	-1.212149
O	-7.485649	3.779494	-3.037128
O	-8.795197	2.044007	-4.206519
H	-8.331952	2.877144	-3.777465

```
   O -8.574382 -0.950797 -4.158086
   H -8.824150 -1.361927 -4.986373
   O -6.457238  0.836152 -5.215978
   O -5.544255  3.378920 -5.088041
   O -5.652236  5.982245 -3.692232
   H -6.018840  6.487719 -2.963352
   O -4.678086  3.528679 -2.436451
   H -4.249448  4.043908 -1.695580
  Si -5.169830  1.817033 -5.298726
   O -4.418547  1.707568 -6.753798
   H -4.194126  0.827846 -7.065232
   O -4.126008  1.405404 -4.064708
   H -4.371548  0.625460 -3.540256
  Al -5.872125  4.276262 -3.647463
  Al -5.620568  5.146228  0.324679
  Al -1.023863  5.182862 -2.776035
  Al -3.198496 -0.027008 -1.191134
  Al -7.722391  0.553395 -4.071762
   H -4.141174  2.754226 -2.713447
   H -5.331527  2.956966  1.623273
   H  0.308470  4.138679 -1.045398
   H -3.424614  0.240929  1.342098
   H -9.747244  2.051860 -4.059146
-------------------------------------

34_SiAl_Mono_11MR
-------------------------------------
Atom         x         y         z
   O  3.972214 -2.106748  1.953054
   H  4.127561 -2.681109  1.183824
   O  1.578952 -1.982145  3.229896
   H  1.038077 -2.766794  2.981961
   O  2.637529  0.188858  2.257566
   O  1.716779 -1.747649  0.582635
   O  0.159730  1.592803  1.953372
   H -0.595316  1.135587  2.410849
   O  2.151891  2.591735  3.898369
   H  2.341352  2.153481  4.727213
   O  2.362879  2.923394  1.152708
   O  1.637722 -2.152504 -2.196856
   H  0.916862 -1.484652 -2.104415
   O  3.613154 -3.533854 -0.455360
   H  3.946170 -4.376948 -0.764389
   O  0.677195 -4.193563 -0.510487
   O -1.206465  5.593830  1.946204
   H -0.935230  6.476933  2.208589
   O -1.243708  5.608046 -0.790259
   O -0.997916  3.391500  0.555304
   O -0.451405 -5.710573 -2.468499
   H  0.205990 -5.483888 -3.130644
   O -1.625012 -5.465585 -0.114599
   H -1.325636 -6.345394  0.134561
   O -1.541187 -3.342841 -1.675164
   O -0.913273  1.508154 -1.637599
   H -0.594250  0.543240 -1.390071
   O -3.109630  3.435337 -1.464044
```

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   H -2.853831  4.361076 -1.534472
   O -4.195249  2.008258  2.232880
   O -3.035235 -0.836963 -1.269557
   H -3.089311  0.006240 -0.684915
   O -0.293524 -0.793175 -0.967890
   H  0.347741 -0.788779 -0.228142
   O -1.938966 -2.238247  0.963193
   O -2.704533  1.078499  0.302365
   O -4.175355 -0.622900  1.726496
   H -3.661067 -1.407602  1.485490
   O -2.019808  0.507293  2.854474
   O  0.150279 -0.328035  4.371857
   O -0.097125 -3.801129  2.192973
   H  0.197819 -4.159174  1.339335
   O -2.746658 -4.382355  2.346523
   H -2.734966 -4.930041  1.549822
   O -1.707410 -2.294961  3.608130
   O -2.461093 -0.385907  5.647065
   H -2.837410  0.468318  5.859875
   H -0.837931  6.381723 -1.188570
  Si -3.257892  0.734691  1.816408
  Si -1.636698 -3.175486  2.266697
  Si -0.709349 -4.664831 -1.238640
  Si -0.575978  4.967518  0.570796
  Si  2.505181 -1.377644  1.962821
   O  3.673612  5.053223  0.296986
   H  3.758676  5.996740  0.143457
   O  2.502607  5.073279  2.743206
   O  1.036994  5.172551  0.519912
   H  2.460529  4.348978  3.395270
  Si  2.404480  4.533743  1.195248
  Al  1.938836  1.758706  2.383143
  Al  1.968318 -3.036638 -0.574044
  Al -1.661788 -1.914362 -0.709884
  Al -1.670880 -0.650815  4.144165
  Al -2.026322  2.474956 -0.542689
   H -0.487628  1.839360 -2.434664
   H -0.229461  2.344027  1.412298
   H -3.897656 -1.124259 -1.591005
   H  2.328045 -1.831233 -2.790210
   H  0.803254 -1.039767  3.957441
   H  0.470576 -0.030113  5.230779
   H -4.459375  2.106961  3.150644
-------------------------------------

35_SiAl_Mono_12MR
-------------------------------------
Atom         x         y         z
   O  3.752410 -2.335256  3.009507
   H  4.040608 -2.727646  2.163769
   O  1.174150 -2.145154  3.864074
   H  0.702869 -2.901368  3.456982
   O  2.459717  0.027003  3.394860
   O  1.831568 -1.547041  1.331155
   O  0.656711  2.195246  3.434962
   H  0.631687  2.964609  4.026662
```

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 O  3.559058  2.776697  3.050850
 H  4.100501  2.797933  3.840676
 O  1.967386  1.684418  1.033076
 O  2.262784 -1.300588 -1.430141
 H  1.229831 -1.089024 -1.651623
 O  3.840050 -3.140553  0.339558
 H  4.307880 -3.799194 -0.173942
 O  1.010834 -3.641351 -0.488097
 O -0.320565  4.855664  3.016118
 H -0.054509  5.755919  3.217807
 O -2.523845  4.756357  1.391234
 O -0.774372  2.860450  1.515792
 O  0.530681 -5.379250 -2.520468
 H  1.241638 -4.991655 -3.036448
 O -0.868677 -5.544071 -0.280271
 H -0.378762 -6.309705  0.032256
 O -1.295200 -3.477063 -1.789077
 O -0.187225  0.112263  1.270513
 H -0.738389 -0.749500  1.141654
 O -0.422256  1.721514 -1.263606
 H  0.302501  2.326723 -1.473775
 O -4.222241  2.525114  1.758864
 O -2.910612 -0.881643 -1.338176
 H -2.900821 -0.057708 -0.676127
 O -0.114107 -0.866256 -1.726327
 H -0.233866  0.109950 -1.768635
 O -1.395976 -1.966580  0.663112
 O -2.593335  0.935758  0.315532
 O -4.954422  0.098375  1.247151
 H -4.906923 -0.845145  1.416630
 O -2.851143  0.491784  2.916838
 O -0.535952 -0.301380  4.372413
 O -0.195838 -3.798936  2.209712
 H  0.328661 -4.005289  1.421942
 O -2.734299 -4.189222  1.376223
 H -2.342088 -4.860471  0.794968
 O -2.126934 -2.301851  3.193363
 O -3.024012 -0.817958  5.548720
 H -3.935628 -1.090951  5.651959
 H -2.853139  5.614135  1.110395
Si -3.636417  1.009674  1.611489
Si -1.651747 -3.065064  1.870848
Si -0.113498 -4.487388 -1.309153
Si -0.898573  4.500754  1.515033
Si  2.354262 -1.498168  2.875112
 O  3.340434  1.267806 -1.148482
 H  3.790147  1.543518 -1.953504
 O  3.886351  3.457326  0.452597
 O -0.085349  5.219160  0.339555
 H  4.067134  3.298359  1.404784
Si  2.711663  2.453620 -0.178246
 O  2.753339  5.729973 -0.075970
 H  2.862499  6.535159  0.441289
 O  0.789632  5.975650 -2.256979
 H  1.371301  5.963359 -3.017750
 O  1.736706  3.425287 -1.035059
```

Al	1.173391	5.079908	-0.845720
Al	2.308330	1.616645	2.752858
Al	2.272982	-2.516263	-0.066723
Al	-1.395379	-1.896321	-1.100785
Al	-2.297269	-0.757154	3.984445
Al	-0.921189	1.532748	0.381500
H	0.740552	-0.191530	1.125713
H	3.378271	5.006539	0.221006
H	0.009358	2.448174	2.650304
H	-3.276008	-0.632262	-2.194725
H	2.731167	-0.447038	-1.312483
H	0.166146	-1.021939	4.252550
H	-0.159831	0.563906	4.138095
H	-3.637085	3.289704	1.634696

36_SiAl_Multi_Mono-ring

Atom	x	y	z
O	-6.827363	1.845965	0.058893
O	-8.209360	-0.240841	1.041619
O	-5.426788	-1.169218	1.147067
O	-4.375842	0.453557	-0.754541
Si	-8.251253	1.309014	0.581935
Si	-4.455852	-1.028351	-0.133337
O	-4.250963	3.216756	0.178598
H	-4.601896	3.744468	0.895896
O	-5.332894	2.395056	-2.338627
H	-5.489109	3.277153	-2.696512
O	-8.682066	2.310276	1.822619
H	-9.511451	2.099330	2.257035
O	-9.426777	1.489635	-0.569748
H	-9.541156	0.741947	-1.160231
O	-7.316544	-2.759114	0.002802
H	-6.589197	-2.673127	-0.672208
O	-7.528965	-2.290739	2.900179
H	-6.946005	-2.951265	3.275315
O	-2.913956	-1.491818	0.196075
H	-2.807203	-2.324698	0.661587
O	-5.147075	-2.090525	-1.238395
H	-4.822216	-2.115232	-2.141845
Al	-5.210562	1.952907	-0.494164
Al	-7.110448	-1.516768	1.419632
H	-4.818140	1.878000	-2.970822
H	-8.160391	-2.934166	-0.427898

37_SiAl_Multi_Branched_Mono-ring

Atom	x	y	z
O	-6.717121	2.006037	0.421858
O	-8.016132	-0.128592	1.453341
O	-5.410930	-1.410144	1.142895
O	-4.573111	0.393792	-0.692686
Si	-8.133509	1.329516	0.782574
Si	-4.679789	-1.146727	-0.267958

O	-4.268839	3.318083	-0.247834
O	-5.898205	2.132581	-2.332615
H	-6.274700	2.948947	-2.680846
O	-9.010131	2.281393	1.792141
O	-9.005153	1.159565	-0.631731
O	-7.694447	-2.649716	0.264288
H	-6.992862	-2.764616	-0.411029
O	-7.354315	-2.299929	3.197545
H	-6.818645	-3.038400	3.487868
O	-3.182924	-1.809778	-0.346752
H	-3.047334	-2.639940	0.116069
O	-5.669981	-1.941282	-1.404500
H	-5.216988	-2.439922	-2.092858
Al	-5.289251	1.966767	-0.552493
Al	-7.063296	-1.553000	1.678638
H	-6.471846	1.359985	-2.582695
H	-8.477208	-2.307728	-0.232242
H	-3.386846	3.344093	-0.619645
H	-9.004246	3.223327	1.607682
Si	-8.945686	0.107255	-1.859350
O	-9.370889	-1.415559	-1.369200
H	-10.225770	-1.762415	-1.641995
O	-7.387555	-0.008497	-2.394571
H	-6.837369	-0.793377	-2.199172
O	-9.900867	0.586023	-3.082959
H	-10.441619	1.369582	-2.957444

38_SiAl_Multi_Di-ring

Atom	x	y	z
Si	-0.777140	2.052345	-0.326918
O	0.250559	0.794541	0.035140
O	-0.067625	-0.966441	2.243596
O	-2.296404	1.554859	-0.279710
Si	-1.018650	-1.793334	1.180814
O	-2.457292	-1.070762	0.998683
O	-2.888723	-0.580976	-1.812872
H	-3.098718	-1.485595	-2.069140
O	-4.884637	0.201338	0.209019
O	-0.341767	2.797712	-1.713390
H	-0.391171	2.190872	-2.463123
O	-0.441746	3.141394	0.894547
H	-0.911339	3.979665	0.934167
O	0.751153	1.799572	2.656301
H	0.275577	2.528715	2.145449
O	2.626960	-0.011090	1.332230
O	-0.205590	-1.874136	-0.236993
O	-1.331304	-3.306345	1.758427
H	-0.568042	-3.874610	1.882904
Si	3.369381	-0.055983	-0.125346
O	2.308752	-0.475169	-1.274853
O	4.653933	-1.086955	-0.038996
H	4.511475	-1.900086	0.450837
O	0.893537	-2.170160	-2.634365
H	0.464866	-2.996506	-2.376826

```
   O -0.552033  0.093073 -2.452127
   H -0.383874 -0.101046 -3.379974
   O  3.994897  1.405805 -0.554093
   H  4.679494  1.762901  0.016300
  Al  0.572755 -0.714568 -1.296872
  Al -3.193797  0.063719 -0.082325
  Al  0.955947  0.276047  1.626090
   H -5.404061  0.845720 -0.272283
   H  0.456934  1.775507  3.575049
   H -1.955678 -0.318189 -2.174635
   H  1.839121 -2.347376 -2.722396
-------------------------------------

39_SiAl_Multi_Branched_Di-ring
-------------------------------------
Atom         x         y         z
  Si -0.857234  0.136692  2.001982
   O  0.067604 -0.606683  0.831514
   O -0.761641 -2.964586 -0.500217
   O -2.302285  0.502290  1.417972
  Si -1.466566 -1.884630 -1.523988
   O -2.800471 -1.222706 -0.886052
   O -2.553417  1.673704 -0.984892
   H -2.691982  1.820209 -1.927248
   O -4.955649  0.370717  0.093252
   O -0.088811  1.329823  2.784260
   H  0.083131  2.190953  2.367065
   O -0.963189 -1.089467  3.144602
   H -1.327334 -0.892324  4.012245
   O  0.235957 -3.069534  2.244853
   H -0.282650 -2.415750  2.826831
   O  2.122882 -2.382643  0.111301
   O -0.341126 -0.734156 -1.837031
   O -1.936031 -2.634013 -2.914166
   H -1.239558 -3.051593 -3.425904
  Si  3.159918 -1.136340 -0.091689
   O  2.328289  0.194912 -0.521288
   O  4.300168 -1.560563 -1.203191
   O  1.036633  1.299389 -2.591647
   H  0.900076  0.739522 -3.365356
   O -0.105648  1.888425 -0.239436
   O  3.982957 -0.753256  1.279418
  Al  0.605019  0.363387 -0.864695
  Al -3.247303  0.210526 -0.023828
  Al  0.460013 -2.359221  0.559985
   H -5.336695  1.080835  0.610293
   H -0.015480 -3.982868  2.425627
   H -1.604480  1.902657 -0.730014
   H  1.887064  1.750144 -2.672270
   H  4.571869 -1.425444  1.630322
   H  3.984819 -2.042335 -1.971507
  Si  0.772216  3.264177 -0.118495
   O  0.250034  4.479327 -1.074302
   O  0.643176  3.640286  1.483732
   O  2.307625  2.987918 -0.618013
   H -0.581172  4.908816 -0.858298
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   H  1.100578  4.405010  1.843053
   H  2.668194  2.109109 -0.408534
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40_SiAl_Multi_Tri-ring
-------------------------------------
Atom         x         y         z
  Si  1.591595  2.430557  0.839505
   O  2.114271  2.094163 -0.655423
   O  2.852704 -0.386163 -2.061370
   O  1.935736  1.214134  1.872945
  Si  2.689731 -1.525471 -0.941654
   O  1.638095 -1.107644  0.202959
   O  3.337623 -1.262191  2.374838
   H  3.856652 -1.613143  1.605871
   O  2.289283  3.821720  1.397955
   H  3.222932  3.757913  1.610231
   O  0.240890  0.574914 -2.243852
   H  0.003169 -0.414977 -2.133520
   O  4.090371 -1.844017 -0.084150
   H  4.920432 -1.999177 -0.542252
  Si -1.122742 -1.151800  2.260745
   O  0.427945 -1.168759  2.774189
   O -1.496883  0.362875  1.793228
   O -0.013845  2.731633  0.828980
   O -2.884313  2.783581  1.303753
   H -3.703042  2.432452  0.875085
   O -2.117395 -1.650048  3.479950
   H -2.033974 -1.176127  4.310432
   O -1.381951 -2.181824  1.026795
   O -3.087669 -1.058999 -1.098272
  Si -3.277168  0.534249 -1.249898
   O -1.892870  1.317798 -0.865858
   O -4.356871  1.178199 -0.155176
   H -5.252903  0.834233 -0.110208
   O -3.831956  0.942395 -2.736465
   H -3.548869  0.401166 -3.477253
   O -2.327322 -3.836066 -0.902610
   H -2.549540 -4.389206 -0.142556
   O -0.487375 -1.838178 -1.856313
   H  0.298891 -2.404431 -1.837695
   O  2.185305 -2.902410 -1.717083
   H  2.262981 -3.727293 -1.229573
   O  2.402794  2.134498 -3.472881
   H  2.441067  1.728273 -4.339092
   H -0.509790  1.062374 -1.827414
  Al  2.002582  1.153958 -2.102769
  Al  1.711271 -0.496354  1.826479
  Al -1.411869  1.744539  0.782198
  Al -1.741431 -2.064507 -0.651834
   H  3.473451 -1.802018  3.161337
   H -2.885143  3.748019  1.305849
   H -2.715867 -4.209695 -1.703077
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41_SiAl_Multi_Branched_Tri-ring

Atom	x	y	z
Si	-0.680664	-3.174895	0.012961
O	-1.243883	-2.865311	-1.479199
O	-3.155856	-0.599192	-1.452466
O	-1.134801	-1.963072	0.999050
Si	-3.529534	0.242563	-0.145104
O	-2.232193	0.659825	0.746472
O	-2.744886	-0.831190	3.009575
H	-3.616757	-0.812353	2.551986
O	-1.230862	-4.631099	0.559577
H	-2.182219	-4.756059	0.546160
O	-0.360261	-0.221075	-1.760297
H	-0.395372	0.663677	-1.330561
O	-4.462681	-0.593367	0.954656
H	-5.234796	-1.081779	0.656309
Si	1.579434	0.200032	2.544686
O	-0.050056	0.227216	2.653771
O	2.051072	-1.193345	1.842351
O	0.947385	-3.285399	0.041817
O	3.765312	-2.748847	0.139769
H	4.372738	-2.136294	-0.351285
O	2.245808	0.335841	4.046799
H	2.005337	-0.344602	4.679317
O	2.127547	1.483518	1.709910
O	3.064426	1.615064	-1.050940
Si	3.236278	0.119851	-1.626776
O	2.057804	-0.841777	-1.013930
O	4.621654	-0.647363	-1.112392
H	5.482866	-0.276275	-1.322411
O	3.256872	0.096904	-3.262803
H	2.856910	0.840682	-3.719819
O	2.122764	3.995193	0.243343
H	2.563093	4.465827	0.960396
O	0.256143	2.076757	-0.449850
O	-4.308698	1.614851	-0.649251
H	-4.819849	2.103686	0.002073
O	-1.895460	-1.546149	-3.904090
H	-2.330674	-0.867216	-4.420020
H	0.562148	-0.561175	-1.589713
Al	-1.774060	-1.370353	-2.190912
Al	-1.356262	-0.459768	1.782582
Al	2.059559	-2.004540	0.327444
Al	1.910611	2.142954	0.138897
H	-2.817343	-0.443016	3.889550
H	3.907106	-3.663619	-0.131234
H	1.343100	4.510814	-0.102135
Si	-0.970370	3.144732	-0.445472
O	-1.743899	3.309837	0.985623
O	-0.198670	4.595619	-0.728275
O	-1.978493	2.762812	-1.673583
H	-2.097488	2.450526	1.267785
H	-0.708461	5.405962	-0.812587
H	-2.909093	2.591446	-1.457176

42_SiAl_Multi_Tetra-ring

Atom	x	y	z
Si	-1.393744	-2.311705	-1.753034
O	-2.511321	-1.180780	-2.088529
O	-3.752824	0.138838	0.201417
O	-1.452275	-2.707829	-0.173985
Si	-3.369880	0.102953	1.781273
O	-2.540587	-1.254632	2.138386
O	-0.795649	-3.566619	2.498001
H	-1.243288	-4.420039	2.488222
O	-1.690468	-3.664842	-2.659611
H	-2.518886	-4.111664	-2.471972
O	-4.839482	0.249258	-2.463274
H	-5.028811	-0.488948	-3.056385
O	-2.566618	1.753376	-1.911600
O	-2.524761	1.423993	2.195196
O	-4.753812	0.013433	2.683688
H	-5.359635	0.750843	2.583669
Si	-1.341297	2.665162	-1.374864
O	-0.742927	2.139812	0.025037
O	-0.062212	2.638772	-2.437545
H	-0.242933	2.904769	-3.342765
O	-0.859787	3.848248	2.330312
H	-1.158054	4.056507	3.216221
O	0.269231	1.215685	2.531126
H	1.216669	1.572104	2.523115
O	-1.817562	4.247280	-1.321801
H	-2.723831	4.407815	-1.049606
Si	1.823629	-1.815564	1.403228
O	0.299972	-1.248729	1.629393
O	2.116746	-2.163137	-0.143284
O	0.082105	-1.803915	-2.191307
O	2.732319	-2.642680	-2.873895
H	2.852741	-3.595196	-2.774449
O	1.795630	-3.225207	2.305649
H	2.528993	-3.842538	2.240169
O	2.875436	-0.751865	2.006447
O	3.964793	0.947906	-0.146769
Si	3.379962	1.176078	-1.642450
O	2.401421	-0.027774	-2.115218
O	4.728351	1.249664	-2.596125
H	4.576208	1.461725	-3.519634
O	2.581314	2.605359	-1.739594
H	1.637882	2.580248	-1.981640
O	5.331015	0.731717	2.228888
H	6.106918	0.684705	1.654796
O	2.701290	1.990485	2.339662
H	2.869510	2.923534	2.192306
Al	-1.058403	2.232004	1.738259
Al	-3.247501	0.232636	-1.436625
Al	-1.230721	-2.095452	1.415775
Al	1.708141	-1.549780	-1.712387
Al	3.595899	0.737363	1.509301
H	0.286231	0.252269	2.275006

H	-5.178005	1.064121	-2.855215
H	0.188816	-3.685760	2.579599
H	3.509512	-2.266864	-3.306576
H	5.567487	0.430840	3.115476

43_SiAl_Multi_Branched_Tetra-ring

Atom	x	y	z
O	2.441399	0.770901	2.175238
Si	2.853386	2.166723	1.444613
O	3.750748	1.861351	0.120760
O	2.981296	-1.874196	1.106483
Si	2.970455	-1.864335	-0.517304
O	4.017977	-0.781566	-1.113652
O	3.305418	-3.411105	-1.072883
H	4.070251	-3.880712	-0.730974
O	2.966703	-1.421867	3.935026
H	3.780748	-1.046897	4.293312
O	3.713180	3.126770	2.479324
H	4.583822	2.805301	2.722999
O	1.500994	2.998448	1.086096
O	2.386227	1.301778	-2.381529
O	5.248721	1.353110	-2.282684
H	5.399301	2.157249	-2.794238
O	0.195007	1.189346	-0.743657
Si	0.782396	1.388994	-2.239176
O	-1.141971	1.911998	1.819605
H	-1.360746	0.965306	1.894269
O	0.325319	3.002398	-2.537215
H	0.594421	3.433687	-3.352009
O	0.081723	0.444316	-3.367635
H	-0.863699	0.264028	-3.206113
O	-0.843368	3.690126	-0.436810
H	-0.922083	4.599827	-0.125087
O	1.485595	-1.580315	-1.107941
O	-0.448401	-2.833050	0.642566
Si	-0.777074	-1.950303	1.956939
O	0.553658	-1.407665	2.688517
O	-1.718380	-2.875619	2.997584
H	-1.400553	-3.743454	3.260284
O	0.821907	-4.143461	-1.579954
H	1.808935	-4.138473	-1.467119
Si	-2.720016	-1.503747	-2.124567
O	-1.264105	-2.208563	-2.074643
O	-3.453687	-1.482783	-0.681522
O	-1.805012	-0.728441	1.613700
O	-4.066326	-2.124240	2.072913
O	-4.313115	0.628800	1.116299
O	-3.658448	-2.254834	-3.252413
O	-2.554063	0.044341	-2.688245
Al	-0.006923	2.311503	0.573323
Al	3.694755	0.913248	-1.316653
Al	2.168586	-0.916158	2.298375
Al	0.037443	-2.526154	-0.995099
Al	-3.397044	-0.818072	0.904409

H	-0.420360	3.657507	-1.364193
H	5.833285	0.652559	-2.599382
H	2.402555	-1.717729	4.661103
H	0.466545	-5.027213	-1.434645
H	-2.868729	0.753946	-2.097733
H	-3.669377	-3.214078	-3.226336
Si	-4.186517	2.121318	0.510478
O	-3.498142	3.175130	1.554498
O	-3.255010	2.032097	-0.870150
O	-5.640762	2.715947	0.038847
H	-2.622923	2.841810	1.849908
H	-2.612683	2.748643	-0.953358
H	-6.356294	2.688744	0.678010
H	-4.799607	-2.724474	1.895955
H	-3.338932	-2.586656	2.572798

44_SiAl_Multi_Penta-ring

Atom	x	y	z
O	1.262434	1.356446	-1.586377
Si	2.872150	1.594915	-1.525580
O	3.360103	1.971001	-0.025404
O	0.024123	3.114757	0.356700
Si	0.038225	2.365613	1.796768
O	1.501641	1.841062	2.222920
O	-0.591989	3.423785	2.940668
H	-0.212773	4.302988	3.020459
O	0.662274	3.938761	-2.322043
H	1.606532	3.784318	-2.597452
O	3.076535	2.939075	-2.510751
H	3.931445	3.376560	-2.535133
O	3.663484	0.306706	-2.104420
O	3.470165	-0.328472	1.736103
O	4.146897	2.230624	2.717353
H	5.021889	1.914349	2.973690
O	3.690230	-2.047661	-0.331005
Si	3.554628	-1.890908	1.283376
O	4.930817	-2.577508	1.894010
H	5.007343	-2.567638	2.850724
O	4.311304	-2.350890	-2.980357
H	4.849769	-3.066337	-2.618098
O	-1.059297	1.161580	1.847746
O	-3.267005	1.858042	0.026026
Si	-3.055777	1.717868	-1.581229
O	-1.469727	1.964087	-1.942407
O	-4.005725	2.818451	-2.361913
H	-4.014471	3.704334	-1.993042
O	-3.108176	2.627807	2.792474
H	-2.272016	3.115652	3.024869
Si	-3.391887	-1.661206	1.455595
O	-3.580341	-0.189592	2.108657
O	-2.612036	-1.601103	0.046119
O	-3.471994	0.259394	-2.143992
O	-4.856272	-1.876477	-1.508731
H	-5.404206	-1.112840	-1.728323

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   O -2.594413 -2.737407 -2.720687
   H -3.335698 -3.329943 -2.857655
   O -4.853813 -2.383639  1.128146
   H -5.519414 -2.441094  1.818279
   O -2.587364 -2.645029  2.522000
   H -1.848284 -2.155592  2.949577
  Si  0.297761 -1.676078 -1.433132
   O  0.688905 -1.228526  0.062137
   O -1.002394 -0.788534 -2.029272
   H -0.908151  0.171013 -2.191161
   O -0.373775 -3.199361 -1.378929
   H -1.178167 -3.295680 -1.947616
   O -0.267292 -1.311526  2.863507
   H -0.503554 -0.391980  2.645770
   O -0.428166 -3.578581  1.191579
   H -0.540246 -3.630214  0.197705
   O  2.245794 -2.663301  1.886985
   O  1.592155 -1.660935 -2.393401
  Al -2.918159 -1.344018 -1.676453
  Al -2.778449  1.246942  1.558414
  Al  0.014705  2.523803 -1.268453
  Al  2.997414  1.304967  1.531548
  Al  3.212005 -1.345211 -1.829091
  Al  0.637564 -2.078240  1.586902
   H -5.106330 -2.169797 -0.605690
   H -3.858424  3.232627  2.769739
   H  0.165294  4.391025 -3.012942
   H  3.760883  2.729580  3.448715
   H  4.145737 -2.515203 -3.917019
   H -1.321237 -3.500442  1.598665
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45_SiAl_Cage_Trigonal_prism
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Atom         x         y         z
  Si  1.569482 -1.562712  0.811615
   O  1.646550 -1.274805 -0.823861
  Si  1.496638  0.075126 -1.757103
   O -0.018488  0.108541 -2.387862
   O  0.111839 -2.204404  1.137380
  Si -1.528864  0.068469 -1.737418
   O -1.762830 -1.301566 -0.907909
   O -2.578754 -2.808909  1.481954
   H -3.535149 -2.742702  1.598914
   O  2.773202 -2.577305  1.262513
   H  2.663668 -3.507280  1.051400
   O  2.481837  0.006822 -3.057499
   H  3.428414  0.007178 -2.897176
   O  1.755687  1.366778 -0.809178
   O -1.656809  1.342796 -0.699848
   O -2.631011  0.166130 -2.937711
   H -2.553890  0.892968 -3.560321
   O -0.092047  2.098200  1.328705
  Si -1.550477  1.497277  0.951178
   O  2.607248  2.677669  1.672444
   H  2.297680  3.475691  2.120618
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   O -2.661318  2.574864  1.485415
   H -3.586248  2.346946  1.367738
   O -1.768065  0.005132  1.567851
   O  1.790049 -0.135110  1.556134
  Al  1.451865  1.441502  0.905962
  Al -1.438524 -1.515535  0.791231
   H -2.252185 -3.621626  1.890077
   H  3.572643  2.658351  1.661219
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46_SiAl_Cage_Tetragonal_prism
------------------------------------
Atom         x         y         z
  Si -2.411493 -0.450922 -1.426237
   O -1.975086 -1.865369 -0.744506
   O  0.875286 -2.533328 -0.768420
   O -1.230055  0.066613 -2.419813
  Si  2.095434 -1.527578 -1.158747
   O  1.621681 -0.422766 -2.252346
   O  0.602795  1.381174 -4.213189
   H  0.929032  0.851722 -4.951301
   O -3.812676 -0.653154 -2.280269
   H -3.768961 -1.274542 -3.010147
   O  3.303571 -2.387154 -1.890565
   H  3.646636 -3.130468 -1.390076
  Si  0.664498  2.750038 -0.069380
   O  0.549284  2.228030 -1.609567
   O -0.771127  2.580135  0.681012
   O -2.754827  0.660354 -0.290174
   O -3.407393  2.372556  1.756979
   H -3.316794  3.181777  2.275251
   O  1.104091  4.344030 -0.048886
   H  0.435883  4.959608 -0.357786
   O  1.847413  1.958796  0.713300
   O  1.149556 -0.128421  2.587947
  Si -0.335537 -0.776410  2.707049
   O -1.490470  0.305327  2.319884
   O -0.498215 -1.216585  4.293092
   H -1.342540 -1.605568  4.530616
   O -0.476009 -2.090889  1.755767
   O  3.898521  0.616846  2.179864
   H  4.183850  1.420612  2.631838
   O  2.669056 -0.803320  0.183862
   O -1.173997 -4.332984  0.105474
   H -0.605892 -5.100649  0.241814
  Al -0.618736 -2.528742  0.094152
  Al  0.357810  0.735059 -2.456352
  Al -1.957296  1.385401  1.059545
  Al  2.221485  0.395870  1.341718
   H  0.879933  2.298814 -4.332132
   H -1.944857 -4.591072 -0.415983
   H  4.667583  0.179647  1.791980
   H -4.238100  2.400542  1.264961
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47_SiAl_Cage_Pentagonal_prism

Atom	x	y	z
Si	2.243890	-1.802021	1.619875
O	2.452286	-0.270304	2.129103
O	2.525599	1.754543	0.018717
O	2.398676	-1.877720	0.005937
Si	2.391006	1.665325	-1.597091
O	2.413114	0.127175	-2.111731
O	3.158831	-2.449595	-2.711188
H	3.818691	-1.978755	-3.235866
O	3.368604	-2.781710	2.336116
H	4.278060	-2.627384	2.071804
O	3.289826	2.238672	2.747146
H	3.803564	1.708210	3.369655
O	0.541934	1.952786	2.129923
O	1.028436	2.421301	-2.073994
O	3.697956	2.387463	-2.310467
H	3.844676	3.304935	-2.070620
Si	-0.879591	2.575665	1.676778
O	-0.883901	2.971350	0.108483
O	-1.288280	4.023240	-2.380469
H	-0.991413	4.348667	-3.239285
O	-1.267556	3.883383	2.603365
H	-0.662982	4.627084	2.552986
Si	-1.013269	-2.562846	-1.682787
O	0.452649	-2.059118	-2.145401
O	-1.057744	-2.891021	-0.101167
O	0.804335	-2.380573	2.101192
O	-1.425747	-3.868864	2.581682
H	-0.804195	-4.284544	3.193206
O	-1.481485	-3.876008	-2.563176
H	-0.941381	-4.662898	-2.462792
Si	-2.658435	0.059274	-1.664709
O	-2.148565	-1.439196	-2.067554
O	-2.989937	0.083616	-0.065809
Si	-2.764453	0.102547	1.546249
O	-1.846899	-1.125203	2.040100
O	-4.279127	0.015763	2.180064
H	-4.337825	-0.047482	3.136250
O	-2.094620	1.521373	1.999422
O	-4.034207	0.383437	-2.502519
H	-4.778575	-0.204739	-2.356178
O	-1.573882	1.173479	-2.065051
Al	-0.819316	-2.415495	1.533272
Al	2.066496	1.330030	1.617152
Al	1.977311	-1.460559	-1.604360
Al	-0.598067	2.486574	-1.517746
H	-1.581830	4.767965	-1.839879
H	3.118939	3.105374	3.136063
H	2.859254	-3.224487	-3.203027
H	-2.318957	-3.936450	2.941338

48_SiAl_Cage_Hexagonal_prism

Atom	x	y	z
O	0.999901	1.413841	-1.543705
Si	2.616575	1.358969	-1.685575
O	3.355244	1.876574	-0.335784
O	0.112365	3.613244	0.057444
Si	0.156875	2.869449	1.503416
O	1.664892	2.510849	1.961081
O	-0.564230	3.862207	2.654889
H	-0.254783	4.764898	2.763214
O	0.717873	3.868655	-2.758744
H	1.604011	3.510412	-3.040838
O	2.915703	2.469977	-2.912528
H	3.820661	2.743505	-3.082504
O	3.116428	-0.115689	-2.118029
O	3.172963	-0.022558	1.837899
O	4.370910	2.513666	2.281015
H	5.195086	2.103443	2.570952
O	2.990072	-2.045178	0.060876
Si	2.916057	-1.612594	1.625739
O	4.139972	-2.460258	2.355701
H	4.234512	-2.315920	3.299744
O	3.953147	-2.807301	-2.510892
H	4.828770	-3.037944	-2.177422
O	-0.813065	1.565785	1.507501
O	-3.298596	1.968052	0.062146
Si	-3.048567	1.749671	-1.533221
O	-1.696406	2.529271	-2.002909
O	-4.338315	2.341764	-2.383562
H	-4.521634	3.276213	-2.264569
O	-2.897921	2.746347	2.808294
H	-2.113439	3.355335	2.919411
Si	-2.933493	-1.640293	1.791624
O	-3.151395	-0.065882	2.147544
O	-3.074952	-1.905131	0.193607
O	-2.960613	0.175651	-1.903363
O	-4.313846	-2.326593	-2.174423
H	-4.730015	-2.098186	-3.014432
O	-4.138805	-2.536789	2.488445
H	-4.134017	-2.560850	3.447839
Si	-0.097860	-2.693593	-1.544173
O	-0.042920	-1.977009	-0.095065
O	-1.468726	-2.263112	-2.291243
O	-0.145578	-4.341347	-1.181086
H	-0.122353	-4.993553	-1.885256
O	-1.491393	-2.131683	2.381541
O	0.026770	-4.340358	1.369790
H	-0.063551	-4.606129	0.408628
O	1.491822	-2.026401	2.311061
O	1.269011	-2.373710	-2.355901
Al	-2.778397	-1.469641	-1.448919
Al	-2.549273	1.418915	1.519626
Al	-0.086483	2.772806	-1.454832
Al	3.006077	1.608954	1.340562
Al	2.701012	-1.715545	-1.603900

Al	-0.004847	-2.457523	1.568053
H	-4.993700	-2.613323	-1.551100
H	-3.724448	3.234569	2.887829
H	0.238163	4.236443	-3.509103
H	4.125297	3.211027	2.902485
H	3.626962	-3.519051	-3.076201
H	-0.497385	-4.922031	1.931514

49_SiAl_Cage_Heptagonal_prism

Atom	x	y	z
O	0.995324	-3.628273	0.175144
O	4.279549	-2.058856	0.497778
O	2.716491	3.979761	0.338357
O	-2.420873	-2.210674	0.020844
O	4.918631	1.315079	0.305076
O	-3.089167	1.146625	0.326240
O	-0.530056	-2.672021	2.154677
O	4.081137	-0.331414	2.542072
O	2.424920	-2.353402	-1.695975
O	-1.516132	2.061253	2.310074
O	-2.378151	-0.442827	-1.993897
O	3.653969	2.293249	-1.853445
O	1.990830	-1.837129	1.873150
O	4.469029	-0.250771	-1.804520
O	3.398757	2.519729	2.490602
O	-0.163438	-1.784624	-1.353896
O	-1.826972	2.438529	-1.962308
O	-2.428021	-0.443842	2.361882
Si	0.954329	-3.108696	1.733957
Si	3.635740	-1.761085	1.949353
Si	2.518117	3.766548	1.938027
Si	-1.809954	-1.840695	-1.428372
Si	4.787999	1.268484	-1.311534
Si	-2.749495	1.087154	1.912756
Si	0.987689	-2.961874	-1.328001
O	5.995553	1.592284	2.970125
H	6.129567	2.434947	3.421718
O	3.995509	-2.999162	2.996409
H	4.914283	-3.259167	3.094814
O	3.102560	5.096529	2.737626
H	2.703954	5.933537	2.490054
O	1.488146	-4.318284	2.706764
H	2.404481	-4.193219	2.994093
O	-4.055208	1.646179	2.768694
H	-4.888300	1.207266	2.582992
O	-3.296509	-3.037047	2.613312
H	-3.195335	-3.979073	2.796746
O	0.568421	-4.118196	-2.414619
H	-0.368935	-4.083996	-2.656028
O	-2.072500	-3.080191	-2.501316
H	-2.971034	-3.393854	-2.626664
O	-4.386762	1.517741	-2.235934
H	-4.438026	2.304121	-2.794507
O	2.197704	4.731925	-2.380341

H	2.702474	5.548883	-2.303928
O	6.208477	1.779666	-1.994717
H	6.997846	1.328071	-1.688345
O	5.192923	-2.870143	-2.085453
H	5.062421	-3.804958	-2.285848
O	-1.017389	3.927110	0.114301
O	0.791457	2.627644	-1.382928
O	0.947705	3.558051	2.301177
Si	-0.649830	3.371865	-1.363886
O	-1.556286	4.932640	2.544566
H	-1.843854	5.645586	1.959833
O	-0.396046	4.682696	-2.388712
H	-1.059105	5.375949	-2.433758
Al	-2.037108	-1.974901	1.688918
Al	-2.763940	1.118297	-1.354844
Al	-0.671975	3.449877	1.744085
Al	2.398346	3.270670	-1.200323
Al	4.431897	1.257972	1.946841
Al	3.959945	-1.765161	-1.173737
H	-3.858872	-2.636221	3.287984
H	-4.995338	0.847575	-2.570813
H	-1.379269	5.290456	3.422838
H	1.232255	4.934344	-2.535174
H	6.370750	0.883148	3.507543
H	5.782298	-2.478856	-2.742652

50_SiAl_Cage_Heptagonal_prism

Atom	x	y	z
O	0.958358	-3.510472	-0.112405
O	4.314177	-2.139005	0.224364
O	3.855538	4.320407	0.548128
O	-2.172773	-2.384280	0.301956
O	5.503657	1.072091	0.391384
O	-3.804342	0.880767	0.003261
O	-0.349913	-2.404228	2.263508
O	4.245593	-0.617597	2.415160
O	2.067595	-1.460823	-1.456490
O	-2.732943	2.570621	2.144741
O	-2.784720	-0.622675	-1.988682
O	4.628419	2.575145	-1.669628
O	2.549701	-2.665635	2.196535
O	4.634054	-0.085889	-1.849202
O	3.282928	2.104813	1.964632
O	-0.425129	-2.279805	-2.046418
O	-2.731862	2.042314	-2.145932
O	-1.695106	-0.140026	1.696687
Si	4.031189	-2.119668	1.825760
Si	3.315824	3.725899	1.955535
Si	5.389744	1.215197	-1.224308
Si	-1.734296	-1.760199	1.734174
Si	-3.557312	0.748639	-1.598875
Si	1.040530	-2.713796	-1.522634
O	5.693736	1.773474	3.171781
H	5.416905	2.718561	3.337313

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   O  5.075172 -3.168668  2.573640
   H  6.005416 -3.023418  2.387826
   O  4.463643  4.059599  3.144000
   H  4.773425  4.962688  3.248095
   O  0.774620 -4.904807  2.346218
   H  1.094275 -5.726980  1.954492
   O -4.211981  0.210714  2.767262
   H -3.923536 -0.710511  3.015556
   O -2.965926 -2.063003  2.843704
   H -3.279826 -2.964152  2.952285
   O  1.779170 -3.722400 -2.654263
   H  1.440505 -4.614151 -2.767081
   O -3.028871 -3.482542 -2.012849
   H -3.279574 -4.162804 -1.374499
   O -5.020305  0.655794 -2.372708
   H -5.613312  1.394713 -2.219921
   O  4.808889  5.435406 -1.852646
   H  5.483161  5.904813 -1.345656
   O  6.912562  1.338317 -1.867849
   H  7.518288  0.633749 -1.627886
   O  4.204495 -2.812945 -2.563428
   H  3.382956 -3.317042 -2.819455
   O -2.605329  4.086168 -0.045187
   O  2.300136  4.292473 -1.937445
   O  1.894028  4.373243  2.369903
  Si -2.453891  4.070259  1.573345
   O -3.546185  5.131518  2.229370
   H -4.455289  5.006845  1.948512
   O -2.275112  4.776092 -2.812934
   H -1.442946  5.295468 -2.992921
   O  0.771591  5.480202 -0.088338
   O -0.221021  3.441815 -1.539524
   O -1.002630  4.599745  2.064222
  Si  0.795933  4.704268 -1.511795
   O  0.724835  6.847939  2.403639
   H  0.027246  7.513600  2.442125
   O  0.133529  5.723450 -2.680639
   H  0.471006  6.619563 -2.755654
  Al  0.554531  5.142654  1.590996
  Al  3.806482  3.985208 -1.144693
  Al  4.598633  0.970035  1.856815
  Al  3.802316 -1.481699 -1.284975
  Al  1.035528 -3.187229  1.582772
  Al -1.998471 -2.018662 -1.378213
  Al -3.013644  0.988039  1.532022
  Al -1.963667  3.444060 -1.510685
   H  1.312816  6.957780  3.161397
   H  4.376799  6.055469 -2.453773
   H  6.654019  1.696964  3.186870
   H  4.749594 -2.627853 -3.336097
   H -0.040412 -5.080234  2.833255
   H -2.958712 -3.878193 -2.890245
   H -4.540144  0.689375  3.536288
   H -2.744594  4.583302 -3.632006
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(3) Pure-silicates with an external cation (The most stable position only)

51_Si_Cage_Trigonal_Na_Vertex

Atom	x	y	z
Si	-2.099625	0.017126	-1.399726
O	-2.533357	-0.255032	0.164128
Si	-1.899699	0.271551	1.589315
O	-0.881574	-0.858985	2.175462
O	-1.124221	-1.184569	-1.910870
Si	0.322041	-1.773245	-1.400907
Si	0.483162	-1.544243	1.567432
O	0.115765	-2.289735	0.150953
O	0.821366	-2.957378	-2.390266
H	0.196543	-3.635181	-2.659225
O	-3.366751	0.043743	-2.405624
H	-4.078540	0.668149	-2.242956
O	-3.027626	0.505703	2.725933
H	-3.747873	1.116449	2.550010
O	-1.059507	1.630099	1.217083
O	1.551990	-0.366586	1.226708
O	1.039160	-2.675515	2.588442
H	1.163818	-2.447125	3.512787
Si	-0.405423	2.179080	-0.195040
O	1.159064	1.774993	-0.256553
Si	2.086115	0.388190	-0.173166
O	-0.621756	3.776725	-0.380048
H	0.006660	4.375300	0.030978
O	3.613756	0.637875	-0.265805
O	1.437571	-0.595153	-1.370429
O	-1.258969	1.427762	-1.384815
Na	5.520734	1.588401	-0.008791

52_Si_Cage_Trigonal_K_Vertex

Atom	x	y	z
Si	2.213438	-0.347503	-1.488807
O	2.765021	-0.010343	0.024356
Si	2.179381	-0.370271	1.520719
O	1.330311	0.904207	2.079372
O	1.355516	0.921926	-2.045640
Si	0.038283	1.731815	-1.490450
Si	0.038143	1.732304	1.491661
O	0.419701	2.313433	0.003583
O	-0.366358	2.909587	-2.530441
H	0.328214	3.455930	-2.906250
O	3.405193	-0.597142	-2.554651
H	4.009038	-1.331142	-2.416208
O	3.349027	-0.649127	2.604178
H	3.948737	-1.386188	2.464416
O	1.180687	-1.653304	1.302407
O	-1.207372	0.703453	1.305724
O	-0.287185	3.004867	2.444554
H	-0.421106	2.860117	3.384431

```
  Si  0.359553 -2.191086 -0.025046
   O -1.132742 -1.572486 -0.021172
  Si -1.901738 -0.089088 -0.002143
   O  0.345101 -3.811459 -0.108516
   H -0.317676 -4.292330  0.393079
   O -3.449818 -0.172689  0.001025
   O -1.218533  0.723683 -1.305689
   O  1.222856 -1.645217 -1.316138
   K -5.800909 -0.883573 -0.003483
-------------------------------------

53_Si_Cage_Trigonal_Ca_LateralEdge
-------------------------------------
Atom         x         y         z
  Si  1.164467 -1.512727 -1.502595
   O  1.844655 -1.530839  0.000234
  Si  1.164744 -1.511914  1.503184
   O  1.190241  0.019070  2.083175
   O  1.190254  0.018042 -2.083262
  Si  1.115360  1.550731 -1.502023
  Si  1.115291  1.551547  1.501416
   O  1.798183  1.567329 -0.000328
   O  1.873953  2.551834 -2.535691
   H  2.674417  2.239603 -2.964247
   O  2.024431 -2.384354 -2.574124
   H  2.045717 -3.337992 -2.462104
   O  2.024983 -2.382723  2.575168
   H  2.051981 -3.335818  2.459794
   O -0.353957 -2.121967  1.320849
   O -0.416049  2.118547  1.319552
   O  1.873725  2.553273  2.534477
   H  2.675945  2.242874  2.961055
  Si -1.244759 -1.594588  0.000512
   O -0.799840 -0.008073  0.000084
  Si -1.290099  1.565102 -0.000324
   O -2.797006 -1.802512  0.000676
   O -2.847290  1.729750 -0.000406
   O -0.415924  2.118004 -1.320331
   O -0.354305 -2.122466 -1.319892
  Ca -4.224327 -0.053305  0.000084
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54_Si_Cage_Tetragonal_Na_Vertex
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Atom         x         y         z
  Si  0.478250  2.557724  0.325540
   O  1.791713  1.666486  0.040672
  Si  2.570631  0.201646  0.185338
   O  1.856437 -0.515656  1.507230
   O -0.277761  2.027867  1.678824
  Si -1.362587  0.951986  2.243422
  Si  0.644569 -1.401980  2.096763
   O -0.591781 -0.446453  2.573784
   O -2.140402  1.520446  3.551552
   H -1.624185  1.773101  4.321053
   O  0.830955  4.142516  0.459454
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   H  1.497536  4.402946  1.099688
   O  1.083920 -2.236448  3.424889
   H  1.829983 -2.836700  3.353192
  Si -2.914216 -0.208917 -0.188098
   O -2.509396  0.682785  1.117211
   O -2.323078  0.533176 -1.515269
  Si -1.097236  1.448662 -2.091876
   O -0.572029  2.448103 -0.922210
   O -1.597313  2.394073 -3.315024
   H -1.946096  1.975053 -4.105596
   O -4.521180 -0.413460 -0.293395
   H -5.079220  0.362388 -0.389138
  Si -0.920318 -2.581724 -0.316264
   O -2.268340 -1.696244 -0.051586
   O -0.212633 -2.030058 -1.677463
  Si  0.881757 -0.946222 -2.223627
   O  0.104494  0.455458 -2.563805
   O  1.491506 -1.596546 -3.587284
   H  2.184107 -1.114354 -4.045333
   O  2.020043 -0.685421 -1.111137
   O -1.281435 -4.161702 -0.429739
   H -1.873198 -4.446618 -1.130510
   O  0.093112 -2.425844  0.943052
   O  4.119702  0.309191  0.277855
  Na  6.209718 -0.017311 -0.036454
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55_Si_Cage_Tetragonal_K_TopEdge
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Atom         x         y         z
  Si  0.518314 -1.296789 -2.359044
   O -0.904176 -1.847179 -1.764465
  Si -1.716419 -1.624676 -0.361742
   O -0.846053 -2.306313  0.843787
   O  1.709998 -1.810583 -1.366501
  Si  2.606860 -1.435424 -0.056671
  Si  0.254460 -1.833947  1.958254
   O  1.733448 -1.776454  1.278374
   O  4.020348 -2.232524 -0.058944
   H  4.009123 -3.192756 -0.068994
   O  0.746035 -1.814185 -3.880447
   H  0.811837 -2.757911 -4.046081
   O  0.352123 -2.914798  3.166624
   H -0.427295 -3.073013  3.705012
  Si  2.429355  1.631265  0.355690
   O  2.968318  0.149875 -0.079009
   O  1.508598  2.219041 -0.851445
  Si  0.329617  1.871154 -1.933063
   O  0.506440  0.320916 -2.397632
   O  0.512158  2.767239 -3.280725
   H  0.330750  3.708393 -3.221626
   O  3.672308  2.623997  0.686858
   H  4.314200  2.802369 -0.005069
  Si  0.064894  1.253556  2.344699
   O  1.558385  1.503847  1.720654
   O -1.041346  1.920614  1.372001
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  Si -2.004281  1.597244  0.052873
   O -1.116291  2.127468 -1.252103
   O -3.470683  2.107513  0.123287
   O -1.933055 -0.065409 -0.064349
   O -0.017941  1.853149  3.857201
   H  0.001197  2.807036  3.967065
   O -0.162659 -0.355752  2.497473
   O -3.218533 -2.261884 -0.455416
   H -3.343774 -3.193075 -0.653848
   K -4.898664 -0.054897 -0.023799
-------------------------------------

56_Si_Cage_Tetragonal_Ca_TopEdge
-------------------------------------
Atom         x         y         z
  Si -0.220792 -2.199726 -1.579181
   O  1.009900 -1.321657 -2.197376
  Si  1.731654  0.021173 -1.527010
   O  1.002651  1.374062 -2.165729
   O -1.589033 -1.311114 -1.663685
  Si -2.518034  0.007610 -1.470892
  Si -0.244614  2.226083 -1.545460
   O -1.613157  1.348148 -1.635827
   O -3.779484  0.009593 -2.496586
   H -3.603428  0.043470 -3.439984
   O -0.389278 -3.590351 -2.413690
   H -0.407970 -3.537595 -3.372302
   O -0.516327  3.558951 -2.444785
   H  0.189899  4.205571 -2.515608
  Si -2.482666 -0.007268  1.512457
   O -3.168357 -0.008598  0.026160
   O -1.582314 -1.353593  1.642509
  Si -0.214102 -2.239117  1.528522
   O  0.025413 -2.660797 -0.031339
   O -0.376011 -3.650200  2.328776
   H -0.378865 -3.622580  3.288562
   O -3.626903  0.063071  2.665773
   H -4.252954 -0.662512  2.729212
  Si -0.203757  2.208142  1.567036
   O -1.575133  1.325759  1.671652
   O  1.024798  1.327701  2.186407
  Si  1.740935 -0.019201  1.518757
   O  1.016769 -1.372702  2.163058
   O  3.308781 -0.024097  1.582466
   O  1.082059 -0.003939 -0.002130
   O -0.360489  3.606672  2.390491
   H -0.376343  3.560815  3.349559
   O  0.030437  2.651821  0.012459
   O  3.299208  0.027028 -1.599022
  Ca  4.840035  0.003952 -0.012766
-------------------------------------
```

57_Si_Cage_Pentagonal_Na_TopEdge

Atom	x	y	z
Si	1.615995	-1.432353	2.135808
O	1.956037	0.152363	2.334297
Si	1.578443	1.708985	2.067057
O	2.137614	2.152018	0.594007
O	2.259256	-1.982710	0.755743
Si	2.367817	-1.540796	-0.846831
Si	2.089916	1.543113	-0.924173
O	1.675244	-0.013772	-0.855490
O	3.795915	-1.616057	-1.460172
O	2.169665	-2.284541	3.412592
H	3.119424	-2.338282	3.543346
O	2.206326	2.667082	3.222039
H	3.148793	2.613936	3.399058
O	-0.033099	1.912350	2.120670
O	0.979068	2.383521	-1.775528
O	3.554597	1.690784	-1.649649
H	3.875596	2.576527	-1.844361
Si	-1.416752	2.375287	1.399117
O	-1.115092	2.692269	-0.166702
Si	-0.643344	2.569222	-1.712295
O	-1.086964	3.945441	-2.454975
H	-0.859690	4.061228	-3.381013
O	-2.068231	3.663085	2.150414
H	-1.526443	4.447649	2.264727
Si	-0.381511	-2.649629	-1.600086
O	1.226422	-2.467532	-1.619313
O	-0.902134	-2.789716	-0.061037
Si	-1.260227	-2.409247	1.474988
O	-0.005425	-1.611452	2.140954
O	-1.667145	-3.733150	2.331207
H	-1.029692	-4.448590	2.394790
O	-0.818543	-3.956960	-2.472541
H	-0.391678	-4.792869	-2.269650
Si	-2.144627	-0.123180	-2.213233
O	-1.129781	-1.386400	-2.305339
O	-2.879369	-0.127511	-0.762666
Si	-3.195593	-0.116770	0.824519
O	-2.572227	-1.449739	1.524304
O	-4.813161	-0.090696	0.987689
H	-5.183533	-0.085029	1.873951
O	-2.519278	1.191913	1.520466
O	-3.231825	-0.164572	-3.424845
H	-3.737862	-0.970795	-3.551481
O	-1.333359	1.270287	-2.406999
Na	5.069760	-0.034462	-2.211867

58_Si_Cage_Pentagonal_K_TopEdge

Atom	x	y	z
Si	1.064761	-1.318518	2.448920
O	1.390592	0.269107	2.639765
Si	1.088620	1.823401	2.280159

```
   O  1.872835  2.213553  0.898263
   O  1.936919 -1.937639  1.234446
  Si  2.342007 -1.550859 -0.337367
  Si  2.098408  1.539999 -0.577451
   O  1.684942 -0.017176 -0.518600
   O  3.852567 -1.670304 -0.681257
   O  1.364652 -2.120873  3.838880
   H  2.279625 -2.216766  4.113828
   O  1.553976  2.801733  3.494226
   H  2.458238  2.737373  3.811298
   O -0.509310  2.059721  2.092890
   O  1.138831  2.329318 -1.640385
   O  3.662223  1.694272 -1.045107
   H  3.999153  2.586815 -1.170103
  Si -1.757267  2.404368  1.108278
   O -1.194597  2.601012 -0.402028
  Si -0.474724  2.476699 -1.847756
   O -0.825960  3.833481 -2.671383
   H -0.510857  3.921015 -3.574281
   O -2.564398  3.718801  1.626887
   H -2.070356  4.529058  1.773644
  Si -0.249797 -2.715714 -1.503437
   O  1.333990 -2.490117 -1.268928
   O -1.014631 -2.823552 -0.065879
  Si -1.639952 -2.363612  1.358812
   O -0.535658 -1.478519  2.167989
   O -2.154907 -3.646562  2.218669
   H -1.518101 -4.324996  2.456139
   O -0.511798 -4.060985 -2.389457
   H -0.093682 -4.874469 -2.097000
  Si -1.885058 -0.213504 -2.496618
   O -0.902602 -1.497873 -2.365676
   O -2.835282 -0.123592 -1.181345
  Si -3.418830 -0.099659  0.328103
   O -2.964488 -1.448538  1.122207
   O -5.038687 -0.028284  0.208399
   H -5.552742  0.063110  1.014457
   O -2.831309  1.187864  1.135953
   O -2.769477 -0.300299 -3.861086
   H -3.265833 -1.105572 -4.026732
   O -1.013807  1.152043 -2.626176
   K  5.627540 -0.147617 -1.508126
-------------------------------------

59_Si_Cage_Pentagonal_Ca_TopEdge
-------------------------------------
Atom         x         y         z
  Si -3.181301  0.043153  0.431060
   O -2.770562 -1.314541  1.232339
  Si -1.758666 -2.594340  1.168367
   O -1.321788 -2.817918 -0.380664
   O -2.513359 -0.002581 -1.044463
  Si -1.713051 -0.011001 -2.455992
  Si -0.349539 -2.671665 -1.683038
   O -0.812616 -1.364045 -2.538630
   O -2.737918  0.059448 -3.723778
```

```
   O -4.801916  0.195771  0.365717
   H -5.311811 -0.531664  0.000821
   O -2.485989 -3.916800  1.780475
   H -3.309543 -4.204071  1.378471
   O -0.464367 -2.332101  2.107020
   O  1.193300 -2.561064 -1.205653
   O -0.546806 -3.939672 -2.690009
   H -0.192416 -4.789578 -2.417925
  Si  0.927132 -1.526152  2.391161
   O  1.998357 -1.869603  1.223076
  Si  2.201994 -1.528574 -0.394085
   O  3.703896 -1.634645 -0.847120
   O  1.515339 -1.940569  3.855889
   H  1.804739 -2.847016  3.984896
  Si -0.275545  2.627877 -1.751120
   O -0.781206  1.312456 -2.578633
   O -1.250071  2.796884 -0.453346
  Si -1.671673  2.647474  1.109222
   O -2.644284  1.344087  1.244209
   O -2.421761  3.984212  1.658315
   H -3.251741  4.238554  1.247586
   O -0.343770  3.951675 -2.700356
   H -1.195057  4.198670 -3.069273
  Si  2.254388  1.450841 -0.464172
   O  1.269297  2.484149 -1.302527
   O  2.080030  1.868041  1.138222
  Si  1.012089  1.630397  2.328882
   O -0.362089  2.469301  2.048561
   O  1.723097  2.176650  3.691897
   H  1.231837  2.108085  4.514120
   O  0.585910  0.061980  2.458806
   O  3.753819  1.487626 -0.935070
   O  1.517391 -0.029946 -0.594463
   H -3.309504 -0.696337 -3.879754
  Ca  5.231821 -0.108957 -1.288071
-------------------------------------

60_Si_Cage_Hexagonal_Na_TopEdge
-------------------------------------
Atom         x         y         z
   O  0.719830 -3.498486 -0.078514
   O  3.690266 -0.802500  0.094512
   O -0.724090  3.270411 -0.104618
   O -2.333629 -2.271022  0.067331
   O  2.427891  2.393516  0.133594
   O -3.268048  0.961841 -0.041920
   O -0.495960 -2.310078  1.973048
   O  2.113256  0.383103  1.873497
   O  1.622456 -1.372037 -1.409409
   O -1.986002  2.181796  1.953292
   O -2.704913 -0.711559 -2.038250
   O  0.849589  2.304180 -2.002268
   O  2.152696 -2.247400  1.775679
   O  3.028991  0.778856 -1.904608
   O  0.636760  2.562778  2.075088
   O -0.718823 -2.472440 -2.043773
```

```
   O -1.733408  1.752915 -2.050805
   O -2.358304 -0.440997  2.008425
  Si  0.825415 -3.139721  1.512753
  Si  3.066903 -0.918127  1.583719
  Si  3.203825 -0.818076 -1.499408
  Si -0.764076  3.161786  1.514996
  Si -2.242805 -2.192832 -1.553178
  Si  2.392940  2.201183 -1.486873
  Si -0.633908  2.885958 -1.681028
  Si -2.059143 -1.991895  1.644674
  Si -3.008055  0.831817 -1.640782
  Si -3.005623  0.984502  1.560905
  Si  0.801746 -2.753557 -1.532895
  Si  2.109027  1.996310  1.675474
   O  3.253158  2.589355  2.673930
   H  3.444284  3.530232  2.646522
   O  4.250204 -1.050965  2.699855
   H  4.957343 -0.401571  2.684634
   O -0.938662  4.626654  2.201626
   H -1.754172  5.107742  2.040243
   O  0.858311 -4.503888  2.398566
   H  1.598010 -5.105703  2.283396
   O -4.377687  1.295355  2.379415
   H -5.090236  0.652968  2.336254
   O -3.058026 -2.879857  2.574951
   H -3.006396 -3.837299  2.516866
   O  1.570043 -3.720372 -2.617176
   H  1.161144 -4.563009 -2.836729
   O -3.158767 -3.340478 -2.254300
   H -4.107563 -3.318474 -2.105987
   O -4.333281  1.248716 -2.488630
   H -4.641859  2.156588 -2.434278
   O -0.984149  4.173700 -2.615875
   H -0.405354  4.938852 -2.569099
   O  3.188354  3.430990 -2.207321
   H  4.132953  3.504831 -2.050623
   O  4.121996 -1.635744 -2.455136
  Na  3.537819 -3.236410 -3.806097
-------------------------------------

61_Si_Cage_Hexagonal_K_TopEdge
-------------------------------------
Atom         x         y         z
   O  0.744479 -3.308119 -0.121151
   O  3.538992 -1.330828 -0.172762
   O -0.717101  3.244209 -0.164606
   O -2.416817 -2.257118  0.143056
   O  2.471261  2.559785 -0.028602
   O -3.294643  1.029818  0.003540
   O -0.492863 -2.230985  1.967658
   O  2.172054  0.298950  1.349185
   O  1.511175 -1.475986 -1.913659
   O -1.930804  2.225423  1.955208
   O -2.839207 -0.711986 -1.964688
   O  0.800224  2.206671 -2.072135
   O  2.169859 -2.257898  1.876448
```

```
   O  2.976512  0.695845 -1.856427
   O  0.714159  2.442395  1.938710
   O -0.907095 -2.527718 -2.039207
   O -1.796184  1.720224 -2.066876
   O -2.378503 -0.386650  2.042773
  Si  0.827280 -3.061644  1.491328
  Si  3.193260 -1.028082  1.431942
  Si  3.031062 -0.918382 -1.647758
  Si -0.675688  3.131005  1.456261
  Si -2.394686 -2.199576 -1.480028
  Si  2.361048  2.175089 -1.612308
  Si -0.666015  2.833445 -1.735904
  Si -2.069217 -1.941147  1.699533
  Si -3.086583  0.847631 -1.597534
  Si -2.993539  1.052063  1.599679
  Si  0.647594 -2.833226 -1.671270
  Si  2.170558  1.905585  1.441782
   O  3.323084  2.381894  2.509022
   H  3.372402  3.320278  2.715225
   O  4.435709 -0.851669  2.349474
   O -0.721688  4.601776  2.151193
   H -1.501533  5.145192  2.014096
   O  0.761411 -4.495207  2.271178
   H  1.506566 -5.092499  2.169860
   O -4.333754  1.410186  2.450533
   H -5.055231  0.776471  2.451832
   O -3.018123 -2.818158  2.692496
   H -2.934693 -3.774873  2.672559
   O  1.265790 -3.967973 -2.664472
   H  0.893123 -4.852733 -2.639116
   O -3.376187 -3.327206 -2.123442
   H -4.317861 -3.261786 -1.945920
   O -4.422847  1.284329 -2.417739
   H -4.716097  2.196977 -2.358771
   O -0.996543  4.114196 -2.686184
   H -0.381020  4.851548 -2.687005
   O  3.136287  3.284048 -2.517813
   H  4.079380  3.405919 -2.382796
   O  4.096928 -1.577827 -2.693729
   H  3.930574 -1.465341 -3.632843
   K  5.289638  0.997631  3.776528
-------------------------------------

62_Si_Cage_Hexagonal_Ca_TopEdge
-------------------------------------
Atom         x         y         z
   O  0.724152 -3.285080 -0.052522
   O  3.545743 -1.401112 -0.011713
   O -0.708107  3.196510 -0.093788
   O -2.424551 -2.260438  0.108808
   O  2.532384  2.599033  0.134542
   O -3.240008  1.015300 -0.012331
   O -0.595508 -2.280132  2.024209
   O  2.040673  0.292729  1.298026
   O  1.577029 -1.459484 -1.816389
   O -1.906193  2.137756  2.007590
```

O	-2.817632	-0.712954	-2.000721
O	0.895115	2.151585	-1.935379
O	2.069487	-2.250604	2.003028
O	3.086742	0.689845	-1.658666
O	0.730086	2.452308	2.044799
O	-0.846483	-2.489601	-2.028344
O	-1.698499	1.686107	-2.056620
O	-2.499559	-0.447602	2.062764
Si	0.751428	-3.075242	1.565813
Si	3.049117	-1.001611	1.527849
Si	3.096420	-0.926597	-1.494165
Si	-0.660927	3.079521	1.530826
Si	-2.356646	-2.194006	-1.511599
Si	2.445534	2.166856	-1.425836
Si	-0.576271	2.789969	-1.659729
Si	-2.159581	-1.987588	1.688986
Si	-3.020759	0.849196	-1.612513
Si	-3.009275	1.025748	1.595811
Si	0.691596	-2.807796	-1.604924
Si	2.231992	1.906809	1.619130
O	3.335039	2.228645	2.693052
O	4.237294	-0.745718	2.524399
O	-0.797769	4.558493	2.207072
H	-1.600730	5.055601	2.032739
O	0.696919	-4.523201	2.317737
H	1.450863	-5.109170	2.215588
O	-4.373125	1.446169	2.381001
H	-5.141606	0.877556	2.289589
O	-3.146896	-2.901320	2.608878
H	-3.032309	-3.854750	2.585908
O	1.335974	-3.949939	-2.573368
H	0.958768	-4.832937	-2.554068
O	-3.297172	-3.335652	-2.191377
H	-4.243625	-3.295642	-2.032426
O	-4.335621	1.333708	-2.441714
H	-4.611729	2.250090	-2.362256
O	-0.860178	4.077242	-2.620142
H	-0.270547	4.832305	-2.552534
O	3.214073	3.260926	-2.364409
O	4.185317	-1.585655	-2.517129
H	4.085023	-1.404184	-3.454766
Ca	4.849470	0.997850	3.720948
H	4.133172	3.455175	-2.164960

63_Si_Cage_Heptagonal_Na_Vertex

Atom	x	y	z
O	1.005795	-3.524874	0.070874
O	3.970350	-1.956347	0.224861
O	2.666861	3.991370	0.065466
O	-1.997575	-2.224400	0.001252
O	4.511775	1.393058	0.220014
O	-3.017435	1.282024	0.212292
O	-0.436547	-2.578513	2.107731
O	3.571076	-0.187735	2.156199

```
   O  2.402982 -2.349782 -1.873045
   O -1.346076  2.193024  2.091848
   O -1.454931 -0.078404 -1.454413
   O  3.123216  2.284399 -1.888281
   O  2.200965 -2.440309  2.167941
   O  3.957917 -0.218641 -1.805545
   O  3.010274  2.387940  2.163929
   O -0.239927 -2.393598 -1.976676
   O -1.915409  2.526614 -1.868614
   O -1.876912 -0.378537  1.939014
  Si  0.933808 -3.336803  1.682805
  Si  3.634613 -1.776341  1.805436
  Si  3.847534 -1.780503 -1.386544
  Si  2.360539  3.792605  1.655266
  Si -1.629264 -1.706621 -1.502398
  Si  4.324689  1.311689 -1.393463
  Si  2.106235  3.453738 -1.381592
  Si -1.856639 -1.965738  1.605158
  Si -2.545427  1.137361 -1.344052
  Si -2.506030  1.109207  1.754472
  Si  1.084758 -3.226741 -1.523755
  Si  4.152496  1.285883  1.801954
   O  5.489955  1.481199  2.711968
   H  5.974723  2.307460  2.642379
   O  4.737972 -2.549648  2.721136
   H  5.658546 -2.286449  2.644001
   O  3.077952  4.968239  2.525149
   H  2.802219  5.876380  2.378047
   O  0.904323 -4.777886  2.440301
   H  1.660063 -5.361589  2.337129
   O -3.736208  1.387618  2.784671
   H -4.541723  0.873565  2.686892
   O -3.107412 -2.630708  2.406392
   H -3.276099 -3.570203  2.298902
   O  1.215646 -4.609852 -2.372483
   H  0.502595 -5.250774 -2.312505
   O -2.802418 -2.105530 -2.558520
   H -3.453025 -1.406660 -2.713078
   O -3.793716  0.623781 -2.272236
   H -4.610263  1.127618 -2.319216
   O  2.037836  4.652891 -2.475443
   H  1.098584  4.942221 -2.592370
   O  5.671154  1.823571 -2.153954
   H  6.501223  1.384138 -1.952733
   O  5.069164 -2.543052 -2.146073
   H  5.161199 -3.491335 -2.024214
   O -1.294264  4.046768  0.193286
   O  0.608377  2.840033 -1.146616
   O  0.762798  3.759000  1.916561
  Si -0.842883  3.705591  1.715732
  Si -0.829756  3.668001 -1.354630
   O -1.455364  4.804334  2.754621
   H -2.398820  4.980663  2.721103
   O -0.645759  4.891247 -2.320681
  Na -1.872206  6.161241 -3.584719
-------------------------------------
```

64_Si_Cage_Heptagonal_K_Vertex

Atom	x	y	z
O	0.943567	-3.489595	0.109712
O	4.004428	-1.945422	0.091536
O	2.418321	3.890059	0.274905
O	-2.096976	-2.188647	0.174999
O	4.674054	1.400910	0.264352
O	-3.222163	0.947254	0.063858
O	-0.353018	-2.363174	2.155887
O	3.956936	-0.315974	2.181985
O	2.147283	-2.043742	-1.789326
O	-1.787473	2.348877	1.855012
O	-2.263829	-0.538991	-1.899389
O	3.371929	2.532319	-1.781163
O	2.283791	-2.352469	2.093412
O	3.878075	-0.056876	-1.796167
O	3.046527	2.158872	2.211451
O	-0.450655	-2.470465	-1.900647
O	-1.021656	1.731092	-1.178051
O	-1.956703	-0.274815	2.040626
Si	0.957027	-3.211043	1.712631
Si	3.777226	-1.857283	1.699723
Si	3.691615	-1.633296	-1.474301
Si	2.236149	3.517937	1.844901
Si	-1.955406	-2.067244	-1.441004
Si	4.444986	1.401317	-1.345719
Si	2.371405	3.744943	-1.346528
Si	-1.848718	-1.868390	1.749363
Si	-2.468503	0.999083	-1.397968
Si	-2.763777	1.084372	1.624829
Si	0.974940	-3.123485	-1.474447
Si	4.327358	1.224916	1.843286
O	5.620640	1.590616	2.762806
H	5.971011	2.484038	2.721144
O	4.809829	-2.844309	2.481613
H	5.752257	-2.684363	2.387670
O	2.868036	4.689544	2.787580
H	2.538637	5.585813	2.684158
O	0.898880	-4.613304	2.539008
H	1.626451	-5.232267	2.436943
O	-4.062064	1.327108	2.579216
H	-4.764644	0.672554	2.569558
O	-2.986599	-2.586702	2.668068
H	-3.120571	-3.533286	2.574515
O	1.315932	-4.445019	-2.363116
H	0.752184	-5.217373	-2.273212
O	-2.953316	-3.112131	-2.192087
H	-3.898926	-3.012392	-2.056447
O	-3.344118	1.823839	-2.488305
H	-2.910206	2.702938	-2.656292
O	2.832743	5.144462	-2.048642
H	3.700768	5.491342	-1.828271
O	5.829435	1.766685	-2.122716
H	6.592469	1.200612	-1.982526
O	4.737847	-2.427257	-2.437860

H	4.759409	-3.386780	-2.397518
O	-0.780385	4.051012	0.053866
O	0.882866	3.423110	-1.878245
O	0.660168	3.270030	2.165231
Si	-0.832355	3.641470	1.621190
Si	-0.708732	3.353292	-1.451978
O	-1.337630	4.901547	2.528127
H	-2.183497	5.300272	2.309414
O	-1.721978	3.943251	-2.498151
K	-2.104645	5.668632	-4.264648

65_Si_Cage_Heptagonal_Ca_TopEdge

Atom	x	y	z
O	1.030667	-3.592219	0.074634
O	3.964656	-1.990389	0.243436
O	2.645307	4.020415	0.003635
O	-1.942485	-2.235600	0.017480
O	4.424181	1.352844	0.227327
O	-3.008680	1.179181	0.247793
O	-0.397615	-2.657798	2.123851
O	3.410219	-0.220641	2.135403
O	2.461703	-2.477281	-1.880776
O	-1.205220	2.153730	1.968640
O	-1.425477	-0.097693	-1.461452
O	2.923114	2.181914	-1.850773
O	2.246876	-2.589368	2.199180
O	3.898971	-0.262948	-1.797525
O	2.790958	2.339303	2.076797
O	-0.181730	-2.403708	-1.958564
O	-1.981582	2.500673	-1.829368
O	-1.771704	-0.412715	1.973433
Si	0.957420	-3.438671	1.689358
Si	3.614437	-1.806572	1.819920
Si	3.862667	-1.823695	-1.371068
Si	2.305781	3.817759	1.575116
Si	-1.578743	-1.728861	-1.491099
Si	4.181806	1.289973	-1.385198
Si	2.054668	3.541255	-1.477250
Si	-1.796968	-1.997529	1.623496
Si	-2.550547	1.085320	-1.318778
Si	-2.398404	1.072928	1.759914
Si	1.110029	-3.294734	-1.519693
Si	3.977021	1.262491	1.787317
O	5.266176	1.494696	2.759777
H	5.764656	2.310883	2.671286
O	4.777092	-2.463367	2.753160
H	5.665260	-2.101313	2.701846
O	3.136839	4.891960	2.482776
H	3.042466	5.824111	2.271749
O	0.893042	-4.892759	2.418908
H	1.644026	-5.483480	2.320837
O	-3.558156	1.417159	2.850680
H	-4.390294	0.939136	2.806938
O	-3.068852	-2.632690	2.416439

H	-3.259647	-3.567580	2.305753
O	1.174674	-4.680149	-2.372504
H	0.436358	-5.290858	-2.303622
O	-2.747544	-2.154379	-2.542222
H	-3.418051	-1.472141	-2.686626
O	-3.798214	0.539285	-2.231522
H	-4.627247	1.023425	-2.263389
O	2.132316	4.674323	-2.565210
O	5.503460	1.861476	-2.156253
H	6.355092	1.481741	-1.926282
O	5.134420	-2.530194	-2.104308
H	5.269255	-3.472129	-1.973757
O	-1.411126	4.113085	0.185782
O	0.521909	2.995804	-1.175463
O	0.712733	3.958761	1.853025
Si	-0.879722	3.735675	1.673487
Si	-0.952330	3.721945	-1.367081
O	-1.587516	4.697409	2.787578
H	-2.542995	4.789895	2.756324
O	-0.971552	4.938973	-2.360149
Ca	0.616029	5.983845	-3.483625

66_Si_Cage_Octagonal_Na_Vertex

Atom	x	y	z
O	1.002623	-3.424660	0.098154
O	4.098348	-1.986219	0.124301
O	3.722883	4.364775	0.353601
O	-2.127855	-2.268218	0.134850
O	5.277000	1.079129	0.304059
O	-3.543440	0.834449	0.080247
O	-0.346352	-2.269279	2.094990
O	4.156065	-0.364550	2.223533
O	2.240010	-1.949808	-1.758671
O	-2.438591	2.270790	2.050527
O	-2.303708	-0.525215	-1.854737
O	3.952823	2.522270	-1.528473
O	2.286638	-2.214634	2.075848
O	4.105119	-0.091231	-1.763250
O	3.405211	2.164028	1.835819
O	-0.365754	-2.305913	-1.875202
O	-2.379521	2.109502	-1.940070
O	-2.142574	-0.346076	1.993076
Si	0.982430	-3.109986	1.695662
Si	3.836087	-1.881086	1.726727
Si	3.810789	-1.653856	-1.443036
Si	3.360815	3.796853	1.833488
Si	-1.915982	-2.055040	-1.465281
Si	4.910925	1.239367	-1.279456
Si	3.639495	4.101847	-1.260067
Si	-1.887576	-1.924678	1.707511
Si	-3.208414	0.778948	-1.512525
Si	-3.170813	0.876228	1.663728
Si	1.043076	-3.011880	-1.475733
Si	4.669422	1.118248	1.819504

O	5.800122	1.603012	2.884152
H	5.734761	2.531022	3.148976
O	4.741004	-2.970545	2.528807
H	5.693144	-2.958179	2.401997
O	4.524876	4.214390	2.907877
H	4.766216	5.135911	3.032552
O	0.932157	-4.496142	2.548125
H	1.659153	-5.117369	2.455006
O	-4.523581	0.791645	2.567677
H	-5.119032	0.049765	2.434281
O	-2.947255	-2.740820	2.636674
H	-2.984187	-3.697914	2.562788
O	1.356216	-4.315951	-2.398944
H	0.794606	-5.090136	-2.310828
O	-2.796774	-3.137171	-2.305067
H	-3.748498	-3.150914	-2.175121
O	-4.581035	0.623148	-2.375993
H	-5.248202	1.310414	-2.303123
O	4.704128	5.066408	-2.031499
H	5.632346	4.997866	-1.793903
O	6.264917	1.484222	-2.149928
H	6.979474	0.845522	-2.085605
O	4.801669	-2.521719	-2.399935
H	4.809847	-3.477844	-2.306343
O	-2.589388	3.911516	-0.021146
O	2.174691	4.453507	-1.834127
O	1.887512	4.306051	2.271556
Si	-2.243593	3.819393	1.569382
Si	-1.891068	3.592412	-1.474941
O	-3.196116	4.834546	2.416924
H	-4.147139	4.774736	2.295589
O	-2.323981	4.697771	-2.584799
H	-1.585628	5.347959	-2.697637
O	0.844823	5.552044	0.147442
O	-0.269151	3.623999	-1.270018
O	-0.712356	4.242104	1.878732
Si	0.675822	4.996276	-1.408013
Si	0.617292	5.164277	1.702780
O	0.543041	6.498749	2.637629
H	-0.114079	7.164823	2.420726
O	0.013235	6.022559	-2.396454
Na	0.324828	7.932025	-3.378506

67_Si_Cage_Octagonal_K_Vertex

Atom	x	y	z
O	1.005218	-3.415513	0.083358
O	4.102967	-1.981887	0.124194
O	3.715911	4.364038	0.354668
O	-2.124044	-2.249950	0.114267
O	5.273986	1.080079	0.305042
O	-3.541739	0.848553	0.087898
O	-0.350206	-2.269080	2.081288
O	4.156164	-0.363717	2.226000
O	2.260234	-1.957650	-1.774571

```
 O -2.430894  2.267559  2.066740
 O -2.274390 -0.480051 -1.852642
 O  3.939057  2.517289 -1.524017
 O  2.282472 -2.209005  2.067489
 O  4.120244 -0.093985 -1.770311
 O  3.403596  2.164482  1.839547
 O -0.350602 -2.275619 -1.886549
 O -2.420782  2.151020 -1.939352
 O -2.152065 -0.351273  1.997279
Si  0.980902 -3.105914  1.681750
Si  3.834244 -1.878638  1.725489
Si  3.826987 -1.656130 -1.446505
Si  3.358584  3.797355  1.836097
Si -1.900931 -2.018517 -1.481860
Si  4.910041  1.243337 -1.278634
Si  3.622532  4.096986 -1.258020
Si -1.891149 -1.925001  1.692025
Si -3.212567  0.800143 -1.506139
Si -3.171378  0.879399  1.672138
Si  1.048879 -3.002245 -1.490259
Si  4.668294  1.119388  1.821185
 O  5.800209  1.604478  2.884446
 H  5.735545  2.532925  3.147968
 O  4.733162 -2.971421  2.529915
 H  5.685790 -2.961335  2.406576
 O  4.526361  4.215974  2.906246
 H  4.769372  5.137507  3.027489
 O  0.931692 -4.494918  2.529786
 H  1.658791 -5.115600  2.433910
 O -4.525973  0.798999  2.573784
 H -5.121866  0.057244  2.441648
 O -2.951650 -2.757648  2.605594
 H -2.990650 -3.712784  2.510190
 O  1.340814 -4.309678 -2.415766
 H  0.758037 -5.069305 -2.338784
 O -2.785473 -3.083663 -2.339385
 H -3.737240 -3.096762 -2.209611
 O -4.584674  0.605908 -2.362812
 H -5.286940  1.252715 -2.257015
 O  4.682215  5.062051 -2.036291
 H  5.610175  5.001768 -1.795430
 O  6.262906  1.506271 -2.145679
 H  6.981869  0.872026 -2.087159
 O  4.828000 -2.524645 -2.392329
 H  4.837932 -3.480313 -2.294435
 O -2.607489  3.922753  0.009132
 O  2.154324  4.442518 -1.824902
 O  1.886798  4.306480  2.279125
Si -2.245982  3.820849  1.595432
Si -1.916977  3.622321 -1.452562
 O -3.194839  4.825217  2.459875
 H -4.147014  4.756911  2.352837
 O -2.342769  4.749442 -2.542693
 H -1.591325  5.387706 -2.655786
 O  0.841170  5.556052  0.158403
 O -0.294192  3.636940 -1.252624
```

O	-0.714132	4.247957	1.894389
Si	0.660835	5.003039	-1.397887
Si	0.616700	5.167507	1.713530
O	0.547503	6.501563	2.649794
H	-0.105524	7.171153	2.431389
O	0.009475	6.035082	-2.386615
K	0.442225	7.989421	-3.860566

68_Si_Cage_Octagonal_Ca_TopEdge

Atom	x	y	z
O	0.937171	-3.408526	0.092741
O	4.055277	-2.021372	0.100944
O	3.729172	4.364484	0.424964
O	-2.064596	-2.376924	0.163108
O	5.285281	1.066123	0.349145
O	-3.759896	0.659910	0.053309
O	-0.340497	-2.319515	2.168911
O	4.108212	-0.410393	2.210669
O	2.173779	-1.928501	-1.758666
O	-2.612731	2.365861	1.787522
O	-2.447780	-0.650111	-1.835490
O	4.071990	2.579444	-1.501729
O	2.296449	-2.317632	2.091028
O	4.005920	-0.038782	-1.690887
O	3.384092	2.131609	1.854505
O	-0.421543	-2.352996	-1.923465
O	-1.919161	1.877511	-1.370034
O	-1.811258	-0.162391	1.653468
Si	0.966062	-3.167800	1.700479
Si	3.825744	-1.933639	1.709786
Si	3.741743	-1.621521	-1.446219
Si	3.345526	3.763434	1.887257
Si	-1.968882	-2.138210	-1.453735
Si	4.924151	1.227985	-1.235455
Si	3.719419	4.137563	-1.193310
Si	-1.786376	-1.791590	1.653014
Si	-3.168297	0.798511	-1.499715
Si	-3.110338	0.848914	1.530431
Si	0.995100	-3.015665	-1.485630
Si	4.641158	1.076048	1.850604
O	5.747915	1.532237	2.952024
H	5.687538	2.456718	3.229615
O	4.780388	-3.000193	2.484086
H	5.729394	-2.953454	2.342907
O	4.489408	4.155927	2.990314
H	4.736978	5.073053	3.134224
O	0.900368	-4.583780	2.500549
H	1.616595	-5.212146	2.377050
O	-4.194066	0.464123	2.690317
H	-4.189184	-0.468450	2.943489
O	-3.001204	-2.208696	2.670342
H	-3.264414	-3.128280	2.759675
O	1.364596	-4.322879	-2.384769
H	0.824857	-5.112272	-2.295138

```
   O -2.830684 -3.287230 -2.227810
   H -3.783101 -3.294704 -2.104357
   O -4.272767  1.211482 -2.540595
   O  4.766313  5.153163 -1.914826
   H  5.697951  5.084200 -1.690899
   O  6.289444  1.343453 -2.113530
   H  6.937845  0.637072 -2.052732
   O  4.739691 -2.422546 -2.453328
   H  4.754468 -3.382582 -2.422097
   O -2.335025  4.191009 -0.154117
   O  2.253942  4.470670 -1.796727
   O  1.865765  4.270987  2.305367
  Si -2.255984  3.912519  1.438688
  Si -1.919229  3.511950 -1.617282
   O -3.242242  4.934280  2.246264
   H -4.152850  5.004327  1.949288
   O -2.859549  3.992220 -2.784256
   O  0.742374  5.390728  0.157807
   O -0.319174  3.896441 -1.813877
   O -0.753637  4.204759  2.007478
  Si  0.762314  5.030029 -1.433376
  Si  0.577034  5.100841  1.747562
   O  0.551819  6.493540  2.592339
   H -0.150844  7.123105  2.411441
   O  0.416197  6.363246 -2.308737
   H  0.920517  7.162693 -2.138670
  Ca -4.568965  3.014833 -3.772817
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(4) Aluminosilicates with an external cation (The most stable position only)

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69_SiAl_Cage_Trigonal_Na_TopEdge
-------------------------------------
Atom         x         y         z
  Si -1.391184  0.197759  1.620791
   O -0.942763  1.679916  1.061443
  Si -0.548783  2.254649 -0.451894
   O  1.069864  2.354336 -0.555996
   O -0.077486 -0.562082  2.247929
  Si  1.401537 -0.988947  1.668572
   O  2.210397  0.347557  1.230498
   O  2.178773 -1.888000  2.790353
   H  2.372329 -1.475463  3.635365
   O -2.414993  0.342604  2.890544
   H -3.259579  0.767387  2.723634
   O -1.115780  3.787227 -0.612079
   H -2.068957  3.894748 -0.647022
   O -1.177541  1.227364 -1.533238
   O  2.033010 -0.256900 -1.495751
   O  3.797728  1.936989 -0.665154
   H  3.821953  2.875993 -0.892047
   O -0.320672 -1.508423 -1.817090
  Si  1.195626 -1.642001 -1.277686
   O -3.197822 -0.922419 -2.018049
```

```
   H -3.324873 -1.188577 -2.927540
   O  1.953912 -2.931132 -1.957719
   H  1.751216 -3.107606 -2.878987
   O  1.204202 -1.953335  0.354838
   O -2.015891 -0.645432  0.387351
  Al -1.648496 -0.461292 -1.354639
  Al  2.188509  1.050055 -0.364625
   H  4.673458  1.546909 -0.782104
  Na -4.151454 -1.503084 -0.016443
-------------------------------------

70_SiAl_Cage_Trigonal_K_TopEdge
-------------------------------------
Atom         x         y         z
  Si -1.176844  0.371187  1.616100
   O -0.533735  1.794330  1.092987
  Si -0.074084  2.347764 -0.409509
   O  1.543643  2.237648 -0.520685
   O  0.026024 -0.563712  2.231734
  Si  1.445811 -1.154633  1.651302
   O  2.415584  0.080851  1.242009
   O  2.101583 -2.161298  2.759763
   H  2.306739 -1.799385  3.624797
   O -2.173561  0.623260  2.891665
   H -2.957324  1.155279  2.737027
   O -0.428974  3.947231 -0.527667
   H -1.358646  4.180448 -0.575281
   O -0.842810  1.444650 -1.510630
   O  2.183354 -0.456385 -1.495542
   O  4.211335  1.464050 -0.625800
   H  4.374693  2.387359 -0.858812
   O -0.319269 -1.371304 -1.830643
  Si  1.165210 -1.718304 -1.304344
   O -3.083637 -0.421601 -2.110518
   H -3.190881 -0.470076 -3.059944
   O  1.741265 -3.076473 -2.029036
   H  1.427506 -3.244644 -2.920085
   O  1.144661 -2.067214  0.320873
   O -1.905650 -0.355176  0.368795
  Al -1.522418 -0.179707 -1.366550
  Al  2.493453  0.804030 -0.342610
   H  5.013826  0.944749 -0.762183
   K -4.522061 -0.950788  0.011864
-------------------------------------

71_SiAl_Cage_Trigonal_Ca_LateralEdge
-------------------------------------
Atom         x         y         z
  Si  1.481668  1.264365 -1.543209
   O -0.105089  1.672571 -1.322223
  Si -1.043120  1.779610  0.039454
   O -2.054227  0.486597  0.067985
   O  1.533851 -0.280989 -2.103093
  Si  0.966853 -1.704638 -1.504762
   O -0.645503 -1.640626 -1.373523
   O  1.494294 -2.924882 -2.462747
```

```
   H  1.185374 -2.933613 -3.371552
   O  2.123773  2.144443 -2.769497
   H  2.310962  3.067343 -2.583753
   O -2.048833  3.074716 -0.090757
   H -1.643423  3.944443 -0.077528
   O -0.074146  1.838275  1.324186
   O -0.545574 -1.629365  1.424299
   O -3.241810 -1.790037  0.112914
   O  1.709536 -0.300382  2.084757
  Si  1.079193 -1.667949  1.514633
   O  2.516332  2.345840  2.649073
   H  2.600972  3.282802  2.471607
   O  1.577252 -2.944746  2.430004
   H  2.020801 -2.710963  3.247678
   O  1.629613 -1.964413 -0.027911
   O  2.258645  1.433245 -0.145881
  Al  1.630770  1.366003  1.518704
  Al -1.566840 -1.241573  0.064641
   H -3.534897 -2.700694  0.129115
  Ca -4.379006  0.243585  0.106731
-------------------------------------

72_SiAl_Cage_Tetragonal_Na_TopEdge
-------------------------------------
Atom         x         y         z
  Si -0.163385  2.677911 -0.897255
   O -1.347549  2.562318  0.222001
   O -2.962582  0.122364  0.071410
   O -0.524384  1.711893 -2.164357
  Si -2.618611 -1.234834 -0.760744
   O -1.790836 -0.896929 -2.118004
   O -0.431443 -0.028468 -4.464438
   H -1.232100 -0.090920 -4.999897
   O -0.078069  4.247028 -1.427596
   H -0.871041  4.577591 -1.854868
   O -4.024792 -1.946838 -1.262401
   H -4.642040 -2.180590 -0.565886
  Si  1.984312 -1.389669 -1.123195
   O  1.122871 -0.701559 -2.322820
   O  2.622955 -0.252160 -0.154793
   O  1.288144  2.333876 -0.281374
   O  3.819164  1.775572  1.072411
   O  3.217063 -2.283606 -1.783287
   H  3.751118 -1.825878 -2.436163
   O  1.082891 -2.451890 -0.286093
   O  0.114096 -1.582061  2.310850
  Si  0.068657 -0.029847  2.804336
   O  1.273360  0.848169  2.175993
   O  0.229487 -0.102538  4.453620
   H  0.377715  0.741828  4.884562
   O -1.375913  0.639410  2.438199
   O -0.353066 -4.249168  1.435577
   O -1.786739 -2.269995  0.184200
   O -3.589622  2.346689  1.755492
   H -4.453985  2.009276  2.020220
  Al -2.174785  1.299638  1.060507
```

Al	-0.414764	0.042579	-2.573578
Al	2.178806	1.219727	0.728201
Al	-0.207791	-2.453723	0.858718
H	0.279713	-0.517543	-4.898644
H	-1.201310	-4.697433	1.323720
H	-3.687362	3.248556	1.423602
H	3.991158	2.575886	1.565926
H	0.086587	-4.595053	2.222138
Na	4.891690	0.040065	0.108597

73_SiAl_Cage_Tetragonal_K_TopEdge

Atom	x	y	z
Si	0.308198	-2.087793	1.908526
O	1.667248	-1.202233	2.095144
O	3.217038	0.005488	-0.074173
O	0.260300	-2.693422	0.393410
Si	2.665713	-0.151202	-1.599801
O	1.803415	-1.517043	-1.767480
O	0.321761	-3.933123	-2.185171
H	1.081891	-4.519000	-2.285193
O	0.350083	-3.351704	2.983623
H	1.108991	-3.932107	2.895042
O	3.940525	-0.303770	-2.643141
H	4.512925	0.462966	-2.714874
Si	-1.896611	-0.216284	-1.652954
O	-1.102625	-1.604389	-1.967618
O	-2.182129	-0.025336	-0.079840
O	-1.019127	-1.243218	2.268096
O	-3.552726	0.200072	2.246359
O	-3.428670	-0.286540	-2.303959
H	-3.512566	-0.447578	-3.245736
O	-1.085875	1.050929	-2.277986
O	0.086605	2.761104	-0.211047
Si	0.236324	2.464232	1.384790
O	-1.011392	1.620769	1.977908
O	0.277247	3.967099	2.087072
H	0.266831	3.968571	3.046401
O	1.647929	1.700265	1.684733
O	0.352226	3.461370	-2.852746
O	1.789905	1.161780	-2.000475
O	3.914879	0.245114	2.671535
H	4.774659	0.632800	2.466900
Al	2.454426	0.196092	1.466330
Al	0.335480	-2.277873	-1.273474
Al	-1.895223	0.142544	1.644118
Al	0.283179	1.949873	-1.717336
H	-0.279921	-4.059848	-2.929672
H	0.836109	3.488812	-3.687338
H	4.038693	-0.507271	3.264310
H	-3.722174	0.289491	3.183734
H	0.355677	4.340919	-2.454095
K	-4.901948	-0.004582	-0.000873

74_SiAl_Cage_Tetragonal_Ca_TopEdge

Atom	x	y	z
Si	0.318104	-2.302503	-1.609058
O	1.703024	-1.502778	-1.817392
O	1.758892	1.391055	-1.900413
O	-0.960195	-1.449049	-2.152392
Si	0.405610	2.242846	-1.689077
O	-0.936095	1.449346	-2.149379
O	-3.510891	0.025362	-2.181631
H	-3.826492	0.029237	-3.084651
O	0.384832	-3.747510	-2.431976
H	0.675954	-3.671958	-3.342967
O	0.453907	3.595356	-2.657796
H	1.299323	4.048908	-2.656509
Si	-1.916834	0.060664	1.616814
O	-2.227905	0.009769	0.020364
O	-1.163343	-1.269299	2.140095
O	0.086254	-2.742799	-0.052822
O	0.199611	-3.737064	2.501399
H	-0.120760	-3.836521	3.406322
O	-3.522212	0.086487	2.104660
H	-3.777534	0.158424	3.026415
O	-1.150979	1.412394	2.058381
O	1.731054	1.334560	2.001579
Si	2.599594	-0.004449	1.670149
O	1.716744	-1.349104	1.961582
O	3.852677	0.037862	2.760559
H	4.462741	-0.700163	2.700314
O	3.173788	-0.006554	0.164342
O	0.331900	3.813910	2.393237
H	-0.012246	3.959623	3.282930
O	0.267066	2.736124	-0.133156
O	4.072860	-0.200126	-2.573514
H	4.658264	0.557370	-2.600913
Al	2.668043	-0.067387	-1.524362
Al	-1.791557	0.006942	-1.702848
Al	0.237084	-2.111780	1.538210
Al	0.313975	2.158253	1.483004
H	0.244553	4.627357	1.880222
H	0.036576	-4.554481	2.013536
Ca	-4.598849	0.025424	-0.111808

75_SiAl_Cage_Pentagonal_Na_TopSurface

Atom	x	y	z
Si	-2.768069	-0.908753	1.674816
O	-1.630809	-1.989603	2.123631
O	-0.110791	-2.893342	-0.223497
O	-2.786640	-0.757776	0.070340
Si	-0.143796	-2.625744	-1.819645
O	-1.366174	-1.686250	-2.307995
O	-3.976500	-0.649162	-2.568060
O	-4.239452	-1.400846	2.256893
H	-4.529230	-2.267343	1.963589

```
   O -0.162482 -4.282557  2.295245
   H -0.914838 -4.504468  2.858964
   O  1.308213 -1.905574  2.102890
   O  1.252498 -1.887381 -2.274470
   O -0.296144 -4.060383 -2.628739
   H  0.329931 -4.745824 -2.385419
  Si  2.630455 -1.064775  1.712889
   O  2.869598 -1.057231  0.109024
   O  3.959847 -0.985663 -2.400404
   O  3.954801 -1.648113  2.497563
   H  4.144474 -2.581031  2.375904
  Si -1.444032  2.477559 -1.288276
   O -1.642531  1.005331 -1.926020
   O -2.002603  2.566152  0.231433
   O -2.509246  0.546752  2.366597
   O -1.974794  3.272681  2.881739
   H -2.282477  3.167319  3.790553
   O -2.141889  3.650929 -2.215509
   H -3.090101  3.576229 -2.345014
  Si  1.671016  2.291829 -1.248572
   O  0.153820  2.878630 -1.326329
   O  2.178204  2.289298  0.307692
  Si  1.715425  1.836318  1.812373
   O  0.137465  1.551476  1.873021
   O  2.194098  3.072779  2.781062
   H  2.029951  2.971219  3.721612
   O  2.530592  0.486910  2.248586
   O  2.680156  3.240743 -2.125768
   H  2.773717  4.156671 -1.853517
   O  1.732563  0.801879 -1.879387
  Al -1.555793  1.832478  1.730618
  Al -0.151227 -2.574425  1.462052
  Al -2.508909 -0.524838 -1.624640
  Al  2.325520 -0.789962 -1.489070
   H  0.635156 -4.681244  2.664824
   H -4.768433 -0.235291 -2.224124
   H -2.354748  4.077831  2.507029
   H  4.757515 -1.256705 -1.927585
   H  4.061170 -1.175832 -3.341455
  Na -0.033196  0.078971 -3.345301
-------------------------------------

76_SiAl_Cage_Pentagonal_K_TopSurface
-------------------------------------
Atom         x         y         z
  Si -2.902674  0.050162  1.788853
   O -2.095497 -1.230167  2.401000
   O -0.740676 -2.859578  0.369561
   O -3.028328 -0.072195  0.188868
  Si -0.718252 -2.781417 -1.248577
   O -1.716788 -1.678127 -1.871149
   O -4.183239 -0.462520 -2.439462
   O -4.399838  0.122138  2.499277
   H -4.971925 -0.628211  2.325033
   O -1.043336 -3.642366  3.111975
   H -1.801776 -3.597629  3.708458
```

```
   O  0.807712 -1.607475  2.477239
   O  0.805632 -2.442756 -1.760074
   O -1.181216 -4.242617 -1.877382
   H -0.713586 -5.008033 -1.536232
  Si  2.313987 -1.233320  2.030886
   O  2.611521 -1.710097  0.510546
   O  3.529917 -2.574246 -2.036791
   O  3.419445 -1.890574  3.061282
   H  3.433370 -2.849087  3.108806
  Si -0.891618  2.390193 -1.706142
   O -1.751080  1.093932 -2.122273
   O -1.012025  2.774744 -0.144979
   O -2.176769  1.443094  2.224736
   O -1.510552  4.081718  2.327535
   H -2.347149  4.097740  2.809902
   O -1.275412  3.689615 -2.651368
   H -2.207019  3.917546 -2.689262
  Si  2.127086  1.570996 -1.547086
   O  0.687852  2.105440 -2.107728
   O  2.268991  1.931813  0.032149
  Si  2.136043  1.858458  1.655166
   O  0.639303  2.195486  2.139992
   O  3.221280  2.960071  2.209610
   H  3.218204  3.126680  3.155073
   O  2.581460  0.378239  2.178074
   O  3.337504  2.288301 -2.390291
   H  3.403152  3.244677 -2.335825
   O  2.228548 -0.013954 -1.826462
  Al -0.961645  2.447352  1.540434
  Al -0.733171 -2.177707  1.944777
  Al -2.711373 -0.266729 -1.509497
  Al  2.182238 -1.606401 -1.144375
   H -0.331116 -4.131054  3.542674
   H -4.852548  0.218238 -2.364457
   H -1.353921  4.949848  1.935508
   H  4.454220 -2.626130 -1.763069
   H  3.296547 -3.367271 -2.536786
   K  0.030823 -0.398756 -3.569566
-------------------------------------

77_SiAl_Cage_Pentagonal_Ca_TopSurface
-------------------------------------
Atom         x         y         z
  Si -2.933395  0.650671  1.573346
   O -2.619403 -0.859930  2.098560
   O -1.527447 -2.475072 -0.090667
   O -2.811461  0.701037 -0.036043
  Si -1.321809 -2.303204 -1.675907
   O -1.861864 -0.886770 -2.293242
   O -3.479588  1.510077 -2.742388
   O -4.447975  1.099168  2.069761
   H -5.170475  0.573242  1.720294
   O -2.445752 -3.569598  2.410771
   H -3.282066 -3.392210  2.860526
   O -0.013520 -2.175838  2.369593
   O  0.265861 -2.271997 -2.102954
```

```
   O -2.119626 -3.500785 -2.481793
   H -2.091592 -4.371539 -2.079293
  Si  1.561296 -2.073899  2.003024
   O  1.811508 -2.226554  0.423370
   O  3.007709 -3.007222 -2.102339
   O  2.413921 -3.190953  2.869864
   H  2.134531 -4.102869  2.763663
  Si  0.082027  2.747292 -1.365936
   O -0.731546  1.480830 -2.009145
   O -0.504780  3.133508  0.086122
   O -1.926295  1.732713  2.257644
   O -0.517574  4.006790  2.797823
   H -1.291765  4.173009  3.350857
   O  0.070689  4.051664 -2.368047
   H -0.757464  4.532405 -2.437283
  Si  2.665783  1.040847 -1.098031
   O  1.666954  2.322278 -1.290719
   O  3.002576  0.848271  0.486386
  Si  2.381376  0.881720  2.001894
   O  0.988847  1.675822  2.051621
   O  3.544719  1.612218  2.902508
   H  3.352443  1.732535  3.835368
   O  2.185980 -0.647813  2.536996
   O  4.066378  1.305512 -1.907763
   H  4.632804  2.013599 -1.591984
   O  1.964235 -0.276946 -1.738767
  Al -0.484185  2.480137  1.687855
  Al -1.550036 -2.112041  1.589537
  Al -2.338646  0.723690 -1.690447
  Al  1.828010 -2.025954 -1.288444
   H -1.965855 -4.249819  2.899813
   H -4.414719  1.392753 -2.572862
   H -0.073602  4.842147  2.606310
   H  3.825706 -3.220490 -1.653052
  Ca  0.211546 -0.205491 -3.364876
-------------------------------------

78_SiAl_Cage_Hexagonal_Na_TopEdge
-------------------------------------
Atom         x         y         z
   O  0.775269 -1.383583  1.713945
  Si  2.378979 -1.304513  1.976178
   O  3.255153 -1.865360  0.743335
   O  0.096157 -3.641218  0.050488
  Si  0.341180 -2.926705 -1.393530
   O  1.890087 -2.610493 -1.681482
   O -0.268327 -3.942690 -2.597366
   H  0.058769 -4.842851 -2.664614
   O  0.449240 -3.794962  2.926521
   H  1.327668 -3.425713  3.235650
   O  2.574784 -2.363313  3.279063
   H  3.465435 -2.633815  3.516416
   O  2.809497  0.192040  2.420516
   O  2.897066  0.081739 -1.353868
   O  4.705056 -1.872247 -1.806389
   O  2.761856  2.212279  0.316617
```

```
  Si  2.774461  1.681324 -1.221850
   O  4.185347  2.189277 -1.967271
   H  4.349790  3.130291 -2.050897
   O  3.421582  2.914544  2.990550
   H  4.308278  3.201837  2.740498
   O -0.620947 -1.619677 -1.542449
   O -3.257056 -2.048162 -0.385492
  Si -3.261052 -1.871315  1.233155
   O -1.924254 -2.540958  1.878452
   O -4.601356 -2.609822  1.865654
   H -4.684628 -3.546856  1.676059
   O -2.541155 -2.818798 -3.063034
   H -1.749817 -3.433078 -3.061586
  Si -2.905707  1.559796 -2.025171
   O -2.900732 -0.014538 -2.435356
   O -3.252070  1.758239 -0.449114
   O -3.386485 -0.311295  1.654415
   O -4.728472  2.200769  1.784964
   H -5.202887  1.999092  2.600543
   O -4.117165  2.343594 -2.839136
   H -3.981356  2.439060 -3.784394
  Si -0.496260  2.626448  1.614059
   O -0.264391  1.995660  0.143108
   O -1.914466  2.107584  2.195888
   O -0.577197  4.290183  1.330175
   H -0.612278  4.905078  2.066876
   O -1.473230  2.227895 -2.445265
   O -0.186233  4.451248 -1.183501
   H -0.365197  4.649780 -0.216258
   O  1.504477  2.271250 -2.057854
   O  0.792562  2.321035  2.549365
  Al -3.135609  1.331100  1.217460
  Al -2.345355 -1.489888 -1.743372
  Al -0.260396 -2.769101  1.513691
  Al  3.161319 -1.611681 -0.995493
  Al  2.334053  1.779412  1.933361
  Al -0.093233  2.587356 -1.475841
   H -5.361629  2.470182  1.107335
   H  5.138014 -2.724703 -1.813607
   H  2.997227  3.607548  3.512636
   H -0.714997  5.025793 -1.748407
   H  0.442896 -4.756707  2.976622
   H -3.354397 -3.309658 -3.222615
  Na  5.079075  0.165358 -2.687392
--------------------------------------

79_SiAl_Cage_Hexagonal_K_TopSurface
--------------------------------------
Atom         x         y         z
   O -0.644531 -1.468601 -1.795400
  Si -2.260815 -1.645455 -1.867720
   O -2.894104 -2.307682 -0.544439
   O  0.446258 -3.614076 -0.218878
  Si  0.309880 -2.969537  1.263331
   O -1.198115 -2.792385  1.787570
   O  1.207355 -3.905132  2.342451
```

```
   H  1.033981 -4.847427  2.409426
   O -0.089931 -3.817905 -3.052022
   H -1.051087 -3.592422 -3.247508
   O -2.428157 -2.760882 -3.132770
   H -3.278615 -3.195065 -3.239581
   O -2.970007 -0.254362 -2.292474
   O -2.733301 -0.460772  1.636346
   O -3.983778 -3.094052  2.023569
   H -4.894947 -2.959976  1.761594
   O -3.328596  1.581064 -0.073326
  Si -3.101411  1.104599  1.463069
   O -4.528831  1.467557  2.225525
   H -4.595520  1.170590  3.135750
   O -4.361579  2.210413 -2.638378
   H -5.263342  2.247633 -2.296709
   O  1.095998 -1.536368  1.358287
   O  3.631917 -1.366432 -0.101603
  Si  3.326654 -1.192250 -1.694811
   O  2.167229 -2.236397 -2.158574
   O  4.706330 -1.494787 -2.556030
   H  5.052608 -2.387074 -2.484954
   O  3.350020 -2.466777  2.554904
   H  2.660728 -3.190173  2.621355
  Si  2.531753  1.908597  1.786990
   O  3.057152  0.410181  2.146536
   O  2.642755  2.223989  0.197866
   O  2.909384  0.333737 -2.045339
   O  3.877178  3.027795 -2.080027
   H  4.323635  2.952680 -2.932231
   O  3.495144  3.031025  2.526437
   H  3.518597  2.996548  3.485384
  Si -0.343981  2.826715 -1.638106
   O -0.367738  2.089997 -0.198418
   O  1.087931  2.549190 -2.340188
   O -0.474611  4.462166 -1.246125
   H -0.453994  5.134055 -1.931642
   O  0.989043  2.060183  2.327567
   O -0.507123  4.397816  1.312986
   H -0.476943  4.702499  0.358226
   O -1.880731  1.934073  2.191852
   O -1.655696  2.352961 -2.463650
  Al  2.467420  1.896577 -1.487617
  Al  2.790403 -1.111974  1.380292
  Al  0.578244 -2.701608 -1.697852
  Al -2.750857 -2.164510  1.203528
  Al -2.916935  1.379769 -1.735825
  Al -0.432823  2.536270  1.464598
   H  4.504480  3.349559 -1.419757
   H -4.184827  3.003265 -3.160778
   H -0.114500  5.044258  1.909616
   H  0.067826 -4.765122 -3.126382
   H  4.239453 -2.835227  2.594687
   K -0.476443 -0.293636  3.209385
-------------------------------------
```

80_SiAl_Cage_Hexagonal_Ca_TopEdge

Atom	x	y	z
O	0.511246	-1.466042	1.791783
Si	2.094998	-1.361050	2.154027
O	3.033070	-1.876637	0.935507
O	-0.086162	-3.642032	-0.005753
Si	0.213150	-2.859029	-1.400921
O	1.773569	-2.512172	-1.596190
O	-0.317416	-3.823967	-2.679308
H	0.008250	-4.724045	-2.755197
O	0.175608	-3.944131	2.869160
H	1.036151	-3.561436	3.231207
O	2.225375	-2.510657	3.397492
H	3.102798	-2.762999	3.695485
O	2.516762	0.085757	2.703698
O	3.069309	0.081201	-1.204648
O	4.634243	-1.924574	-1.544417
O	2.612161	2.078396	0.601632
Si	2.731129	1.653741	-0.935773
O	4.172176	2.232946	-1.612614
H	4.351950	3.173894	-1.660288
O	3.404757	2.790814	3.208982
O	-0.747518	-1.552002	-1.544938
O	-3.405124	-2.118895	-0.518378
Si	-3.388778	-1.820403	1.085995
O	-2.178332	-2.649137	1.794874
O	-4.830616	-2.282622	1.755088
H	-5.057896	-3.209626	1.655527
O	-2.580364	-2.691243	-3.210214
H	-1.786910	-3.300408	-3.199694
Si	-2.940272	1.654601	-2.100485
O	-3.033417	0.062126	-2.419228
O	-3.347614	1.983224	-0.560618
O	-3.241990	-0.235213	1.373932
O	-4.860070	2.123956	1.651984
H	-5.316836	1.870410	2.462720
O	-4.047154	2.467610	-3.026102
H	-3.885300	2.450907	-3.971960
Si	-0.581924	2.622865	1.682734
O	-0.442405	1.944153	0.213443
O	-2.092347	2.279082	2.180710
O	-0.491302	4.291135	1.369528
H	-0.196343	4.872290	2.075048
O	-1.438713	2.192450	-2.469559
O	-0.181749	4.389999	-1.130718
H	-0.312597	4.598252	-0.149899
O	1.495215	2.166603	-1.854556
O	0.603184	2.225908	2.689183
Al	-3.169101	1.453483	1.078667
Al	-2.466352	-1.439996	-1.805280
Al	-0.494471	-2.853495	1.493131
Al	3.046851	-1.637142	-0.789107
Al	2.285815	1.786448	2.310074
Al	-0.133773	2.523120	-1.390144
H	-5.511313	2.326989	0.968625

H	5.070519	-2.775240	-1.582312
H	3.281960	2.834614	4.157943
H	-0.738671	4.955898	-1.676693
H	0.205057	-4.906378	2.850884
H	-3.379671	-3.177273	-3.440258
Ca	5.210048	0.185715	-2.320136

81_SiAl_Cage_Heptagonal_Na_TopSurface

Atom	x	y	z
O	0.927801	-3.619340	0.258943
O	4.374343	-2.214179	0.408710
O	2.603632	4.061947	0.485781
O	-2.319892	-2.216480	0.077907
O	5.145689	1.469855	0.318055
O	-3.117732	1.167996	0.257637
O	-0.435988	-2.452334	2.240700
O	4.302276	-0.416504	2.416303
O	2.417886	-2.509854	-1.693099
O	-1.733534	2.179656	2.333489
O	-2.366157	-0.511288	-1.990472
O	3.860205	2.616153	-1.724590
O	2.119763	-1.809262	1.807973
O	3.478322	0.028563	-1.182736
O	3.321641	2.328704	2.422285
O	-0.116799	-1.818499	-1.404267
O	-1.641838	2.292224	-2.002283
O	-2.507227	-0.372079	2.348140
Si	0.998215	-3.011850	1.786891
Si	3.773029	-1.832131	1.854698
Si	2.445134	3.639502	2.050960
Si	-1.776074	-1.887753	-1.403686
Si	4.574487	1.253109	-1.194932
Si	-2.881200	1.136341	1.865046
Si	0.979111	-3.066927	-1.286129
O	6.008503	1.590421	3.048192
H	6.227362	2.464355	3.393841
O	4.073785	-3.054771	2.943018
H	4.966707	-3.404877	2.985936
O	3.051824	4.859963	2.995944
H	2.703155	5.734606	2.810099
O	1.491680	-4.202316	2.803033
H	2.424986	-4.118822	3.050090
O	-4.269259	1.628789	2.624774
H	-5.068332	1.163595	2.367461
O	-3.194147	-2.998389	2.684337
H	-3.065776	-3.935793	2.873891
O	0.506603	-4.269791	-2.294970
H	-0.433068	-4.227010	-2.526370
O	-2.070310	-3.162164	-2.423889
H	-2.973353	-3.474858	-2.516780
O	-4.259446	1.553363	-2.375543
H	-4.236845	2.307906	-2.978105
O	2.211794	4.937122	-2.228285
H	2.634686	5.793092	-2.096466

```
   O  5.803709  0.868090 -2.223750
   H  5.823478 -0.088298 -2.416072
   O  5.214212 -1.828165 -2.344039
   H  5.801680 -2.584225 -2.323289
   O -0.878352  3.816146  0.068765
   O  0.975405  2.605617 -1.453409
   O  0.877965  3.393145  2.408228
  Si -0.514412  3.280900 -1.411525
   O -1.472194  5.041698  2.394342
   H -1.671691  5.739768  1.757463
   O -0.327995  4.603421 -2.434137
   H -1.059022  5.218321 -2.537248
  Al -1.988867 -1.892184  1.742031
  Al -2.716208  1.077281 -1.402110
  Al -0.707482  3.427242  1.746401
  Al  2.482076  3.449140 -1.117967
  Al  4.535360  1.222747  1.912765
  Al  3.887921 -1.698376 -1.198503
   H -3.779900 -2.611984  3.347585
   H -4.940964  0.933138 -2.663069
   H -1.314429  5.434264  3.261553
   H  1.244805  5.050249 -2.459701
   H  6.265596  0.919689  3.693724
  Na  1.233366  0.231340 -1.648333
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82_SiAl_Cage_Heptagonal_K_TopSurface
-------------------------------------
Atom         x         y         z
   O  0.925748 -3.621756  0.239216
   O  4.336368 -2.209207  0.450612
   O  2.701521  4.028668  0.446221
   O -2.378013 -2.188249  0.049463
   O  5.005102  1.383264  0.283028
   O -3.114178  1.162625  0.293538
   O -0.495517 -2.511847  2.212077
   O  4.209032 -0.390619  2.438328
   O  2.393922 -2.387124 -1.663743
   O -1.670724  2.127274  2.352078
   O -2.359560 -0.453994 -1.997519
   O  3.594848  2.338259 -1.793256
   O  2.053100 -1.808074  1.828712
   O  4.113801 -0.232168 -1.669294
   O  3.367016  2.409104  2.488513
   O -0.149160 -1.802353 -1.396420
   O -1.773493  2.412016 -1.971170
   O -2.523198 -0.399391  2.370066
  Si  0.958407 -3.032798  1.775375
  Si  3.706476 -1.815450  1.874119
  Si  2.477277  3.682182  2.023483
  Si -1.802065 -1.850888 -1.419477
  Si  4.690862  1.235340 -1.303989
  Si -2.857596  1.121298  1.896724
  Si  0.977814 -3.015894 -1.285917
   O  5.985972  1.730458  2.955870
   H  5.886040  2.425530  3.618683
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```
   O  4.010329 -3.024892  2.981545
   H  4.901687 -3.380325  3.009686
   O  3.025782  4.955183  2.932327
   H  2.642988  5.809077  2.719467
   O  1.460192 -4.225469  2.785511
   H  2.385640 -4.117885  3.053019
   O -4.219520  1.653931  2.677225
   H -5.035229  1.211059  2.433272
   O -3.259167 -3.020213  2.638760
   H -3.131248 -3.958721  2.823356
   O  0.537923 -4.206719 -2.329005
   H -0.400171 -4.171771 -2.566585
   O -2.095132 -3.110360 -2.458985
   H -2.995244 -3.433125 -2.544927
   O -4.341778  1.529390 -2.306042
   H -4.374290  2.314462 -2.867978
   O  2.188182  4.855114 -2.263558
   H  2.675259  5.683657 -2.195214
   O  6.063070  1.577492 -2.168913
   H  6.814236  1.003480 -2.004193
   O  5.234931 -2.792490 -2.232979
   H  5.463273 -3.686128 -1.975538
   O -1.024443  3.908028  0.130256
   O  0.826497  2.671953 -1.366021
   O  0.902578  3.423474  2.326456
  Si -0.640245  3.379953 -1.350484
   O -1.489255  4.993792  2.549271
   H -1.725101  5.721664  1.959811
   O -0.398739  4.704207 -2.358347
   H -1.085201  5.372504 -2.428902
  Al -2.035214 -1.912674  1.720185
  Al -2.751690  1.113617 -1.377584
  Al -0.721656  3.438080  1.770828
  Al  2.406304  3.381092 -1.118552
  Al  4.483089  1.231654  1.912658
  Al  4.058273 -1.938196 -1.264558
   H -3.834891 -2.635420  3.311716
   H -4.964684  0.871138 -2.638424
   H -1.287730  5.343786  3.425482
   H  1.222103  5.027199 -2.452476
   H  6.671026  1.113973  3.242206
   K  1.507164  0.218180 -2.337854
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83_SiAl_Cage_Heptagonal_Ca_TopSurface
-------------------------------------
Atom         x         y         z
   O  0.879107 -3.495678  0.184635
   O  4.342434 -2.268266  0.468675
   O  2.634483  4.039217  0.444656
   O -2.328010 -2.184957  0.042028
   O  5.144904  1.390432  0.306382
   O -3.086908  1.132896  0.272529
   O -0.480229 -2.467208  2.233387
   O  4.267194 -0.401578  2.410757
   O  2.321820 -2.073474 -1.602737
```

```
 O -1.690021  2.114530  2.360013
 O -2.541487 -0.470855 -2.033865
 O  3.511477  2.202572 -1.697306
 O  2.076496 -1.786754  1.837098
 O  4.114965 -0.226405 -1.593797
 O  3.420705  2.407179  2.432632
 O -0.176122 -1.612942 -1.440572
 O -1.749408  2.245289 -2.017861
 O -2.550020 -0.404151  2.383393
Si  0.957171 -2.987345  1.752081
Si  3.727715 -1.827532  1.890750
Si  2.472553  3.655602  2.025906
Si -1.844812 -1.775959 -1.443146
Si  4.753255  1.233959 -1.251922
Si -2.871598  1.111308  1.865971
Si  0.936509 -2.840700 -1.309801
 O  6.036180  1.664530  3.020422
 H  6.014183  2.441697  3.593449
 O  4.007735 -3.022187  3.015035
 H  4.897044 -3.380682  3.067195
 O  3.005665  4.928996  2.939043
 H  2.571161  5.768887  2.774328
 O  1.467565 -4.239991  2.679310
 H  2.382192 -4.136606  2.982347
 O -4.240475  1.654415  2.638909
 H -5.055145  1.227742  2.365063
 O -3.242669 -3.033742  2.611699
 H -3.108796 -3.973822  2.782911
 O  0.613733 -3.999357 -2.416662
 H -0.324554 -4.021345 -2.662592
 O -2.015399 -3.085417 -2.459037
 H -2.894058 -3.455004 -2.573601
 O -4.494119  1.663639 -2.227089
 O  2.155075  4.768890 -2.299986
 H  2.583870  5.628247 -2.216131
 O  6.041280  1.602192 -2.205547
 H  6.908773  1.378964 -1.861142
 O  5.080888 -2.891027 -2.268335
 H  5.535186 -3.653202 -1.909036
 O -0.908228  3.766348  0.068162
 O  0.882636  2.481579 -1.424722
 O  0.915415  3.337139  2.352615
Si -0.615780  3.181011 -1.409568
 O -1.436979  4.982820  2.406975
 H -1.644451  5.683577  1.775769
 O -0.336681  4.492496 -2.442171
 H -1.050659  5.110127 -2.620354
Al -2.027022 -1.895331  1.715298
Al -3.008416  1.137595 -1.467370
Al -0.692983  3.365676  1.739336
Al  2.383667  3.367740 -1.107066
Al  4.559676  1.227501  1.924717
Al  4.062521 -1.954578 -1.225496
 H -3.815196 -2.661024  3.294042
 H -5.309957  1.248301 -1.946608
 H -1.275310  5.369736  3.275877
```

H	1.166469	4.870644	-2.514266
H	6.599647	0.990013	3.420134
Ca	1.751869	0.278468	-2.019995

84_SiAl_Cage_Octagonal_Na_TopEdge

Atom	x	y	z
O	0.945182	-3.518433	-0.121943
O	4.288444	-2.129781	0.227720
O	3.945429	4.368348	0.523986
O	-2.202403	-2.433042	0.283534
O	5.489440	1.064667	0.366994
O	-3.836670	0.851271	0.009104
O	-0.390589	-2.464728	2.256803
O	4.167167	-0.569735	2.390492
O	2.050703	-1.469114	-1.471790
O	-2.758349	2.510351	2.167103
O	-2.802640	-0.638424	-1.984587
O	4.647886	2.562845	-1.707934
O	2.519207	-2.661261	2.192027
O	4.621630	-0.101391	-1.869347
O	3.284693	2.175159	1.919582
O	-0.442290	-2.292484	-2.055181
O	-2.727685	2.027701	-2.114439
O	-1.733826	-0.198505	1.695347
Si	3.991010	-2.085860	1.826274
Si	3.357654	3.799738	1.928243
Si	5.389446	1.195890	-1.250227
Si	-1.772129	-1.819129	1.722713
Si	-3.569317	0.735119	-1.591695
Si	1.024845	-2.723280	-1.532758
O	5.687816	1.782287	3.135845
H	5.426891	2.738455	3.293019
O	5.049934	-3.098558	2.603549
H	5.979520	-2.901619	2.469413
O	4.528911	4.075682	3.118682
H	4.844731	4.971620	3.258344
O	0.792015	-4.930931	2.340734
H	1.198300	-5.740402	2.007710
O	-4.250484	0.148206	2.767007
H	-3.963343	-0.775929	3.007671
O	-3.009918	-2.127767	2.823775
H	-3.323876	-3.029346	2.928460
O	1.763132	-3.734178	-2.663076
H	1.427374	-4.627996	-2.768148
O	-3.044669	-3.497286	-2.053653
H	-3.307081	-4.183172	-1.426153
O	-5.023317	0.660505	-2.384199
H	-5.611317	1.404249	-2.235698
O	4.914023	5.416825	-1.769957
H	5.129858	6.109891	-1.132624
O	6.917138	1.294282	-1.886772
H	7.507659	0.574983	-1.652561
O	4.191184	-2.833119	-2.555313
H	3.369417	-3.334424	-2.816215

O	-2.601862	4.053124	-0.001079
O	2.306305	4.227292	-1.904158
O	1.975104	4.494965	2.351999
Si	-2.365038	3.983513	1.602698
O	-3.321231	5.137702	2.348658
H	-4.268461	5.112134	2.200645
O	-2.247237	4.764247	-2.764109
H	-1.396001	5.264028	-2.941064
O	0.801611	5.490518	-0.072923
O	-0.211286	3.412242	-1.478971
O	-0.888044	4.430865	2.074467
Si	0.814475	4.671879	-1.460533
O	0.247735	6.843867	2.449436
H	0.855092	7.579914	2.385634
O	0.156135	5.664235	-2.666407
H	0.482829	6.564517	-2.739199
Al	0.581243	5.301048	1.654388
Al	3.840498	3.972356	-1.153921
Al	4.569323	1.005848	1.826660
Al	3.784764	-1.488848	-1.291286
Al	1.015872	-3.209857	1.576042
Al	-2.019031	-2.042843	-1.390592
Al	-3.050061	0.932554	1.541210
Al	-1.951134	3.422697	-1.473064
H	4.876066	5.799340	-2.655057
H	6.646889	1.692116	3.127705
H	4.744497	-2.655256	-3.323811
H	-0.040069	-5.148740	2.779224
H	-2.962042	-3.884424	-2.933812
H	-4.589316	0.617917	3.536876
H	-2.718063	4.580763	-3.584380
Na	-1.728589	6.421740	3.432695

85_SiAl_Cage_Octagonal_K_TopSurface

Atom	x	y	z
O	1.005612	-3.255213	0.018583
O	4.508769	-2.211764	0.639615
O	3.749223	4.278692	0.670672
O	-2.135560	-2.343496	0.476177
O	5.501903	1.086171	0.753659
O	-3.837723	0.903307	0.370912
O	-0.361210	-2.468381	2.481158
O	4.148652	-0.583724	2.739043
O	2.445630	-1.282088	-1.153519
O	-2.659954	2.553098	2.484521
O	-2.916295	-0.522405	-1.715228
O	3.806133	1.948612	-1.128647
O	2.542019	-2.680797	2.441973
O	5.133251	-0.379096	-1.474995
O	3.238853	2.155969	2.245995
O	-0.165250	-1.370756	-1.479654
O	-3.016638	2.144162	-1.837507
O	-1.675146	-0.165362	1.956362
Si	4.043506	-2.115696	2.182591

```
Si  3.286527  3.773663  2.144768
Si  5.168412  1.090832 -0.834884
Si -1.726979 -1.788300  1.949007
Si -3.728582  0.801941 -1.247476
Si  1.179207 -2.281428 -1.271732
 O  5.602237  1.812541  3.521900
 H  5.382658  2.780553  3.604514
 O  5.019084 -3.092099  3.112047
 H  5.959159 -2.984894  2.952317
 O  4.495165  4.159970  3.249850
 H  4.825465  5.060823  3.289799
 O  0.803468 -4.949031  2.289474
 H  1.183407 -5.714374  1.841150
 O -4.147728  0.200264  3.133945
 H -3.887760 -0.742313  3.322461
 O -2.981012 -2.113956  3.022496
 H -3.282364 -3.018885  3.133665
 O  1.457679 -3.233810 -2.610529
 H  0.891900 -4.002734 -2.714096
 O -2.218353 -3.286079 -2.065458
 H -2.624680 -4.025984 -1.595507
 O -5.241601  0.638375 -1.898955
 H -5.867341  1.328863 -1.669603
 O  5.054688  4.243538 -1.908534
 H  5.462610  5.114102 -1.842483
 O  6.323904  2.043337 -1.619698
 H  7.254595  1.823629 -1.531252
 O  4.430702 -3.120416 -2.111694
 H  3.622260 -3.399490 -2.553112
 O -2.671339  4.112297  0.319811
 O  2.107675  4.129904 -1.732290
 O  1.891890  4.462547  2.586877
Si -2.464925  4.073191  1.932609
 O -3.575121  5.077141  2.644075
 H -4.486861  4.930847  2.382835
 O -2.463792  4.857472 -2.449264
 H -1.624718  5.337615 -2.686763
 O  0.652511  5.418569  0.119993
 O -0.405882  3.390055 -1.314195
 O -1.020392  4.656219  2.382280
Si  0.636930  4.641783 -1.296737
 O  0.699184  6.928307  2.534451
 H -0.006652  7.584887  2.578087
 O  0.001449  5.667977 -2.466608
 H  0.370371  6.550873 -2.554760
Al  0.515371  5.182033  1.826202
Al  3.568187  3.663262 -0.935412
Al  4.535493  0.994866  2.192085
Al  4.153446 -1.777128 -1.019548
Al  1.052031 -3.149468  1.742031
Al -1.827367 -1.697694 -1.101745
Al -2.985510  0.981548  1.867777
Al -2.151862  3.483177 -1.195632
 H  1.338028  7.097607  3.238385
 H  5.751372  3.516049 -1.920102
 H  6.550003  1.670956  3.622306
```

```
   H -0.022405 -5.208044  2.717164
   H -2.454910 -3.332374 -3.000128
   H -4.407642  0.654482  3.943035
   H -3.013151  4.715137 -3.228288
   K  1.207019  1.096656 -1.553532
-------------------------------------

86_SiAl_Cage_Octagonal_Ca_TopSurface
-------------------------------------
Atom         x         y         z
   O  1.008661 -3.132933  0.013503
   O  4.308793 -2.099179  0.530988
   O  3.890790  4.319675  0.776483
   O -2.200061 -2.381346  0.535079
   O  5.574407  1.063981  0.821697
   O -3.908650  0.897615  0.452454
   O -0.383447 -2.481833  2.498720
   O  4.111692 -0.603663  2.739730
   O  2.261918 -1.022163 -1.189604
   O -2.596770  2.562867  2.499781
   O -3.091046 -0.547608 -1.643064
   O  4.931648  2.494993 -1.340075
   O  2.526470 -2.722193  2.466481
   O  5.021270 -0.174634 -1.492160
   O  3.267920  2.148561  2.202883
   O -0.278708 -1.152259 -1.280390
   O -3.144383  2.121560 -1.807189
   O -1.690140 -0.177092  1.944536
  Si  3.990399 -2.105064  2.112387
  Si  3.330861  3.770308  2.203473
  Si  5.661590  1.137806 -0.802295
  Si -1.757438 -1.798126  1.991386
  Si -3.853678  0.816449 -1.173105
  Si  1.057445 -2.122838 -1.240066
   O  5.554744  1.738421  3.611835
   H  5.334877  2.702028  3.729663
   O  5.059371 -3.112286  2.891127
   H  5.980920 -2.975281  2.661721
   O  4.464819  4.092491  3.399865
   H  4.761781  4.994661  3.541119
   O  0.757741 -4.962282  2.176814
   H  1.171516 -5.713797  1.734995
   O -4.095922  0.261500  3.237802
   H -3.854130 -0.683661  3.426411
   O -2.983183 -2.088332  3.101734
   H -3.283749 -2.988220  3.250095
   O  1.215552 -2.983477 -2.643054
   H  0.780553 -3.839352 -2.676246
   O -2.096644 -3.209499 -2.058866
   H -2.419003 -4.020615 -1.642977
   O -5.394779  0.652174 -1.763964
   H -5.972448  1.403805 -1.615481
   O  4.002432  5.174432 -1.810124
   H  4.308537  5.977321 -1.366916
   O  7.245713  1.312769 -1.260353
   H  7.812107  0.560208 -1.076892
```

```
   O  4.191279 -2.832846 -2.250592
   H  3.387104 -3.066027 -2.722138
   O -2.622446  4.041398  0.274421
   O  2.108713  3.127983 -1.196303
   O  1.920552  4.460936  2.584244
  Si -2.425062  4.061834  1.874886
   O -3.547806  5.074309  2.564953
   H -4.451977  4.927615  2.279244
   O -2.282238  4.795275 -2.482787
   H -1.447782  5.027796 -2.898531
   O  0.724574  5.103678  0.011501
   O -0.430740  2.993466 -1.282901
   O -0.991436  4.681805  2.330186
  Si  0.771751  4.097206 -1.244973
   O  0.764406  6.924552  2.215772
   H  0.052866  7.576233  2.231874
   O  0.712478  4.960097 -2.654392
   H  1.144087  5.818288 -2.656196
  Al  0.557120  5.106832  1.737106
  Al  3.752014  3.599274 -0.788945
  Al  4.551903  0.967277  2.204304
  Al  4.002213 -1.532239 -1.091042
  Al  1.030847 -3.141074  1.748123
  Al -1.944859 -1.641048 -1.007407
  Al -2.979689  0.999841  1.898541
  Al -2.176879  3.489041 -1.320128
   H  1.444984  7.177112  2.852436
   H  4.289640  5.191292 -2.732390
   H  6.496127  1.586897  3.749899
   H -0.066382 -5.246411  2.591796
   H -2.323551 -3.221544 -2.997895
   H -4.272128  0.737287  4.057139
  Ca  0.913606  0.986460 -1.234198
-------------------------------------
```

(5) Pure-silicates with an internal cation

```
87_Si_Cage_Trigonal_Na_Internal
-------------------------------------
Atom         x         y         z
  Si  1.571107 -1.288416 -1.254950
   O  1.720616  0.355763 -1.478249
  Si  1.570971  1.721567 -0.534823
   O -0.030425  2.137500 -0.640092
   O -0.031856 -1.611662 -1.529129
  Si -1.637468 -1.310916 -1.160126
  Si -1.635879  1.692030 -0.467784
   O -1.800637  0.332785 -1.417485
   O -2.669654 -2.249596 -1.941564
   H -2.511258 -2.530794 -2.847326
   O  2.472766 -2.229034 -2.178634
   H  3.433732 -2.198826 -2.147908
   O  2.476866  2.976384 -0.929296
   H  3.437653  2.928681 -0.930710
```

```
   O  1.776113  1.085623  0.989326
   O -1.727956  1.075547  1.056767
   O -2.673865  2.831039 -0.895655
   H -2.531314  3.755670 -0.673938
  Si  1.627064 -0.414904  1.721709
   O  0.052374 -0.515584  2.180130
  Si -1.643004 -0.433164  1.870038
   O  2.723979 -0.729983  2.841960
   H  2.511982 -0.670122  3.777932
   O -2.577951 -0.703105  3.050107
   O -1.739068 -1.430317  0.474507
   O  1.784505 -1.416277  0.390968
  Na -0.029665 -0.007638  0.054159
-------------------------------------

88_Si_Cage_Trigonal_K_Internal
-------------------------------------
Atom         x         y         z
  Si  1.597205 -1.365133 -1.227842
   O  1.795225  0.292257 -1.518445
  Si  1.610250  1.718473 -0.622688
   O -0.028495  2.175739 -0.739545
   O -0.045480 -1.732796 -1.504975
  Si -1.690105 -1.376175 -1.120688
  Si -1.676593  1.704308 -0.537751
   O -1.896197  0.282127 -1.431378
   O -2.706399 -2.343813 -1.882150
   H -2.502292 -2.701138 -2.751658
   O  2.476162 -2.347563 -2.126338
   H  3.437822 -2.314373 -2.115881
   O  2.498106  2.961786 -1.082043
   H  3.459562  2.920929 -1.085416
   O  1.888145  1.134078  0.941320
   O -1.835838  1.140877  1.031566
   O -2.686298  2.847469 -1.010036
   H -2.458035  3.779262 -0.940271
  Si  1.685734 -0.350314  1.758471
   O  0.084150 -0.442296  2.282126
  Si -1.682837 -0.359465  1.919604
   O  2.782141 -0.590057  2.894860
   H  2.522834 -0.704902  3.813894
   O -2.578839 -0.586618  3.134612
   O -1.851558 -1.426332  0.540437
   O  1.877186 -1.417317  0.440615
   K -0.023533 -0.008622  0.049834
-------------------------------------

89_Si_Cage_Trigonal_Ca_Internal
-------------------------------------
Atom         x         y         z
  Si -1.654927  1.817599 -0.152673
   O -1.692418  0.690757 -1.383335
  Si -1.646325 -1.022237 -1.711093
   O  0.117771 -1.183482 -1.894769
   O  0.002408  2.211722 -0.071641
  Si  1.661412  1.817154  0.040668
```

```
  Si  1.744688 -0.977301 -1.483497
   O  1.849715  0.699344 -1.216672
   O  2.667592  3.039239  0.112973
   H  2.504961  3.891779 -0.303333
   O -2.528308  3.139127 -0.221956
   H -3.487741  3.135467 -0.304072
   O -2.529619 -1.650472 -2.777319
   O -1.783580 -1.477951 -0.033058
   O  1.776061 -1.477911  0.122119
   O  2.842856 -1.515733 -2.494298
   H  2.732709 -2.320760 -3.010354
  Si -1.747602 -0.882840  1.538403
   O -0.122439 -1.062587  1.963235
  Si  1.642517 -0.919034  1.767920
   O -2.848144 -1.386926  2.563767
   H -2.654823 -1.991326  3.287292
   O  2.523808 -1.483349  2.870865
   O  1.693058  0.769602  1.335087
   O -1.851091  0.776232  1.166820
  Ca -0.001658 -0.054143 -0.000012
-------------------------------------

90_Si_Cage_Tetragonal_Na_Internal
-------------------------------------
Atom         x         y         z
  Si  0.683014  2.146921  1.560429
   O -0.807498  1.468485  1.643544
  Si -2.162429  0.548810  1.601545
   O -2.809838  0.765727  0.111935
   O  0.780982  2.807453  0.063219
  Si  0.573246  2.245526 -1.466287
  Si -2.250086  0.649078 -1.434760
   O -0.957625  1.663224 -1.516020
   O  0.928509  3.323956 -2.605051
   H  0.476146  4.171319 -2.640741
   O  1.033090  3.173522  2.747241
   H  0.578005  4.017436  2.816462
   O -3.335225  1.101701 -2.535536
   H -4.154950  0.611686 -2.642477
  Si  2.135278 -0.600374 -1.617611
   O  1.550979  0.943524 -1.612176
   O  2.767362 -0.803112 -0.109474
  Si  2.252413 -0.651021  1.438988
   O  1.724187  0.889183  1.603599
   O  3.389195 -0.941812  2.538338
   H  3.837301 -1.791561  2.568273
   O  3.191630 -0.904475 -2.793657
   H  4.045562 -0.463644 -2.810337
  Si -0.702892 -2.249781 -1.681982
   O  0.832976 -1.550489 -1.722887
   O -0.755036 -2.764634 -0.081317
  Si -0.589602 -2.265504  1.445435
   O  0.905812 -1.576753  1.570451
   O -0.836971 -3.486160  2.466573
   H -0.803542 -3.336801  3.415463
   O -1.614897 -0.993692  1.665043
```

```
   O -1.060374 -3.273606 -2.768399
   O -1.636077 -0.844738 -1.572118
   O -3.143599  0.967843  2.804990
   H -4.024291  0.588710  2.873289
  Na -0.025463 -0.095410 -0.055177
-------------------------------------

91_Si_Cage_Tetragonal_K_Internal
-------------------------------------
Atom         x         y         z
  Si -0.390111  0.138608  2.745600
   O -0.159971  1.622236  2.067687
  Si  0.101388  2.659297  0.815043
   O  1.501223  2.166834  0.097525
   O  0.937330 -0.746347  2.334013
  Si  1.996334 -1.453204  1.281658
  Si  2.485635  1.066031 -0.659570
   O  2.605409 -0.212561  0.384066
   O  3.111491 -2.370754  1.985952
   H  3.780800 -1.978775  2.554041
   O -0.702254  0.173061  4.320619
   H -0.079207  0.571247  4.935037
   O  3.969295  1.622246 -0.939479
   H  4.108090  2.345378 -1.557180
  Si -0.100907 -2.646623 -0.850682
   O  1.086822 -2.384692  0.278702
   O -1.501253 -2.163613 -0.102548
  Si -2.487585 -1.071552  0.639950
   O -1.665131 -0.540946  1.964085
   O -3.901213 -1.668193  1.116106
   H -4.529021 -2.013419  0.475088
   O -0.150502 -4.162903 -1.385578
   H -0.315093 -4.888367 -0.776770
  Si  0.412729 -0.141421 -2.891501
   O  0.168951 -1.607169 -2.068784
   O -0.923584  0.750942 -2.344378
  Si -1.982503  1.436837 -1.322468
   O -2.600273  0.219507 -0.378404
   O -3.110399  2.258352 -2.123563
   H -3.813063  2.707710 -1.645362
   O -1.105447  2.375162 -0.271599
   O  0.634243 -0.214898 -4.408433
   O  1.654568  0.542885 -1.958094
   O  0.140481  4.160508  1.385639
   H  0.291804  4.906557  0.798652
   K  0.007772 -0.002064 -0.053906
-------------------------------------

92_Si_Cage_Tetragonal_Ca_Internal
-------------------------------------
Atom         x         y         z
  Si -0.884336  1.737434 -1.968155
   O -1.027796  0.128128 -2.201490
  Si -0.845503 -1.562644 -2.318657
   O  0.789511 -1.621739 -1.851286
   O  0.628898  1.823047 -1.285647
```

```
  Si  2.133531  1.682635 -0.612385
  Si  2.132378 -1.577448 -0.911137
   O  2.390131  0.056227 -0.724238
   O  3.280622  2.635560 -1.186793
   H  3.597532  2.560895 -2.091801
   O -1.167780  2.725476 -3.193744
   H -0.718312  2.623748 -4.037802
   O  3.457138 -2.297017 -1.442401
   H  3.471916 -3.233964 -1.659425
  Si  0.871028  1.477485  2.170933
   O  1.883945  1.990899  0.977159
   O -0.636797  1.658490  1.494669
  Si -2.141343  1.582121  0.811134
   O -1.900866  2.091972 -0.726784
   O -3.300937  2.437927  1.501873
   H -3.635608  2.224044  2.377747
   O  1.091751  2.165561  3.597675
   H  1.088416  3.121137  3.706172
  Si  0.854070 -1.834595  2.108599
   O  1.026904 -0.142438  2.206154
   O -0.781784 -1.842811  1.643650
  Si -2.115916 -1.700093  0.710145
   O -2.374742 -0.049035  0.715714
   O -3.332609 -2.605647  1.213167
   H -4.175655 -2.626167  0.750711
   O -1.538720 -1.923932 -0.808621
   O  1.324435 -2.727979  3.253968
   O  1.540093 -1.995035  0.560809
   O -1.309166 -2.300077 -3.572760
  Ca -0.001042 -0.179943 -0.014043
-------------------------------------

93_Si_Cage_Pentagonal_Na_Internal
-------------------------------------
Atom         x         y         z
  Si -2.780475 -0.323247  1.494633
   O -1.953981 -1.697246  1.826219
  Si -0.575992 -2.495126  1.501702
   O -0.734715 -3.293826  0.082249
   O -3.409250 -0.434425 -0.017965
  Si -2.672159 -0.248215 -1.470013
  Si -0.566052 -2.667953 -1.429344
   O -1.321133 -1.202133 -1.382129
   O -3.635732 -0.571700 -2.720267
   H -4.110244 -1.406574 -2.763554
   O -3.887669  0.022228  2.613613
   H -4.635190 -0.560698  2.770466
   O -0.021955 -3.420913  2.709052
   H -0.492669 -4.193195  3.033837
   O  0.606484 -1.364990  1.257706
   O  1.011397 -2.390044 -1.703204
   O -1.269925 -3.573212 -2.563092
   H -0.912923 -4.433850 -2.797753
  Si  2.252533 -1.258719  1.492247
   O  2.906659 -1.817057  0.098168
  Si  2.360187 -1.500370 -1.420609
```

```
   O  3.555677 -1.877212 -2.441752
   H  3.391617 -1.868291 -3.388413
   O  2.703310 -2.115459  2.785959
   H  2.101990 -2.815901  3.071500
  Si -1.150672  2.594313 -1.437826
   O -2.101477  1.263744 -1.607359
   O -1.359580  3.111720  0.114670
  Si -0.965921  2.359259  1.514573
   O -1.668897  0.873469  1.426092
   O -1.326381  3.214026  2.830720
   H -2.174263  3.660247  2.906621
   O -1.476439  3.742902 -2.523567
   H -2.360487  4.114484 -2.584547
  Si  2.013807  1.718926 -1.700973
   O  0.373634  2.078512 -1.561876
   O  2.603882  2.225964 -0.217177
  Si  2.244086  1.876304  1.319189
   O  0.612918  1.975735  1.497260
   O  3.055558  2.894317  2.281610
   H  3.043668  2.751170  3.231581
   O  2.601790  0.313339  1.671535
   O  2.758435  2.189184 -2.960741
   O  1.872259  0.052335 -1.417443
  Na -0.003749  0.216920 -0.199645
-------------------------------------

94_Si_Cage_Pentagonal_K_Internal
-------------------------------------
Atom         x         y         z
  Si -1.974558  1.896816 -1.561903
   O -0.365904  2.149218 -1.701072
  Si  1.229956  2.462484 -1.534447
   O  1.437395  3.019795 -0.008943
   O -2.385536  2.329461 -0.037780
  Si -2.013500  1.916223  1.503146
  Si  1.187487  2.492208  1.522725
   O -0.402018  2.150241  1.670197
   O -2.907623  2.691193  2.599091
   H -2.867186  3.648946  2.666640
   O -2.859760  2.633575 -2.690367
   H -2.844592  3.591111 -2.770277
   O  1.828892  3.451178 -2.658074
   H  1.497023  4.349239 -2.740494
   O  1.973453  1.019088 -1.646971
   O  1.970008  1.069421  1.658405
   O  1.585596  3.585526  2.639727
   H  2.500449  3.861126  2.741472
  Si  2.754093 -0.413628 -1.506085
   O  3.340346 -0.470129  0.019389
  Si  2.725776 -0.385451  1.538350
   O  3.970191 -0.538484  2.559619
   H  3.799048 -0.607003  3.502567
   O  3.886892 -0.652609 -2.629445
   H  4.641399 -0.060078 -2.686458
  Si -2.437714 -1.310680  1.520951
   O -2.253272  0.316392  1.657400
```

```
   O -2.953518 -1.571154 -0.018988
  Si -2.416559 -1.325544 -1.543585
   O -2.181194  0.287663 -1.697661
   O -3.387255 -1.952689 -2.669325
   H -4.295992 -1.650211 -2.746682
   O -3.456152 -1.920510  2.617693
   H -4.355762 -1.586366  2.667004
  Si  0.488326 -2.786654  1.669440
   O -0.968292 -1.947003  1.679603
   O  0.580032 -3.274682  0.067276
  Si  0.499756 -2.750529 -1.453214
   O -0.940697 -1.995635 -1.686386
   O  0.725565 -3.994322 -2.462833
   H  0.702525 -3.838389 -3.410731
   O  1.601757 -1.550706 -1.663313
   O  0.686178 -3.877741  2.736802
   O  1.549401 -1.481282  1.681053
   K  0.001279 -0.034118  0.025311
-------------------------------------

95_Si_Cage_Pentagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
  Si -1.573095  2.097102  1.575831
   O -2.484991  0.856445  2.125675
  Si -2.689515 -0.674176  1.565369
   O -3.234919 -0.646274  0.019786
   O -1.516046  1.788130 -0.047784
  Si -1.542742  1.988714 -1.697799
  Si -2.686075 -0.743054 -1.519066
   O -2.494625  0.743384 -2.173611
   O -2.016799  3.427533 -2.228548
   H -2.944793  3.679552 -2.228272
   O -2.078513  3.551511  2.025666
   H -3.013841  3.774943  2.031658
   O -3.573280 -1.585149  2.551707
   H -4.457610 -1.325152  2.823391
   O -1.162502 -1.289431  1.458938
   O -1.130493 -1.329926 -1.380822
   O -3.627801 -1.604839 -2.496523
   H -4.041240 -2.418619 -2.195519
  Si -0.038607 -2.518909  1.523647
   O -0.196476 -3.304288  0.085910
  Si -0.071122 -2.621512 -1.396958
   O -0.337003 -3.730513 -2.521843
   H -0.248063 -3.528431 -3.457809
   O -0.117364 -3.465576  2.814236
   H -0.748755 -4.188229  2.873992
  Si  1.620488  2.138189 -1.712906
   O  0.012003  1.671128 -2.053440
   O  1.382222  2.533065 -0.085384
  Si  1.577907  2.177902  1.497723
   O  0.003945  1.882939  1.978612
   O  2.383482  3.216548  2.417495
   H  2.085489  4.123992  2.527158
   O  2.338357  3.117101 -2.643768
```

```
  Si  2.764733 -0.960157 -1.415507
   O  2.197543  0.573232 -1.481977
   O  3.420755 -1.143956  0.056520
  Si  2.830406 -0.885659  1.604593
   O  2.234354  0.694795  1.489161
   O  3.716312 -1.264483  2.796390
   O  1.302869 -1.617026  1.431839
   O  3.679431 -1.446370 -2.647374
   H  4.587808 -1.144348 -2.731417
   O  1.339899 -1.804057 -1.449169
  Ca  0.288241  0.122838 -0.016285
-------------------------------------

96_Si_Cage_Hexagonal_Na_Internal
-------------------------------------
Atom         x         y         z
   O  0.724329 -3.401646  0.043626
   O  3.308188 -1.065019 -0.058123
   O -1.092756  3.557048 -0.105565
   O -2.209998 -1.976494  0.055288
   O  2.745350  2.320922  0.018051
   O -2.515371  0.957591 -0.045492
   O -0.685680 -2.495184  2.102115
   O  2.602723  0.496659  1.947562
   O  1.770309 -2.033453 -1.987803
   O -2.036955  2.285986  2.077150
   O -2.328228 -0.564473 -2.160813
   O  0.813924  2.777350 -1.766655
   O  1.929368 -2.070386  1.987179
   O  2.265711  0.565770 -1.897039
   O  0.465497  1.931868  1.268828
   O -0.786112 -2.736692 -2.031435
   O -1.697738  2.047523 -2.243757
   O -2.197818 -0.344032  2.100324
  Si  0.743240 -3.136019  1.648862
  Si  3.087639 -1.016197  1.552753
  Si  2.888483 -0.912426 -1.624643
  Si -0.768681  3.029575  1.406334
  Si -2.201415 -2.088936 -1.572602
  Si  2.292824  2.159246 -1.549959
  Si -0.737942  3.243990 -1.676635
  Si -2.156396 -1.918814  1.690459
  Si -2.741551  0.934358 -1.654277
  Si -3.025176  1.030772  1.560793
  Si  0.712562 -3.191560 -1.570830
  Si  2.108831  1.969069  1.481027
   O  2.503960  3.062588  2.610037
   H  1.841755  3.751163  2.766903
   O  4.425170 -1.438782  2.367214
   H  5.216676 -0.902684  2.273300
   O -0.132797  4.202022  2.347446
   H -0.636528  4.981550  2.595870
   O  0.920086 -4.507522  2.498933
   H  1.767686 -4.958858  2.477033
   O -4.530148  1.132251  1.865817
   O -3.373093 -2.706877  2.411920
```

H	-3.423512	-3.664485	2.350116
O	1.167108	-4.538096	-2.357894
H	0.603094	-5.314009	-2.305497
O	-3.371343	-3.056240	-2.146536
H	-4.285550	-2.767978	-2.080841
O	-4.266842	1.197606	-2.145798
H	-4.655879	2.066294	-2.011925
O	-1.040612	4.538238	-2.607334
H	-0.552863	5.350479	-2.449269
O	3.292155	2.986649	-2.527028
H	4.205681	2.700642	-2.607052
O	4.189458	-1.048863	-2.591857
H	4.651510	-1.890277	-2.626516
Na	-0.448116	0.039244	0.412015

97_Si_Cage_Hexagonal_K_Internal

Atom	x	y	z
O	0.672828	-2.945832	-0.019700
O	2.862454	-0.885759	-0.016953
O	-0.641125	2.973129	-0.034077
O	-2.222683	-2.055586	-0.017241
O	2.234921	2.047319	-0.034033
O	-2.701047	0.858253	-0.001448
O	-0.805780	-2.557421	2.102695
O	2.529049	0.585724	2.102293
O	1.812716	-1.951178	-2.170291
O	-1.723765	1.925623	2.113875
O	-2.583745	-0.598348	-2.186875
O	0.798314	2.558221	-2.183780
O	1.749338	-1.922074	2.110272
O	2.603575	0.594208	-2.180697
O	0.816465	2.582010	2.087025
O	-0.785675	-2.560338	-2.165950
O	-1.791962	1.950836	-2.194174
O	-2.471435	-0.542314	2.126607
Si	0.664512	-3.042664	1.602781
Si	2.936131	-0.920475	1.605876
Si	2.946964	-0.903775	-1.645631
Si	-0.678989	3.048239	1.595626
Si	-2.260865	-2.102693	-1.645034
Si	2.270014	2.105724	-1.663141
Si	-0.681632	3.013825	-1.661311
Si	-2.296836	-2.064952	1.612768
Si	-2.898003	0.895902	-1.603658
Si	-3.025208	0.970349	1.635671
Si	0.691828	-3.010400	-1.648238
Si	2.299792	2.122489	1.588525
O	3.490573	3.035951	2.188179
H	3.418698	3.993805	2.158361
O	4.334023	-1.444504	2.222415
H	5.131829	-0.918101	2.123069
O	-0.940487	4.536895	2.180022
H	-1.842186	4.861936	2.245919
O	0.946301	-4.514825	2.207240

```
   H  1.829343 -4.891356  2.165359
   O -4.431999  1.400666  2.092293
   O -3.480171 -2.993153  2.215169
   H -3.460299 -3.941798  2.063325
   O  1.116868 -4.464228 -2.229004
   H  0.492307 -5.191659 -2.167955
   O -3.315989 -3.189957 -2.227619
   H -4.256454 -3.012180 -2.144514
   O -4.397594  1.272575 -2.108723
   H -4.739451  2.149332 -1.915647
   O -1.102572  4.465328 -2.254990
   H -0.516102  5.213029 -2.114329
   O  3.330670  3.187248 -2.242516
   H  4.270862  3.012055 -2.150740
   O  4.421867 -1.278848 -2.206313
   H  4.739962 -2.181138 -2.117534
   K -0.072585  0.043171  0.755269
-------------------------------------

98_Si_Cage_Hexagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
   O  0.878750 -3.205191  0.018408
   O  2.372271 -0.696818  0.008375
   O -0.749391  2.854154  0.036009
   O -2.524660 -2.258709 -0.040273
   O  2.363552  2.027591 -0.026108
   O -3.021383  1.008425  0.011280
   O -0.792792 -2.462921  1.952453
   O  2.819284  0.609216  2.167126
   O  1.886340 -2.011548 -2.154910
   O -1.768895  1.869954  2.156673
   O -2.570427 -0.546896 -2.064589
   O  0.669836  2.172484 -1.917533
   O  1.803448 -1.941684  2.180302
   O  2.656249  0.602895 -2.189182
   O  0.765356  2.182058  1.932050
   O -0.719489 -2.471966 -1.972608
   O -1.952261  2.055848 -2.137907
   O -2.703771 -0.612263  2.047524
  Si  0.692312 -3.033117  1.630114
  Si  2.899872 -0.910487  1.565984
  Si  2.889297 -0.868161 -1.566241
  Si -0.684149  3.053977  1.719431
  Si -2.267546 -2.099156 -1.639359
  Si  2.361525  2.185305 -1.723997
  Si -0.724703  2.983959 -1.595229
  Si -2.344397 -2.126683  1.571546
  Si -3.042550  0.946777 -1.612384
  Si -2.996880  0.943318  1.643551
  Si  0.753120 -3.064637 -1.603586
  Si  2.374572  2.096024  1.614566
   O  3.332386  3.195063  2.296154
   H  3.218915  4.129143  2.098880
   O  4.368315 -1.568083  1.691446
   H  5.152738 -1.026045  1.568893
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O	-0.781730	4.466165	2.311479
O	0.847683	-4.440522	2.421820
H	1.703901	-4.875512	2.437079
O	-4.368287	1.491343	2.316441
H	-5.179033	0.990931	2.193569
O	-3.369860	-3.101699	2.372203
H	-3.241006	-4.051588	2.311322
O	1.058312	-4.467795	-2.358841
H	0.481143	-5.218205	-2.195661
O	-3.186504	-3.121805	-2.505470
H	-4.134571	-2.969738	-2.538622
O	-4.503072	1.210533	-2.262949
H	-4.876743	2.095108	-2.231799
O	-0.857898	4.459534	-2.229104
H	-0.130387	5.083988	-2.157776
O	3.175079	3.323277	-2.352109
O	4.451364	-1.274455	-1.673797
H	4.713295	-2.193471	-1.571948
Ca	0.330199	0.680265	0.021430

99_Si_Cage_Heptagonal_Na_Internal

Atom	x	y	z
O	1.002989	-3.498526	0.243823
O	4.042805	-1.992260	0.236370
O	2.824148	4.052681	0.198687
O	-2.105527	-2.078493	0.063300
O	4.776769	1.347755	0.148984
O	-2.910844	1.205683	-0.008944
O	-0.414045	-2.203661	2.096566
O	3.979654	-0.193636	2.175837
O	2.388712	-2.432608	-1.780244
O	-1.616131	2.234571	2.094973
O	-1.876440	-0.331801	-1.922401
O	3.194987	2.337915	-1.775571
O	2.225485	-2.171319	2.180664
O	3.815486	-0.217628	-1.752478
O	3.428287	2.393966	2.174717
O	-0.243408	-2.394984	-1.818532
O	-1.357127	2.250326	-1.899469
O	-2.279587	-0.322369	2.059744
Si	0.924171	-3.079296	1.813835
Si	3.757060	-1.764691	1.821735
Si	3.823401	-1.792857	-1.362896
Si	2.325653	3.478750	1.657826
Si	-1.758150	-1.901564	-1.515387
Si	4.372936	1.277130	-1.425735
Si	2.479527	3.750146	-1.369172
Si	-1.949173	-1.858116	1.667817
Si	-2.493897	1.130307	-1.577631
Si	-2.738206	1.178925	1.611497
Si	1.057227	-3.257873	-1.364457
Si	4.532662	1.275788	1.757449
O	5.924202	1.489726	2.573113
H	6.354167	2.347442	2.529692

```
   O  4.711268 -2.721158  2.728965
   H  5.659781 -2.569904  2.715026
   O  2.111785  4.651157  2.744259
   H  1.102403  4.791548  2.864167
   O  0.824435 -4.395955  2.764968
   H  1.557151 -5.017038  2.773944
   O -4.134634  1.595239  2.342165
   H -4.907176  1.044841  2.191819
   O -3.011822 -2.780440  2.488287
   H -2.902028 -3.734433  2.463878
   O  1.135992 -4.679166 -2.155533
   H  0.398287 -5.288934 -2.073179
   O -2.734236 -2.830257 -2.430140
   H -3.676666 -2.644690 -2.429772
   O -3.799703  1.310344 -2.536002
   H -4.259023  2.153799 -2.529681
   O  2.987062  4.972057 -2.318249
   H  3.923774  5.184666 -2.330087
   O  5.644632  1.666890 -2.364568
   H  6.454935  1.158813 -2.275367
   O  5.042160 -2.469878 -2.203014
   H  5.204936 -3.411009 -2.100848
   O -1.095577  3.931016  0.150231
   O  0.887386  3.602531 -1.611101
   O  0.887553  2.705630  1.380536
  Si -0.604332  3.462195  1.665425
  Si -0.725356  3.671546 -1.407924
   O -0.430093  4.619163  2.706085
   O -1.386572  4.813600 -2.366588
   H -1.117616  5.726188 -2.235597
  Na  0.913198  0.535939  0.342412
-------------------------------------

100_Si_Cage_Heptagonal_K_Internal
-------------------------------------
Atom         x         y         z
   O  0.840488 -3.505479  0.241517
   O  4.190538 -1.887564  0.276322
   O  2.798355  4.246204  0.197254
   O -2.220336 -2.220189  0.035682
   O  5.104860  1.290406  0.190975
   O -3.163292  1.046495 -0.019352
   O -0.581949 -2.292361  2.112184
   O  4.090712 -0.095390  2.222222
   O  2.103091 -1.770414 -1.328940
   O -1.382188  1.867778  1.779060
   O -2.070782 -0.441643 -1.916834
   O  2.979417  2.044250 -1.222681
   O  1.963142 -1.609514  1.691768
   O  4.205428 -0.224970 -1.783012
   O  3.640458  2.513135  2.030702
   O -0.382935 -2.462923 -1.865560
   O -1.048352  1.916302 -1.353968
   O -2.533565 -0.493530  2.039551
  Si  0.889018 -2.861802  1.750350
  Si  3.604096 -1.570267  1.769935
```

```
  Si  3.751745 -1.707585 -1.289408
  Si  2.425772  3.523126  1.638077
  Si -1.924209 -2.024946 -1.549347
  Si  4.448854  1.308718 -1.297060
  Si  2.498098  3.630083 -1.287928
  Si -2.124858 -2.012036  1.649691
  Si -2.459276  1.075754 -1.489668
  Si -2.762864  1.051882  1.572188
  Si  1.030174 -3.018589 -1.302873
  Si  4.733152  1.340642  1.786720
   O  6.061515  1.540415  2.692693
   H  6.535297  2.374956  2.648540
   O  3.984870 -2.742684  2.834179
   H  4.894841 -2.924042  3.084726
   O  2.145752  4.593893  2.812489
   H  1.160366  4.594758  3.035443
   O  1.356185 -3.957643  2.849247
   H  2.287358 -3.920724  3.108783
   O -3.925459  1.759701  2.459633
   H -4.804250  1.372085  2.469370
   O -3.161537 -2.981107  2.439290
   H -3.025068 -3.931297  2.405545
   O  1.729877 -4.155735 -2.231860
   H  1.329700 -5.019521 -2.364898
   O -2.866130 -2.957253 -2.480538
   H -3.814991 -2.806675 -2.488799
   O -3.408841  1.761547 -2.611934
   H -3.212567  2.686006 -2.814158
   O  3.298846  4.416887 -2.456274
   H  4.162252  4.054299 -2.694034
   O  5.297011  2.202255 -2.356341
   H  6.220111  2.020125 -2.552542
   O  4.396385 -2.838987 -2.248818
   H  3.813674 -3.572364 -2.488170
   O -0.947033  3.995219  0.287056
   O  0.907707  3.646234 -1.616314
   O  1.051924  2.658402  1.324305
  Si -0.487094  3.251775  1.717330
  Si -0.670866  3.517040 -1.236917
   O -0.425918  4.193514  2.958577
   O -1.656763  4.230190 -2.319184
   H -1.708150  5.186375 -2.399136
   K  0.920846  0.518439 -0.317749
-------------------------------------

101_Si_Cage_Heptagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
   O  0.924099 -3.480155  0.215232
   O  3.941955 -1.891862  0.232444
   O  2.897262  4.280548  0.213103
   O -2.233653 -2.219083  0.048279
   O  4.821150  1.433560  0.181063
   O -3.118329  1.025027 -0.056080
   O -0.563252 -2.350126  2.106751
   O  3.810657 -0.082184  2.147337
```

```
   O  2.186688 -2.151840 -1.727461
   O -1.250442  1.822319  1.629221
   O -2.038773 -0.435411 -1.935490
   O  3.321800  2.555874 -1.733847
   O  2.105303 -2.130346  2.161319
   O  3.780406 -0.056287 -1.724012
   O  3.503392  2.560812  2.164819
   O -0.426467 -2.530637 -1.867197
   O -0.857347  1.820478 -1.180281
   O -2.455519 -0.480616  2.037304
  Si  0.844568 -3.108851  1.798064
  Si  3.631961 -1.672390  1.817927
  Si  3.687180 -1.637485 -1.357535
  Si  2.402275  3.631856  1.633914
  Si -1.932180 -2.007498 -1.541517
  Si  4.422951  1.406620 -1.398761
  Si  2.557783  3.951968 -1.359611
  Si -2.104230 -2.027019  1.658990
  Si -2.391501  1.123399 -1.549055
  Si -2.699850  1.046792  1.512649
  Si  0.978562 -3.185828 -1.385338
  Si  4.515913  1.339621  1.777993
   O  5.884502  1.417107  2.649867
   H  6.440288  2.196312  2.567238
   O  4.604117 -2.592358  2.740866
   H  5.549357 -2.420958  2.730564
   O  2.058650  4.741077  2.756320
   H  1.093892  4.736719  2.994324
   O  0.857810 -4.446918  2.722724
   H  1.669504 -4.957511  2.781104
   O -3.755278  1.847394  2.449523
   H -4.668187  1.552692  2.499229
   O -3.167093 -2.949407  2.471195
   H -3.037527 -3.901209  2.480441
   O  1.302646 -4.553381 -2.208736
   H  0.658960 -5.265782 -2.185076
   O -2.934065 -2.917957 -2.445976
   H -3.855170 -2.654275 -2.511665
   O -3.109271  2.013399 -2.609604
   O  3.002749  5.180356 -2.321358
   H  3.913408  5.485326 -2.296125
   O  5.714409  1.721281 -2.335607
   H  6.440359  1.092205 -2.342932
   O  4.826651 -2.384352 -2.248012
   H  4.932564 -3.334994 -2.158785
   O -1.024260  4.045433  0.183580
   O  0.961825  3.737806 -1.582319
   O  1.007067  2.807705  1.251804
  Si -0.576263  3.359055  1.628666
  Si -0.623081  3.482412 -1.307878
   O -0.589555  4.255414  2.893175
   O -1.555991  4.052310 -2.488632
   H -2.277905  3.361367 -2.687875
  Ca  0.648335  0.737148  0.270804
-------------------------------------
```

102_Si_Cage_Octagonal_Na_Internal

Atom	x	y	z
O	0.865443	-3.358994	0.106680
O	4.186604	-1.866972	0.161836
O	3.792677	4.357704	0.363286
O	-2.110366	-2.446913	0.099982
O	5.372956	1.054554	0.365795
O	-3.760814	0.990279	0.006246
O	-0.482717	-2.329068	2.156679
O	4.273990	-0.343273	2.326976
O	2.100220	-1.555576	-1.441521
O	-2.719181	2.286386	2.055971
O	-2.360700	-0.514156	-1.721656
O	4.208178	2.544864	-1.524554
O	2.082201	-1.744224	1.809106
O	4.296132	-0.074240	-1.780033
O	3.530684	2.187408	1.892694
O	-0.410196	-2.263970	-1.951099
O	-2.447701	2.101322	-2.009288
O	-1.843824	-0.172725	1.405503
Si	3.480447	3.818981	1.865851
Si	-1.961345	-2.072855	-1.467851
Si	3.767898	4.082184	-1.245411
Si	-3.174515	0.804331	1.529929
Si	4.790308	1.133892	1.886147
O	5.929913	1.626594	2.934556
H	5.877149	2.557698	3.190077
O	4.163225	-3.042738	2.582492
H	5.081379	-3.324399	2.610356
O	4.655187	4.264666	2.910174
H	4.884474	5.189704	3.032707
O	1.366885	-4.187183	2.614501
H	2.309181	-4.248200	2.818262
O	-4.245680	0.144056	2.536904
H	-3.975528	-0.833085	2.688493
O	-3.176791	-2.164095	2.592981
O	1.704535	-3.913039	-2.383665
H	1.297993	-4.777011	-2.491931
O	-2.836853	-3.077330	-2.406379
H	-3.777273	-3.160028	-2.229114
O	-4.600787	0.565654	-2.509118
H	-5.293465	1.230744	-2.517193
O	4.707407	5.150060	-2.030558
H	5.651739	5.155349	-1.853626
O	6.511801	1.434502	-2.031072
H	7.180300	0.746463	-1.981375
O	4.340970	-2.648783	-2.406029
H	3.728170	-3.357790	-2.644624
O	-2.486017	3.887678	-0.049296
O	2.256650	4.299434	-1.813394
O	2.011370	4.337717	2.322950
Si	-2.136901	3.704406	1.532665
Si	-1.929208	3.566556	-1.554586
O	-2.652687	4.982819	2.406546
H	-3.571079	5.264238	2.381238

```
   O -2.450680  4.680958 -2.617662
   H -1.831874  5.403664 -2.790461
   O  0.853569  5.344671  0.168131
   O -0.288047  3.582976 -1.493874
   O -0.514917  3.715622  1.744900
  Si  0.782381  4.809198 -1.369951
  Si  0.609537  4.904230  1.723218
   O  0.107843  6.160448  2.623155
   H -0.843707  6.194709  2.788653
   O  0.175071  5.958369 -2.361042
   H  0.583534  6.826416 -2.416185
  Si -1.975808 -1.847861  1.641169
  Si  1.023975 -2.786727 -1.410030
  Si  0.940773 -2.920849  1.684163
  Si  3.738744 -1.542815 -1.377798
  Si  3.708095 -1.737739  1.714193
  Na  0.199309  0.725868  0.488955
  Si -3.306855  0.789617 -1.547574
  Si  5.109832  1.228780 -1.234045
-------------------------------------

103_Si_Cage_Octagonal_K_Internal
-------------------------------------
Atom         x         y         z
   O  1.012061 -3.464863  0.008046
   O  4.174098 -1.899280  0.261115
   O  3.879901  4.431051  0.184720
   O -2.372565 -2.256798  0.004747
   O  5.392857  1.033862  0.386648
   O -3.663669  0.661402  0.195849
   O -0.566588 -2.510914  1.933202
   O  4.089293 -0.224769  2.318290
   O  2.402170 -1.972509 -1.710831
   O -1.973163  1.928971  1.822561
   O -2.569195 -0.479810 -1.947842
   O  4.342982  2.507573 -1.583667
   O  1.950647 -1.688069  1.717781
   O  4.287647 -0.124719 -1.720431
   O  3.520496  2.313892  1.752277
   O -0.215898 -1.626187 -1.429367
   O -2.659182  2.153929 -1.759864
   O -2.427375 -0.651209  2.129955
  Si  0.936879 -2.978459  1.569926
  Si  3.586864 -1.659577  1.758337
  Si  3.957827 -1.668408 -1.342271
  Si  3.565074  3.951696  1.706291
  Si -1.838853 -1.845072 -1.476327
  Si  5.161744  1.163255 -1.225477
  Si  3.704890  3.989584 -1.385051
  Si -2.121024 -2.161661  1.615323
  Si -3.453908  0.783391 -1.416634
  Si -3.119036  0.763937  1.726646
  Si  0.998332 -2.738336 -1.460639
  Si  4.724757  1.201693  1.862958
   O  5.819597  1.662466  2.969822
   H  5.836723  2.611934  3.154830
```

```
   O  3.983600 -2.897809  2.747081
   H  4.901534 -3.148065  2.882121
   O  4.785079  4.341444  2.721925
   H  5.056076  5.254859  2.845610
   O  1.392000 -4.173295  2.571324
   H  2.312503 -4.137095  2.865715
   O -4.304966  1.182554  2.754609
   H -5.076568  0.617188  2.843970
   O -3.135534 -3.144325  2.416821
   H -3.093137 -4.089829  2.252260
   O  0.746816 -3.821230 -2.643858
   H -0.179222 -3.945494 -2.893509
   O -2.039655 -3.068928 -2.540081
   H -2.913805 -3.417215 -2.735083
   O -4.876408  0.693392 -2.197159
   H -5.516100  1.399196 -2.071878
   O  4.427725  5.086953 -2.346281
   H  5.360194  5.272859 -2.210147
   O  6.589185  1.252329 -2.000677
   H  7.198592  0.512860 -1.931421
   O  4.983187 -2.596266 -2.195730
   H  4.953388 -3.549788 -2.082285
   O -2.543630  3.940065  0.193690
   O  2.140703  3.926333 -1.788708
   O  2.139236  4.545298  2.194310
  Si -1.964207  3.566602  1.671552
  Si -1.987730  3.569253 -1.316807
   O -2.939418  4.310616  2.737294
   O -2.301572  4.734446 -2.386373
   H -1.423144  5.210896 -2.609999
   O  0.901522  5.403478 -0.008535
   O -0.353890  3.377756 -1.151185
   O -0.403107  3.996097  1.832245
  Si  0.694311  4.661623 -1.485656
  Si  0.745157  5.137366  1.580348
   O  0.442607  6.504577  2.409277
   H -0.272399  7.073762  2.113543
   O  0.094147  5.584216 -2.597846
   H -2.775075  4.195454  3.676859
   K  0.698793  1.151317  0.281032
-------------------------------------

104_Si_Cage_Octagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
   O  1.019150 -3.346168  0.154668
   O  4.170302 -1.890635  0.289224
   O  3.842354  4.407125  0.173542
   O -2.346488 -2.204721 -0.009376
   O  5.403717  1.024476  0.292695
   O -3.710932  0.706608  0.085486
   O -0.563138 -2.182575  1.952936
   O  4.272598 -0.215752  2.340436
   O  2.428200 -2.072181 -1.707287
   O -2.245410  1.920576  1.966076
   O -2.515914 -0.456031 -1.992085
```

```
 O  4.033168  2.406422 -1.545359
 O  2.016143 -1.549014  1.819920
 O  4.293271 -0.204188 -1.769959
 O  3.657199  2.314844  1.813320
 O -0.192407 -1.664893 -1.487755
 O -2.591233  2.179949 -1.829746
 O -2.722726 -0.658943  2.123826
Si  0.921552 -2.766624  1.682537
Si  3.649505 -1.613878  1.804079
Si  3.972626 -1.731452 -1.322454
Si  3.610561  3.944501  1.716230
Si -1.818127 -1.832986 -1.502391
Si  5.041780  1.164024 -1.294243
Si  3.656705  3.986462 -1.397835
Si -2.153181 -2.084910  1.606959
Si -3.418200  0.816233 -1.511469
Si -3.356328  0.774874  1.675248
Si  1.008367 -2.779177 -1.380160
Si  4.862703  1.209229  1.819832
 O  6.050961  1.690841  2.819373
 H  6.054769  2.635657  3.023652
 O  4.001366 -2.870798  2.786430
 H  4.909109 -3.159651  2.911752
 O  4.841037  4.427945  2.675326
 H  5.077087  5.356254  2.749599
 O  1.257127 -3.937622  2.760060
 H  2.184717 -3.994090  3.026060
 O -4.679061  1.135401  2.551000
 H -5.466746  0.596233  2.444689
 O -3.009880 -3.229661  2.379450
 H -2.769901 -4.151492  2.256128
 O  0.737371 -3.984699 -2.437117
 H -0.182740 -4.083127 -2.716965
 O -2.063805 -3.076474 -2.535251
 H -2.949221 -3.408543 -2.705502
 O -4.796219  0.733598 -2.369990
 H -5.436790  1.444305 -2.283256
 O  4.592600  4.928603 -2.339435
 H  5.531789  4.982815 -2.145009
 O  6.381463  1.456502 -2.169545
 H  7.095154  0.813902 -2.160062
 O  5.019506 -2.682884 -2.123770
 H  4.993379 -3.631158 -1.972460
 O -2.491403  3.854985  0.214377
 O  2.127115  4.188353 -1.880108
 O  2.162818  4.463315  2.231905
Si -1.921890  3.524849  1.741153
Si -1.991390  3.610147 -1.322862
 O -2.292216  4.564666  2.840104
 O -2.351773  4.811407 -2.332826
 H -1.503531  5.358283 -2.502761
 O  0.892262  5.377170  0.103788
 O -0.324436  3.441599 -1.235967
 O -0.224093  3.449579  1.522313
Si  0.670720  4.824410 -1.446290
Si  0.689513  4.847874  1.630179
```

```
   O -0.069813  5.889713  2.601437
   H -0.988160  5.543955  2.838648
   O -0.017853  5.821150 -2.432047
  Ca  0.445210  1.535976  0.133846
------------------------------------
```

(6) Aluminosilicates with an internal cation

```
105_SiAl_Cage_Trigonal_Na_Internal
------------------------------------
Atom         x         y         z
  Si  1.606673 -1.449072  1.146235
   O  1.717479 -1.472450 -0.542127
  Si  1.555797 -0.368642 -1.780681
   O -0.049508 -0.391200 -2.207551
   O  0.046893 -1.776694  1.487570
  Si -1.650336 -0.280028 -1.728265
   O -1.864215 -1.378484 -0.559517
   O -2.835734 -2.429987  2.041058
   H -2.618636 -2.855151  2.870712
   O  2.604369 -2.512159  1.850523
   H  3.552879 -2.400354  1.744921
   O  2.412311 -0.729513 -3.101657
   H  3.371470 -0.759216 -3.050251
   O  1.835831  1.076734 -1.075092
   O -1.749722  1.201565 -0.964971
   O -2.659768 -0.447382 -2.979306
   H -2.457210 -0.021186 -3.816089
   O -0.012568  2.168861  0.764564
  Si -1.598642  1.728145  0.631940
   O  2.741128  3.018738  1.084249
   H  2.407324  3.889642  1.346386
   O -2.640834  2.912329  1.001397
   H -2.406508  3.818340  0.783980
   O -1.819264  0.372400  1.507247
   O  1.882481  0.141495  1.486969
  Al -1.715141 -1.416480  1.240479
  Al  1.655930  1.639901  0.586757
   H  3.705836  2.998934  1.165993
  Na -0.040484 -0.039557  0.098566
------------------------------------

106_SiAl_Cage_Trigonal_K_Internal
------------------------------------
Atom         x         y         z
  Si -1.758955 -1.398405 -1.142679
   O -1.882061 -1.400054  0.574888
  Si -1.590659 -0.296862  1.821327
   O  0.045519 -0.411260  2.259887
   O -0.204876 -1.852133 -1.529550
  Si  1.681210 -0.372156  1.750720
   O  1.866681 -1.483082  0.563532
   O  2.674078 -2.520494 -2.191340
   H  2.387477 -3.389370 -2.474094
```

```
   O -2.825676 -2.404017 -1.824176
   H -3.764272 -2.237233 -1.701206
   O -2.437940 -0.595133  3.161062
   H -3.398389 -0.591246  3.123985
   O -1.807783  1.169405  1.095374
   O  1.902309  1.115873  0.972086
   O  2.665892 -0.589386  3.010438
   H  2.436772 -0.213235  3.864388
   O  0.161497  2.238439 -0.791272
  Si  1.749226  1.681900 -0.639952
   O -2.592543  3.173918 -1.088220
   H -2.224259  4.045842 -1.297397
   O  2.840153  2.824735 -0.984452
   H  2.589348  3.745986 -0.877117
   O  1.945642  0.300990 -1.524659
   O -1.977673  0.227324 -1.480424
   K  0.026606 -0.027823 -0.108704
  Al  1.651612 -1.512545 -1.270671
  Al -1.582252  1.745213 -0.589399
   H -3.551117  3.179528 -1.229487
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107_SiAl_Cage_Trigonal_Ca_Internal
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Atom         x         y         z
  Si  1.635883 -0.061863 -1.834061
   O  1.818293  1.253547 -0.790738
  Si  1.757657  1.595108  0.893751
   O  0.161239  2.011590  1.113703
   O -0.014892 -0.031813 -2.221200
  Si -1.665415  0.004020 -1.810644
   O -1.752834  1.304641 -0.820503
   O -2.655047 -0.165567 -3.057246
   H -2.546938  0.350106 -3.861349
   O  2.484548 -0.014035 -3.190743
   H  3.445865  0.006939 -3.176841
   O  2.774240  2.731703  1.390750
   H  3.724174  2.582798  1.371861
   O  1.876502  0.051694  1.483888
   O -1.851337 -0.000107  1.503514
   O -2.734858  2.962008  1.509707
   H -2.589003  3.449560  2.320743
   O -0.146192 -1.966566  1.180719
  Si -1.749422 -1.560243  0.954090
   O  2.753285 -2.910913  1.571249
   H  2.604755 -3.390771  2.386353
   O -2.860272 -2.630561  1.394586
   H -2.739011 -3.166400  2.183490
   O -1.831658 -1.277348 -0.731873
   O  1.748278 -1.325722 -0.798100
  Ca  0.003389  0.004695  0.123087
  Al  1.701655 -1.719527  0.986549
  Al -1.688105  1.754539  0.949483
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108_SiAl_Cage_Tetragonal_Na_Internal

Atom	x	y	z
Si	1.990183	-0.312213	1.966301
O	1.004839	-1.600357	1.912493
O	-1.745465	-1.193743	1.574314
O	1.018317	1.012246	1.905540
Si	-2.601752	0.116448	1.138932
O	-1.715111	1.450585	1.460098
O	-0.241167	3.555393	2.811719
H	-0.679334	3.501320	3.670792
O	2.965707	-0.311912	3.288383
H	2.550969	-0.537890	4.124115
O	-4.016516	0.259011	1.965302
H	-4.624573	-0.481158	1.899946
Si	0.538843	2.371016	-1.380586
O	0.282848	3.064790	0.077788
O	1.967503	1.581430	-1.374851
O	2.954933	-0.258116	0.649679
O	4.155677	-0.287264	-1.875324
H	4.328924	-0.276505	-2.825359
O	0.470451	3.483577	-2.589455
H	1.128853	4.181912	-2.574799
O	-0.644264	1.280037	-1.639938
O	-1.155627	-1.365492	-2.409008
Si	0.080114	-2.202090	-1.741370
O	1.352115	-1.186781	-1.518136
O	0.445683	-3.418126	-2.785220
H	1.133326	-4.028437	-2.509507
O	-0.348649	-2.723952	-0.266084
O	-3.089230	0.610217	-3.254138
H	-2.970291	0.485457	-4.204912
O	-2.867442	0.036168	-0.479068
O	-0.728748	-3.850596	2.464069
H	-1.526111	-4.369695	2.356498
Al	-0.490373	-2.449295	1.480018
Al	-0.164593	2.219029	1.525875
Al	2.527006	-0.017544	-1.018665
Al	-1.901629	0.120580	-1.915567
H	0.114045	4.444320	2.679562
H	-3.950775	1.012939	-3.080171
H	4.929250	-0.625676	-1.405112
Na	-0.061808	-0.215797	0.166017

109_SiAl_Cage_Tetragonal_K_Internal

Atom	x	y	z
Si	-2.389261	1.523357	-0.439344
O	-2.620597	-0.042158	-0.892701
O	-0.604564	-1.666960	-2.094939
O	-1.151332	2.110926	-1.351697
Si	0.894331	-1.119700	-2.466271
O	0.859245	0.511030	-2.553811
O	0.989073	3.449546	-2.884834
H	0.595986	3.690208	-3.734036

O	-3.756427	2.411128	-0.639131
H	-4.122601	2.444949	-1.525843
O	1.405505	-1.683653	-3.919149
H	1.413014	-2.636583	-4.035714
Si	2.028194	1.696457	1.094196
O	1.560952	2.235564	-0.390491
O	0.714934	1.666407	2.052502
O	-1.958058	1.565358	1.122806
O	-1.553286	1.869645	3.956368
H	-1.091360	1.729512	4.783418
O	3.250558	2.606079	1.708056
H	3.020247	3.491823	1.997647
O	2.601284	0.169082	0.916013
O	1.027965	-2.160012	1.406915
Si	-0.542230	-2.096315	1.878289
O	-0.849862	-0.635038	2.523179
O	-0.781183	-3.329533	2.937251
H	-1.643007	-3.368116	3.358375
O	-1.482591	-2.262651	0.537723
O	3.849777	-2.488620	0.575779
H	4.391388	-2.641544	1.361165
O	1.899599	-1.557544	-1.248266
O	-3.357660	-2.661468	-1.711720
H	-3.349197	-3.603675	-1.925788
Al	-1.970519	-1.650826	-1.016220
Al	0.533154	2.036047	-1.780385
Al	-0.928223	1.146573	2.511763
Al	2.304186	-1.477824	0.442198
H	1.706852	4.059976	-2.668212
H	-4.233525	-2.291951	-1.888545
H	4.260840	-2.902383	-0.195210
K	-0.019555	0.021894	0.057481

110_SiAl_Cage_Tetragonal_Ca_Internal

Atom	x	y	z
Si	2.167234	-1.682480	-0.826898
O	0.794199	-1.929117	-1.680167
O	-1.616349	-2.172495	-0.344268
O	1.740961	-1.972514	0.722420
Si	-2.039826	-1.653007	1.145022
O	-0.667458	-1.663006	2.022180
O	1.768682	-2.095830	3.744086
H	1.637572	-3.009255	3.998755
O	3.481921	-2.477486	-1.369017
H	3.443018	-3.436172	-1.412774
O	-3.218294	-2.500966	1.882926
H	-4.042542	-2.634846	1.408538
Si	0.982876	1.884208	1.838908
O	1.241607	0.293756	2.094431
O	1.997580	2.352085	0.640322
O	2.435849	-0.060139	-0.897832
O	3.264633	2.588708	-1.930091
H	3.625862	3.443890	-1.657410
O	1.095623	2.827320	3.167861

H	1.951369	2.891590	3.598917
O	-0.554193	1.939551	1.270750
O	-2.151649	2.040366	-1.047199
Si	-1.114392	1.421473	-2.146584
O	0.416695	1.642250	-1.576077
O	-1.390063	2.152843	-3.580251
H	-0.893469	1.842290	-4.341111
O	-1.264730	-0.200717	-2.150638
O	-3.483278	2.657076	1.424581
H	-3.886266	3.431794	1.008007
O	-2.391091	-0.052807	0.921300
O	-1.427806	-3.030349	-3.236883
H	-2.347383	-3.138495	-3.480067
Al	-0.960301	-1.950010	-1.989038
Al	1.085161	-1.467536	2.301869
Al	2.040152	1.633604	-0.941810
Al	-2.152156	1.648830	0.646695
H	-3.885772	2.505323	2.291025
H	3.654090	2.320415	-2.773922
Ca	0.002560	-0.237551	0.017800

111_SiAl_Cage_Pentagonal_Na_Internal

Atom	x	y	z
Si	2.053536	1.806457	1.763673
O	0.523792	2.198057	2.189024
O	-0.918474	2.044245	-0.277074
O	2.137818	1.683157	0.147735
Si	-0.728623	2.376246	-1.876759
O	0.786789	1.977591	-2.269924
O	3.752358	2.238718	-2.324938
H	3.863013	3.189684	-2.311361
O	3.113822	2.914386	2.372033
H	2.970955	3.826018	2.108068
O	-1.670841	3.896668	1.905320
H	-1.111306	4.597872	2.262418
O	-2.285447	1.143468	1.988066
O	-1.862925	1.418987	-2.576197
O	-0.973427	3.960612	-2.242990
H	-1.876810	4.280480	-2.181446
Si	-3.131114	-0.083809	1.349323
O	-3.321718	0.063608	-0.256434
O	-3.691201	-0.689343	-2.935449
H	-3.695238	-0.520941	-3.886363
O	-4.581112	-0.269631	2.094660
H	-5.262796	0.370973	1.879823
Si	2.553770	-1.754492	-1.202464
O	2.373443	-0.254226	-1.770510
O	2.889961	-1.735708	0.391573
O	2.481530	0.372220	2.428178
O	2.006492	-2.443664	3.111652
H	2.546219	-2.471940	3.910252
O	3.649566	-2.645919	-2.037060
H	4.550694	-2.315348	-2.058195
Si	-0.501282	-2.617399	-1.388614

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   O  1.124331 -2.555467 -1.432255
   O -0.955337 -3.144025  0.113497
  Si -0.913858 -2.224287  1.471288
   O  0.305931 -1.154432  1.337935
   O -0.494813 -3.157891  2.771514
   H -1.043926 -3.889603  3.066087
   O -2.342530 -1.499290  1.696620
   O -1.096828 -3.607153 -2.537770
   H -0.741585 -4.496251 -2.612112
   O -1.107244 -1.125639 -1.585744
  Al  2.028016 -1.155440  1.774582
  Al -1.028234  2.198065  1.441000
  Al  2.364555  1.513273 -1.597115
  Al -2.437364  0.008177 -1.739601
   H -4.511206 -1.127364 -2.674065
   H -2.601092  4.126854  2.021201
   H  1.127558 -2.882345  3.247948
  Na  0.393580  0.173295 -0.476314
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112_SiAl_Cage_Pentagonal_K_Internal
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Atom         x         y         z
  Si -2.087092  2.112086  1.419990
   O -2.469083  0.641907  2.027403
   O -2.614333 -1.430227  0.004090
   O -2.060330  2.010428 -0.192387
  Si -2.451544 -1.451880 -1.621437
   O -2.160308  0.037994 -2.163336
   O -2.734473  2.831007 -2.960982
   H -3.680617  2.918118 -2.841673
   O -3.144488  3.252726  1.968477
   H -4.057961  3.143599  1.694782
   O -3.695979 -1.765919  2.715194
   H -4.290643 -1.207525  3.233110
   O -0.813987 -1.681879  2.151559
   O -1.188023 -2.429625 -1.981548
   O -3.825033 -2.010033 -2.341842
   H -4.111881 -2.888729 -2.083005
  Si  0.512300 -2.560875  1.837391
   O  0.564485 -2.900215  0.255753
   O  0.857680 -4.294676 -2.323483
   H  0.227373 -4.742247 -2.903727
   O  0.625259 -3.896176  2.780430
   H -0.111428 -4.511799  2.759339
  Si  1.372388  2.332442 -1.747257
   O -0.114263  1.928303 -2.210780
   O  1.383812  2.630730 -0.150304
   O -0.615782  2.565364  1.961928
   O  1.789880  3.867780  2.480598
   H  1.251655  4.447241  3.035945
   O  2.032806  3.556801 -2.617692
   H  1.502672  4.350824 -2.716386
  Si  2.724419 -0.467563 -1.543485
   O  2.385318  1.054847 -2.026943
   O  2.802953 -0.438426  0.093481
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Si	2.638763	-0.339758	1.714598
O	1.746258	0.958866	2.067488
O	4.145918	-0.300350	2.342981
H	4.232119	-0.144530	3.286725
O	1.843757	-1.675038	2.228559
O	4.121467	-0.985389	-2.207465
H	4.901239	-0.434380	-2.104150
O	1.528725	-1.469400	-1.959173
Al	1.045484	2.453266	1.528380
Al	-2.346901	-1.037030	1.656458
Al	-1.852497	1.756602	-1.921205
Al	0.423167	-2.710742	-1.450380
H	1.731150	-4.696623	-2.415344
H	-4.012450	-2.678508	2.721779
H	2.708648	4.164987	2.485688
K	-0.097754	0.055514	-0.110452

113_SiAl_Cage_Pentagonal_Ca_Internal

Atom	x	y	z
Si	0.707871	-2.910364	1.335801
O	1.729481	-1.622025	1.559425
O	3.710767	-0.094824	-0.056639
O	0.878972	-3.408160	-0.197729
Si	2.935994	-0.021986	-1.504583
O	1.612904	-0.971416	-1.377467
O	0.881325	-3.276576	-3.169495
H	1.254589	-4.158022	-3.180864
O	0.925996	-4.082822	2.452786
H	1.719131	-4.619609	2.381882
O	3.934486	-0.170772	2.817689
H	3.743531	-0.476926	3.715204
O	1.586216	1.070564	1.383364
O	2.424577	1.501728	-1.808385
O	3.877590	-0.588914	-2.721887
H	4.696322	-0.125489	-2.911980
Si	0.962124	2.591632	1.536029
O	1.224316	3.353888	0.126907
O	0.445948	3.516466	-2.735030
H	0.852697	4.281719	-3.158135
O	1.530080	3.394373	2.835674
H	2.422192	3.747607	2.793591
Si	-2.524874	-1.386825	-1.499436
O	-0.915000	-1.630618	-1.460055
O	-3.152950	-1.843585	-0.083030
O	-0.771022	-2.232830	1.525154
O	-3.494039	-2.055362	2.775766
H	-3.178494	-2.109642	3.678149
O	-3.277021	-2.066089	-2.784295
H	-3.475276	-3.003770	-2.725789
Si	-2.023149	1.670860	-1.385684
O	-2.717608	0.252218	-1.744440
O	-2.641473	2.280736	0.008732
Si	-2.137115	1.777301	1.500475
O	-1.958698	0.162782	1.406205

O	-3.240315	2.318077	2.561535
H	-3.057957	2.234297	3.500847
O	-0.647349	2.387886	1.806853
O	-2.104473	2.770302	-2.606344
H	-2.937474	3.049931	-2.996423
O	-0.412966	1.474340	-1.134929
Al	-2.430625	-1.590901	1.506461
Al	2.773275	-0.246388	1.388332
Al	0.657946	-2.456389	-1.674028
Al	1.065009	2.451422	-1.356631
H	-0.522533	3.458615	-2.928643
H	4.835667	0.178278	2.773541
Ca	0.023245	-0.305562	0.301275

114_SiAl_Cage_Hexagonal_Na_Internal

Atom	x	y	z
O	1.349264	-1.667205	1.203921
Si	2.935426	-1.279335	1.284227
O	3.609185	-1.615244	-0.169935
O	0.280909	-3.937093	-0.090082
Si	0.125831	-3.101220	-1.460494
O	1.555495	-2.632942	-2.073316
O	-0.714425	-4.005371	-2.602364
H	-0.422224	-4.897148	-2.807532
O	1.359829	-4.190859	2.633473
H	2.223048	-3.818185	2.842342
O	3.583552	-2.243525	2.466341
H	4.517186	-2.144273	2.665926
O	3.126934	0.287122	1.667817
O	1.806253	0.177441	-1.416978
O	3.780323	-1.010905	-3.004320
H	3.837993	-0.026748	-3.176710
O	2.852898	2.389122	-0.348366
Si	2.263457	1.719878	-1.705180
O	3.486922	1.536636	-2.838745
H	3.989333	2.299000	-3.137262
O	4.089703	2.936093	2.200694
H	5.026413	2.989367	1.974320
O	-0.858010	-1.801166	-1.263433
O	-3.144315	-2.314798	0.360820
Si	-2.334677	-1.820513	1.687296
O	-1.136756	-2.793685	2.121664
O	-3.412948	-1.587672	2.954052
H	-3.867002	-2.337182	3.346989
O	-3.039718	-2.914352	-2.488568
H	-2.261290	-3.510764	-2.698153
Si	-3.246575	1.472890	-1.429376
O	-3.249480	-0.140472	-1.635979
O	-3.244793	1.886614	0.148015
O	-1.806426	-0.292307	1.388119
O	-3.793204	0.941376	2.851930
H	-3.853734	-0.037581	3.063143
O	-4.632648	2.119684	-2.053615
H	-4.780143	1.975813	-2.991102

Si	-0.074024	2.899192	1.549311
O	-0.209189	2.169264	0.084311
O	-1.357426	2.398831	2.402174
O	-0.194258	4.535911	1.200526
H	0.060734	5.193584	1.852758
O	-1.946802	2.114480	-2.199395
O	-0.756781	4.582104	-1.284703
H	-0.589667	4.843540	-0.331734
O	1.040496	2.566481	-2.361203
O	1.377245	2.572022	2.179099
Al	-2.469243	1.317557	1.585485
Al	-2.607627	-1.662149	-1.169173
Al	0.468823	-3.197931	1.513987
Al	2.626685	-1.369184	-1.583402
Al	2.764235	1.933099	1.327699
Al	-0.485655	2.752772	-1.554504
H	-4.658077	1.363900	2.895406
H	-3.875504	-3.385326	-2.576345
H	3.802044	-1.511631	-3.827797
H	3.852406	3.664828	2.788486
H	-1.523641	5.048120	-1.638111
Na	0.079229	-0.160965	0.088870

115_SiAl_Cage_Hexagonal_K_Internal

Atom	x	y	z
O	1.978694	-0.255471	1.315104
Si	2.899424	1.071268	1.571197
O	3.740177	1.386071	0.214424
O	3.077899	-2.524120	-0.002033
Si	2.464496	-2.047281	-1.433075
O	3.045578	-0.603012	-1.880192
O	2.679823	-3.211181	-2.610689
H	3.557181	-3.523752	-2.844137
O	3.567040	-1.968481	2.818340
H	3.875197	-1.042276	3.036689
O	3.936108	0.580242	2.792655
H	4.642275	1.158694	3.091654
O	2.005732	2.326187	2.062594
O	1.650808	1.923178	-1.651693
O	4.428373	1.652204	-2.576213
H	4.716919	2.560263	-2.730574
O	0.698974	3.829318	-0.045398
Si	0.590857	3.172709	-1.536104
O	1.001352	4.380611	-2.587043
H	0.907014	4.171350	-3.518986
O	-0.205118	4.183461	2.736837
H	0.001835	5.114864	2.871673
O	0.839064	-2.001996	-1.315251
O	-0.692506	-3.911825	0.125576
Si	-0.574142	-3.063679	1.511387
O	0.959859	-2.923840	2.013118
O	-1.519396	-3.767499	2.701176
H	-1.375487	-4.680876	2.961248
O	0.177670	-4.191693	-2.691697

```
   H  1.144854 -4.039676 -2.851041
  Si -3.133499 -1.183357 -1.566387
   O -1.969944 -2.272607 -1.941914
   O -3.745818 -1.450858 -0.074798
   O -1.262284 -1.595563  1.315971
   O -3.541556 -2.157931  2.749606
   H -2.917586 -2.920698  2.916695
   O -4.401696 -1.361229 -2.612173
   H -4.187559 -1.295276 -3.545452
  Si -2.412542  2.013527  1.481135
   O -2.998143  2.539721  0.075369
   O -3.073149  0.601528  1.938676
   O -2.621334  3.187422  2.670275
   H -3.478471  3.610637  2.766374
   O -2.485086  0.303947 -1.619530
   O -3.666166  2.653283 -2.771377
   H -3.842360  3.593292 -2.818241
   O -0.876178  2.575229 -1.843045
   O -0.784530  1.873512  1.457877
  Al -2.921953 -1.032118  1.393355
  Al -0.547048 -3.062573 -1.391972
  Al  2.293063 -1.974229  1.457082
  Al  3.115731  1.057097 -1.379264
  Al  0.527920  3.021038  1.477258
  Al -2.541779  2.069854 -1.574352
   H -4.456987 -2.417730  2.901345
   H -0.096540 -5.070110 -2.976958
   H  3.541783 -2.526485  3.604004
   H  4.750281  1.080457 -3.285055
   H -1.179252  3.999071  2.879214
   K -0.098869  0.175098 -0.459810
-------------------------------------

116_SiAl_Cage_Hexagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
   O -1.971701  1.309560  1.182119
  Si -3.084830  0.116323  1.370836
   O -3.957831 -0.033929  0.017165
   O -1.823842  3.655008 -0.281281
  Si -1.461452  2.694119 -1.527170
   O -2.603728  1.638968 -1.932245
   O -1.034938  3.628811 -2.859974
   H -1.687132  4.199793 -3.274369
   O -2.803349  3.788518  2.494658
   H -3.387176  3.177227  2.948795
   O -3.991618  0.446065  2.695971
   H -4.890042  0.108652  2.719419
   O -2.081273 -1.173896  1.576991
   O -1.669259 -0.969950 -1.361898
   O -4.065276 -0.780374 -2.833450
   H -5.003199 -0.638594 -2.962790
   O -1.648234 -3.380117 -0.220226
  Si -1.483783 -2.594859 -1.649430
   O -2.620321 -3.089287 -2.721281
   H -3.282294 -2.399299 -2.924414
```

```
   O -2.795893 -3.962551  2.281556
   H -3.319628 -4.621900  1.807356
   O -0.027722  1.904520 -1.203924
   O  2.018862  3.347769  0.114362
  Si  1.474426  2.708100  1.506104
   O -0.001610  3.176644  1.908036
   O  2.569908  2.975972  2.741072
   H  2.712124  3.863472  3.081175
   O  1.470664  3.657324 -2.758376
   H  0.497779  3.830179 -2.984360
  Si  3.527598 -0.161674 -1.499817
   O  2.777207  1.252327 -1.792648
   O  3.727816 -0.403678  0.102581
   O  1.556365  1.050922  1.328854
   O  3.896645  0.809695  2.784564
   H  3.570622  1.746520  2.947649
   O  5.044857 -0.156482 -2.143304
   H  5.104231 -0.040564 -3.094351
  Si  1.356936 -2.640188  1.628911
   O  1.056894 -1.957070  0.141584
   O  2.257435 -1.544027  2.406076
   O  2.230646 -4.026871  1.309906
   H  2.248484 -4.736317  1.958918
   O  2.641205 -1.366675 -2.168057
   O  2.427529 -4.068807 -1.215459
   H  2.498676 -4.291124 -0.240095
   O  0.003876 -2.845370 -2.276965
   O -0.074358 -3.019180  2.273558
  Al  2.865169 -0.130580  1.569774
  Al  1.657555  2.471577 -1.352753
  Al -1.684134  3.064651  1.383579
  Al -3.164809  0.019517 -1.568755
  Al -1.593186 -2.831676  1.418590
  Al  1.506767 -2.478373 -1.513918
   H  4.843542  0.722256  2.940593
   H  2.029395  4.419817 -2.945068
   H -2.896564 -4.085730  3.234523
   H  3.250365 -4.278614 -1.673576
  Ca -0.280052  0.045575  0.247704
-------------------------------------

117_SiAl_Cage_Heptagonal_Na_Internal
-------------------------------------
Atom         x         y         z
   O  0.997068 -3.672364  0.106648
   O  4.212120 -1.948030  0.689882
   O  2.839695  4.098796  0.173104
   O -2.476160 -2.234120 -0.070620
   O  4.943749  1.363164  0.340277
   O -3.263130  1.133585  0.331513
   O -0.641502 -2.914451  2.075582
   O  3.692804 -0.080687  2.540746
   O  2.454857 -2.181876 -1.575337
   O -0.885861  1.733397  1.462956
   O -2.320045 -0.307342 -1.957803
   O  3.539913  2.099384 -1.827181
```

```
 O  1.787575 -1.814739  1.830860
 O  4.687412 -0.310866 -1.710735
 O  3.573212  2.842295  2.436660
 O -0.138716 -1.662106 -1.206068
 O -1.899784  2.491791 -1.798066
 O -2.217608 -0.465663  2.223782
Si  0.888635 -3.191029  1.676701
Si  3.409805 -1.586238  2.045971
Si  2.671455  4.026247  1.791197
Si -1.791575 -1.723466 -1.448395
Si  4.810554  1.253719 -1.273691
Si -2.361342  1.044070  1.657917
Si  1.019948 -2.845311 -1.316186
 O  5.928236  1.470820  3.046793
 H  6.241163  2.298541  3.433142
 O  3.757144 -2.702767  3.225026
 H  4.675337 -2.834303  3.472717
 O  3.236924  5.427066  2.466364
 H  2.827919  6.235052  2.148724
 O  1.534559 -4.353333  2.633923
 H  2.375626 -4.095680  3.039583
 O -3.059125  1.993899  2.868416
 H -3.996242  1.883555  3.049920
 O -3.444124 -2.909033  2.563686
 H -3.754972 -3.817225  2.464390
 O  0.642220 -3.864190 -2.539459
 H -0.289734 -3.817473 -2.803796
 O -1.928046 -2.895382 -2.619402
 H -2.803268 -3.124106 -2.940268
 O -4.562543  1.397439 -2.261068
 H -5.155233  2.092261 -1.973195
 O  2.168527  4.520865 -2.605347
 H  2.713986  5.309390 -2.698631
 O  6.144731  1.918468 -1.994427
 H  6.987009  1.532764 -1.743776
 O  5.207209 -2.982125 -1.790178
 H  5.047753 -3.927638 -1.900361
 O -0.952649  4.199808  0.079643
 O  0.747576  2.616879 -1.184459
 O  1.104726  3.818794  2.182722
Si -0.688112  3.416833 -1.325077
 O -1.606252  4.051242  2.896862
 H -2.308041  3.355918  3.098356
 O -0.345970  4.551289 -2.524281
 H -1.050707  5.097465 -2.880528
Al -2.067142 -2.067170  1.601583
Al -3.046199  1.207475 -1.419796
Al -0.447618  3.438197  1.563882
Al  2.392706  3.245755 -1.257848
Al  4.377980  1.400467  1.957846
Al  4.023480 -1.735113 -1.014123
 H -4.100798 -2.390415  3.045562
 H -1.259071  4.442858  3.706290
 H  1.192533  4.732361 -2.750785
 H  6.134135  0.743776  3.647885
 H  5.838287 -2.681045 -2.456533
```

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  Na  0.662822  0.512058 -0.086975
-------------------------------------

118_SiAl_Cage_Heptagonal_K_Internal
-------------------------------------
Atom         x         y         z
   O  0.999530 -3.879392  0.341833
   O  4.331063 -2.111686  0.641477
   O  2.829001  4.125505  0.225617
   O -2.407172 -2.198181 -0.161857
   O  4.955040  1.275560  0.228626
   O -3.392092  1.339915  0.252957
   O -0.622954 -2.592475  2.048737
   O  3.899226 -0.191571  2.473425
   O  2.555418 -2.770771 -1.532890
   O -1.065404  1.804306  1.532208
   O -1.671971 -0.033575 -1.567161
   O  3.318078  2.037094 -1.755897
   O  1.906660 -1.802737  1.712899
   O  4.324870 -0.429860 -1.733685
   O  3.545964  2.697589  2.384781
   O  0.067942 -1.900386 -1.130642
   O -1.983682  2.787800 -1.793684
   O -2.496104 -0.376758  2.116727
  Si  0.875534 -3.099325  1.790730
  Si  3.541263 -1.681317  1.984204
  Si  2.649277  3.933239  1.834571
  Si -1.545547 -1.627770 -1.411514
  Si  4.601878  1.129097 -1.350753
  Si -2.570070  1.165971  1.626351
  Si  1.059571 -3.220585 -1.166261
   O  6.028334  1.663106  2.876008
   H  6.049361  2.414221  3.482606
   O  3.787991 -2.792630  3.190311
   H  4.686509 -2.964604  3.481571
   O  3.222783  5.274401  2.615134
   H  2.817094  6.107121  2.364353
   O  1.349941 -4.104236  2.990116
   H  2.255037 -3.940897  3.296049
   O -3.274050  2.098204  2.839920
   H -4.218729  2.023295  2.997173
   O -3.453825 -2.953294  2.426856
   H -3.642438 -3.893700  2.317076
   O  0.460177 -4.284466 -2.256619
   H -0.351825 -3.983337 -2.688537
   O -1.819453 -2.521872 -2.774486
   H -2.723272 -2.660572 -3.067676
   O -4.156055  0.989465 -2.534709
   H -4.957849  1.504443 -2.440125
   O  2.156102  4.612722 -2.554115
   H  2.773490  5.335189 -2.712941
   O  5.863547  1.702338 -2.256656
   H  6.714887  1.291157 -2.091140
   O  5.343071 -3.006489 -1.906651
   H  5.262222 -3.944783 -2.118566
   O -1.052186  4.328575  0.229791
```

```
   O  0.636621  2.824196 -1.138550
   O  1.078204  3.709050  2.204831
  Si -0.767462  3.667306 -1.233078
   O -1.641463  4.064714  3.045150
   H -2.393921  3.419484  3.192695
   O -0.372561  4.881303 -2.330104
   H -1.028110  5.533029 -2.589405
  Al -2.140796 -1.959115  1.537258
  Al -2.843255  1.294202 -1.428938
  Al -0.530055  3.473873  1.657370
  Al  2.313531  3.321473 -1.212246
  Al  4.461510  1.333855  1.872858
  Al  4.016923 -1.978350 -1.056733
   H -4.189109 -2.523677  2.883002
   H -1.298059  4.395338  3.882893
   H  1.204185  4.920357 -2.645982
   H  6.661188  0.995692  3.167952
   H  5.994041 -2.597317 -2.490927
   K  0.642229  0.413998  0.009124
-------------------------------------

119_SiAl_Cage_Heptagonal_Ca_Internal
-------------------------------------
Atom         x         y         z
   O  1.186100 -3.869828  0.045204
   O  4.090657 -1.920758  0.645593
   O  2.758286  4.032924  0.011682
   O -2.394809 -2.205275 -0.357820
   O  5.122284  1.271083  0.466879
   O -3.187861  1.325777  0.614629
   O -0.738918 -3.147160  1.772834
   O  3.437472 -0.003798  2.408496
   O  2.623247 -2.537523 -1.774478
   O -0.704887  1.968642  1.449484
   O -1.496535  0.162484 -1.304802
   O  2.639975  1.154400 -0.534892
   O  1.616521 -1.806337  1.633154
   O  4.611934 -0.349877 -1.654139
   O  3.591074  2.946835  2.335025
   O  0.158496 -1.722234 -1.085112
   O -2.125882  2.859698 -1.622125
   O -1.435348 -0.450270  1.643378
  Si  0.832442 -3.289541  1.555149
  Si  3.228060 -1.533575  1.956434
  Si  2.737209  4.141109  1.637579
  Si -1.466920 -1.455889 -1.430596
  Si  4.250416  0.997407 -0.858786
  Si -2.046079  1.051441  1.718973
  Si  1.150228 -3.036051 -1.365347
   O  5.717724  1.504010  3.275214
   H  5.833604  2.279853  3.838528
   O  3.551885 -2.587751  3.191669
   H  4.457107 -2.663853  3.503670
   O  3.477705  5.542218  2.107612
   H  3.145133  6.345235  1.700548
   O  1.478433 -4.301163  2.664514
```

```
   H  2.305890 -3.992317  3.062564
   O -2.549546  1.564476  3.224797
   H -3.424977  1.314893  3.534128
   O -3.499677 -2.326939  2.365795
   H -4.123677 -3.015488  2.135482
   O  0.470991 -3.949046 -2.536396
   H -0.263478 -3.531800 -3.008824
   O -1.641871 -2.057761 -2.955185
   H -2.526106 -2.277390 -3.260984
   O -4.275030  0.865427 -1.991054
   H -4.268355  0.876357 -2.948705
   O  2.117153  3.682724 -2.843960
   H  2.830742  4.087683 -3.348210
   O  4.203240  2.378328 -1.852630
   H  4.961943  2.953996 -1.992179
   O  5.345646 -3.103812 -1.727803
   H  5.112908 -3.922427 -2.185220
   O -0.892754  4.467542  0.150102
   O  0.521599  2.575182 -1.066600
   O  1.201212  4.114605  2.185173
  Si -0.757198  3.604874 -1.229401
   O -1.555227  4.015285  3.012609
   H -2.028411  3.212730  3.353433
   O -0.248399  4.593761 -2.483200
   H -0.810986  5.297672 -2.814071
  Al -2.084957 -2.088549  1.394029
  Al -2.847944  1.337242 -1.127175
  Al -0.357790  3.689492  1.612960
  Al  2.294795  2.849689 -1.172017
  Al  4.323073  1.432021  2.018514
  Al  4.071886 -1.908269 -1.082587
   H -1.494709  4.703354  3.684573
   H  1.254231  4.171602 -2.956365
   H  6.197811  0.754437  3.648252
   H  6.303572 -2.981400 -1.737579
  Ca  0.524346  0.408270  0.084308
-------------------------------------

120_SiAl_Cage_Octagonal_Na_Internal
-------------------------------------
Atom         x         y         z
   O  0.934329 -3.446222 -0.516876
   O  4.318030 -2.272931 -0.352928
   O  3.642895  4.250643  0.908975
   O -2.053626 -2.295216  0.712825
   O  5.476575  1.205199  0.871108
   O -3.680696  0.848733  0.421460
   O  0.318290 -2.168252  1.974748
   O  3.703477 -0.913546  1.823707
   O  1.864395 -0.991109 -1.197010
   O -2.149296  2.824383  1.891168
   O -3.430918 -0.960048 -1.543960
   O  5.267669  2.956825 -1.165684
   O  2.863069 -3.442343  1.618318
   O  4.403561  0.460122 -1.434284
   O  2.751115  1.828101  1.656611
```

```
 O -0.665387 -1.698302 -1.770023
 O -2.590558  1.549393 -1.904474
 O -1.116012  0.077532  1.524665
Si  4.044323 -2.411786  1.256894
Si  2.745108  3.431995  1.985819
Si  5.537284  1.410216 -0.748399
Si -1.145551 -1.537235  1.831907
Si -3.710335  0.599904 -1.189050
Si  0.850587 -2.227713 -1.563679
 O  4.589385  1.193277  3.613276
 H  4.292306  2.122289  3.834772
 O  5.410394 -3.005620  1.987149
 H  6.228680 -2.561315  1.754994
 O  3.492963  3.494105  3.489329
 H  3.661650  4.347436  3.897272
 O  0.440675 -5.014442  1.876483
 H  0.691281 -5.841784  1.464111
 O -3.254403  0.582571  3.256038
 H -2.870289 -0.301017  3.539355
 O -1.974463 -1.601978  3.301664
 H -2.185720 -2.464158  3.669460
 O  1.450545 -2.743069 -3.058436
 H  1.094719 -3.552526 -3.434231
 O -2.754648 -3.731635 -1.504264
 H -2.968209 -4.380774 -0.821404
 O -5.220900  0.919388 -1.780450
 H -5.573193  1.790010 -1.582925
 O  4.545369  5.730639 -1.206178
 H  4.749720  6.354298 -0.497280
 O  7.048899  1.058452 -1.313055
 H  7.396886  0.195239 -1.078729
 O  3.779479 -1.741175 -3.118712
 H  2.926811 -2.197658 -3.384280
 O -2.599016  4.052522 -0.426471
 O  2.524936  3.709258 -1.727530
 O  1.258624  4.050204  2.085639
Si -2.462765  4.262222  1.184646
 O -3.848577  4.936250  1.781665
 H -4.667569  4.496032  1.544232
 O -1.912784  3.983012 -3.228480
 H -1.045135  4.413140 -3.468605
 O  0.851252  5.368728 -0.484539
 O -0.073308  3.015511 -1.375963
 O -1.280364  5.314108  1.553373
Si  0.995379  4.220236 -1.625239
 O  1.077489  6.931300  1.737164
 H  1.379680  7.565730  1.074291
 O  0.499997  4.851096 -3.102609
 H  0.941577  5.630766 -3.448972
Al  0.400499  5.259985  1.186787
Al  3.947756  3.993195 -0.778751
Al  4.125669  0.742407  1.855154
Al  3.616170 -1.063125 -1.374735
Al  1.151665 -3.547324  1.238207
Al -2.178845 -2.008413 -0.992122
Al -2.499239  1.161271  1.641544
```

Al	-1.813177	3.052564	-1.600320
H	0.865232	7.395302	2.556261
H	5.012804	5.991261	-2.009625
H	5.435586	0.989986	4.026857
H	4.120173	-1.193897	-3.835112
H	-3.219911	-3.955838	-2.319605
H	-3.374209	1.174846	4.006454
H	-2.357320	3.626144	-4.005351
Na	0.922927	0.822840	0.291684

121_SiAl_Cage_Octagonal_K_Internal

Atom	x	y	z
O	0.910889	-3.304048	-0.249574
O	4.192328	-1.942503	0.012243
O	3.795329	4.304913	0.847574
O	-2.306544	-2.599597	0.529600
O	5.705870	1.119533	0.580872
O	-3.950919	0.847177	0.308576
O	-0.253731	-2.479598	2.261917
O	4.324608	-0.740524	2.379726
O	1.790045	-0.978632	-1.264827
O	-1.924374	2.570608	1.519995
O	-3.447834	-0.924824	-1.650039
O	5.214779	2.963717	-1.338199
O	2.656214	-2.808201	2.047772
O	4.336347	0.470629	-1.610474
O	3.130825	1.840203	1.686946
O	-0.717080	-1.834485	-1.786726
O	-2.549967	1.581278	-1.828292
O	-1.495674	-0.230492	1.422704
Si	4.081708	-2.162427	1.621617
Si	2.908184	3.443527	1.904157
Si	5.535553	1.404692	-1.017197
Si	-1.646347	-1.814793	1.789661
Si	-3.765621	0.627630	-1.301417
Si	0.809752	-2.261152	-1.486413
O	5.280392	1.776863	3.383193
H	4.769767	2.598733	3.629163
O	5.217845	-3.263688	2.109424
H	6.130488	-3.013033	1.950356
O	3.545648	3.699603	3.440535
H	3.591792	4.601422	3.770130
O	0.869089	-4.992355	2.083800
H	1.460291	-5.737710	1.923311
O	-3.510683	0.668368	3.137323
H	-3.336402	-0.278239	3.401048
O	-2.721805	-1.783635	3.079154
H	-3.026555	-2.607353	3.468116
O	1.466335	-2.997313	-2.853177
H	1.118046	-3.849456	-3.128304
O	-2.948710	-3.705305	-1.876333
H	-3.214756	-4.419195	-1.282340
O	-5.180890	0.974616	-2.080450
H	-5.562582	1.835483	-1.894825

```
   O  4.615901  5.761317 -1.317795
   H  4.859725  6.377690 -0.615091
   O  6.967530  1.090764 -1.784195
   H  7.374237  0.246764 -1.576482
   O  3.836895 -2.046049 -2.839514
   H  3.004499 -2.528549 -3.111840
   O -2.620114  4.177061 -0.456601
   O  2.471233  3.825843 -1.698764
   O  1.337751  3.778114  1.800094
  Si -2.336168  4.123186  1.154639
   O -3.727694  4.540489  1.955364
   H -4.543946  4.264142  1.532813
   O -1.912152  3.996192 -3.245501
   H -1.047635  4.470678 -3.430512
   O  0.802653  5.493516 -0.411914
   O -0.091194  3.112678 -1.328754
   O -1.185264  5.131002  1.648743
  Si  0.947878  4.357708 -1.546348
   O  1.258868  6.583894  2.257745
   H  1.124117  7.485948  1.965829
   O  0.428491  4.988388 -3.026226
   H  0.770877  5.843154 -3.300530
  Al  0.532737  5.293557  1.328618
  Al  3.967549  4.048794 -0.859624
  Al  4.586239  0.886508  1.880707
  Al  3.542596 -1.018351 -1.290697
  Al  1.096478 -3.222571  1.468783
  Al -2.296739 -2.094075 -1.134031
  Al -2.700375  1.037025  1.489150
  Al -1.827233  3.123306 -1.586160
   H  5.088559  5.992158 -2.127098
   H  6.213280  1.865168  3.606301
   H  4.292323 -1.678105 -3.604963
   H  0.029292 -5.311578  2.436340
   H -3.443861 -3.774822 -2.701998
   H -3.473200  1.254947  3.901594
   H -2.251037  3.564039 -4.037251
   K  0.643489  1.291825  0.592428
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122_SiAl_Cage_Octagonal_Ca_Internal
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Atom         x         y         z
   O  0.840385 -3.327383 -0.355973
   O  4.091338 -1.991329  0.061139
   O  3.917106  4.540196  0.763393
   O -2.456758 -2.702856  0.584964
   O  5.504621  1.107671  0.750307
   O -3.890359  1.004947  0.609528
   O -0.311910 -2.601474  2.199642
   O  3.735191 -0.589235  2.297553
   O  1.696871 -0.878780 -1.091783
   O -1.512273  2.362471  1.264568
   O -3.618930 -0.880367 -1.330108
   O  5.300176  2.893031 -1.258590
   O  2.545652 -2.968195  2.033923
```

```
 O  4.328976  0.433005 -1.539103
 O  3.086592  2.248046  1.877114
 O -0.796613 -1.385174 -1.298196
 O -2.175665  1.335641 -1.421094
 O -1.482543 -0.331404  1.372843
Si  3.860905 -2.090744  1.673896
Si  3.185510  3.861023  2.045450
Si  5.513015  1.332605 -0.863163
Si -1.722774 -1.910123  1.790423
Si -3.639780  0.690343 -0.969442
Si  0.646663 -2.110464 -1.401533
 O  5.128078  1.624922  3.567653
 H  4.935099  2.590494  3.728546
 O  5.125723 -2.908985  2.358710
 H  6.000235 -2.564996  2.164223
 O  4.169009  4.021073  3.397883
 H  4.447352  4.894110  3.685337
 O  0.831255 -5.212324  1.635874
 H  0.730716 -5.799440  0.875394
 O -3.065353  1.036473  3.456833
 H -3.116644  0.138077  3.800891
 O -2.712129 -1.818299  3.125390
 H -3.152800 -2.627245  3.395330
 O  1.051812 -2.624615 -2.934714
 H  0.600566 -3.394112 -3.294303
 O -2.472770 -3.433461 -2.252391
 H -3.071025 -4.167368 -2.110471
 O -4.746506  1.516833 -1.884319
 H -5.595392  1.691361 -1.472367
 O  4.745787  5.668470 -1.574617
 H  4.987247  6.375685 -0.962566
 O  6.991487  0.926452 -1.479076
 H  7.324121  0.058840 -1.239341
 O  3.576621 -1.992374 -2.795815
 H  2.717282 -2.332046 -3.152942
 O -2.430146  4.130331 -0.473926
 O  2.582644  3.739184 -1.713824
 O  1.753134  4.558945  2.326151
Si -2.130225  3.885710  1.121175
 O -3.545766  3.986580  1.970989
 H -4.272216  3.475122  1.600410
 O -1.851336  3.719371 -3.278289
 H -1.012267  4.223505 -3.486267
 O  0.854164  5.250997 -0.352231
 O  0.032974  2.894786 -1.352928
 O -1.112930  4.982351  1.737602
Si  1.043677  4.177589 -1.544985
 O  0.747823  7.105347  1.864884
 H  0.049379  7.771316  1.840248
 O  0.443053  4.828640 -2.975234
 H  0.777253  5.677688 -3.277376
Al  0.539374  5.307984  1.349117
Al  4.077011  4.042450 -0.887084
Al  4.304232  1.006425  1.993703
Al  3.457023 -1.003197 -1.201711
Al  1.005088 -3.350714  1.378411
```

```
  Al -2.419677 -2.138223 -1.088044
  Al -2.574355  1.024785  1.794001
  Al -1.723126  3.002402 -1.576095
   H  1.414008  7.360360  2.515905
   H  5.242415  5.770398 -2.395873
   H  6.017652  1.395407  3.857522
   H  4.184651 -1.760896 -3.507151
   H  1.197652 -5.707237  2.379200
   H -2.223638  3.293998 -4.059544
  Ca -0.072778  0.718417 -0.250717
-------------------------------------
```