

Figure S1. PY adsorption complexes in the open and closed regions of the 32T cluster for Si/Al = 31.

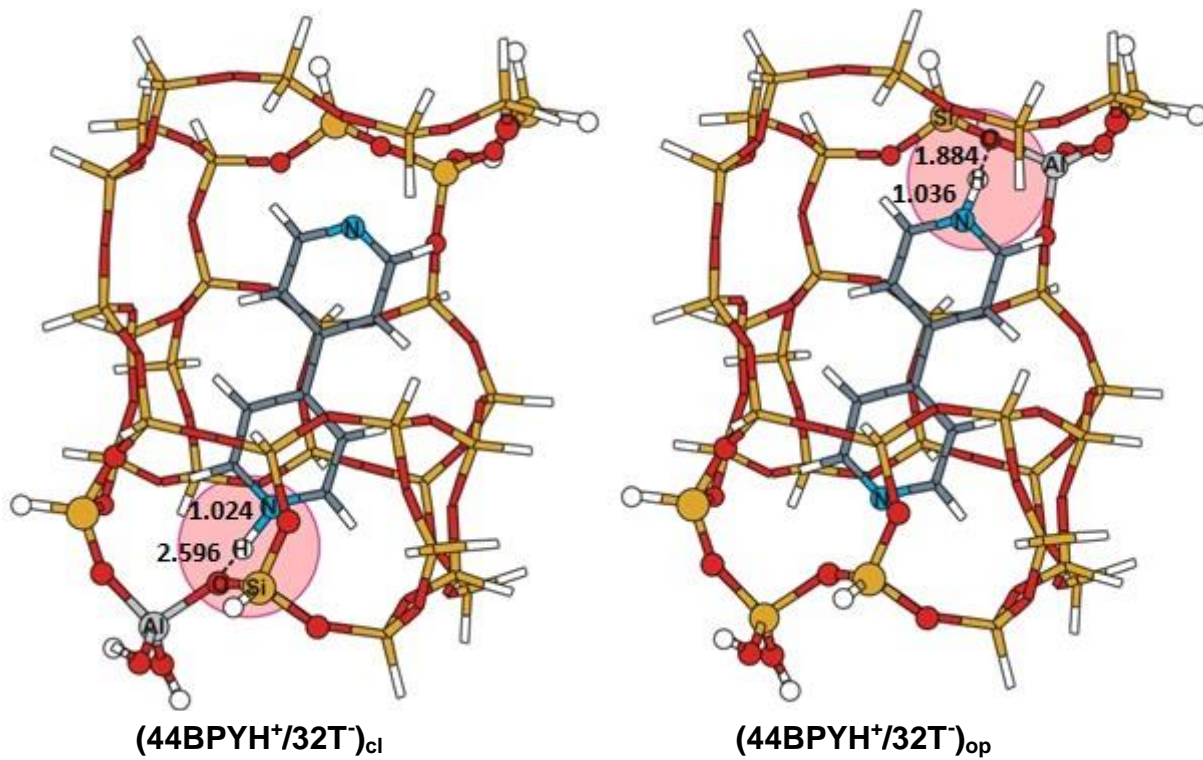


Figure S2. 44BPY adsorption complexes in the open and closed regions of the 32T cluster for Si/Al = 31.

**Table S1:** Cartesian coordinates of the structures of 32T clusters with Si/Al = 15 and 31, and of all the PY and 44BPY adsorption complexes optimized at the B3LYP/6-31+G\* level

**CLUSTERS:**

**1) 32T with Si/Al = 15**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.596271	-2.153698	-4.602513
2	14	0	1.798800	0.679184	-4.576837
3	14	0	2.412553	3.480853	-3.665548
4	14	0	5.050653	4.656814	-2.723424
5	14	0	4.870347	4.091630	0.314493
6	14	0	6.465207	2.413682	2.398154
7	14	0	2.533312	-4.189735	-2.251944
8	8	0	2.735674	-0.588731	-4.245688
9	8	0	2.136059	1.895902	-3.579473
10	8	0	3.991919	3.767641	-3.550636
11	8	0	5.280063	4.009479	-1.268250
12	8	0	5.589483	2.911957	1.143037
13	8	0	6.405770	0.771303	2.449057
14	8	0	3.702097	-4.380541	-1.125768
15	8	0	2.932139	-3.033038	-3.295175
16	14	0	1.721801	2.261950	3.481368
17	14	0	2.531130	-0.567664	3.491592
18	14	0	1.959301	-3.435394	2.506987
19	14	0	-0.694242	-4.634209	1.543320
20	14	0	-0.482347	-3.993676	-1.451117
21	14	0	-2.115664	-2.259075	-3.457150
22	14	0	-1.304240	0.662915	-4.018606
23	14	0	-2.001347	3.335601	-2.800406
24	14	0	0.446340	4.905358	-1.574896
25	14	0	1.833490	4.323853	1.114814
26	8	0	1.598112	0.694577	3.129344
27	8	0	2.224999	-1.790959	2.492235
28	8	0	0.379754	-3.721246	2.392238
29	8	0	-0.929438	-3.972815	0.095409
30	8	0	-1.215110	-2.791416	-2.233996
31	8	0	-2.071148	-0.650321	-3.489734
32	8	0	-1.271034	1.848975	-2.889521
33	8	0	-1.007225	4.392098	-2.070380
34	8	0	0.668500	4.489565	-0.036402
35	8	0	1.404048	3.179748	2.159777
36	1	0	3.540434	-2.495107	-5.685806
37	1	0	2.033921	1.108922	-5.970240
38	1	0	1.909642	3.994622	-4.955762
39	1	0	4.522171	6.027575	-2.570937
40	1	0	6.332011	4.701610	-3.456665
41	1	0	5.235033	5.397571	0.900199
42	1	0	7.863236	2.860212	2.231859
43	1	0	6.218623	-1.121002	4.110316
44	1	0	3.936088	-6.294080	0.493779
45	1	0	2.378106	-5.471837	-2.968640
46	1	0	0.748135	2.604680	4.537796
47	1	0	2.261382	-0.991125	4.880637
48	1	0	2.461841	-3.949230	3.797318

49	1	0	-0.169500	-6.004617	1.375522
50	8	0	-2.086502	-4.687493	2.348688
51	1	0	-0.863343	-5.283437	-2.061763
52	8	0	-3.637515	-2.746369	-3.255789
53	1	0	-1.983005	1.177456	-5.225276
54	1	0	-2.314756	3.832742	-4.216286
55	1	0	0.462093	6.377866	-1.688925
56	1	0	1.967712	5.614538	1.820254
57	8	0	1.089877	-2.453379	-5.079922
58	8	0	-1.541555	-2.841949	-4.843204
59	14	0	-0.266438	-3.013986	-5.812305
60	1	0	-0.509158	-2.286048	-7.074337
61	1	0	-0.054141	-4.447206	-6.099254
62	8	0	0.256760	0.257461	-4.397454
63	8	0	1.628439	4.285259	-2.472870
64	8	0	3.241522	3.932698	0.437943
65	8	0	3.213923	2.570737	3.996316
66	8	0	5.860159	3.029650	3.756458
67	14	0	4.564239	3.222100	4.693599
68	1	0	4.781967	2.527155	5.978579
69	1	0	4.342061	4.661443	4.939480
70	8	0	4.092999	-0.120203	3.300457
71	8	0	2.763458	-4.176079	1.309055
72	8	0	1.145865	-3.806905	-1.529350
73	14	0	-5.063709	-2.299653	-2.655148
74	14	0	-3.695719	-4.675502	2.359756
75	8	0	-5.206787	-2.846478	-1.148164
76	8	0	-5.200526	-0.656625	-2.589075
77	1	0	-6.148282	-2.856823	-3.488689
78	8	0	-4.215361	-3.817978	3.621070
79	8	0	-4.243473	-4.018491	0.996735
80	1	0	-4.197845	-6.060041	2.471338
81	1	0	-7.606426	0.062841	-2.029791
82	1	0	-6.499457	1.195655	-3.849811
83	14	0	-5.411666	-4.061749	-0.110459
84	1	0	-6.724172	-3.925721	0.553131
85	1	0	-5.359747	-5.345443	-0.839131
86	8	0	-5.642888	4.508305	2.039353
87	1	0	-7.759067	4.717088	0.686537
88	1	0	-6.202133	6.559283	0.690553
89	14	0	-5.529494	-3.575742	4.517854
90	8	0	-5.837079	-1.997361	4.602538
91	1	0	-6.676392	-4.269595	3.897595
92	1	0	-5.304387	-4.106661	5.877626
93	14	0	-5.912259	4.338473	3.618669
94	8	0	-5.114991	3.051591	4.160554
95	1	0	-7.359428	4.155692	3.850667
96	1	0	-5.447957	5.545799	4.331632
97	14	0	-5.666475	-0.794520	5.659179
98	8	0	-5.051866	0.499764	4.922916
99	1	0	-6.981879	-0.446590	6.233798
100	1	0	-4.753502	-1.220856	6.739108
101	14	0	-4.707078	2.066410	5.368308
102	1	0	-5.505737	2.396620	6.566069
103	1	0	-3.242407	2.173903	5.525509
104	1	0	-6.105078	4.640522	-3.945901
105	1	0	8.305114	-2.314106	-0.413468

106	1	0	7.374407	-3.765642	3.632819
107	13	0	6.729613	-3.229431	1.304578
108	8	0	5.650582	-1.607698	1.624492
109	8	0	5.439126	-4.341574	0.985526
110	8	0	7.442978	-2.662975	-0.165842
111	8	0	7.591729	-3.307284	2.808475
112	8	0	-3.391898	3.224080	-1.986585
113	13	0	-5.082363	3.579597	-2.015500
114	8	0	-5.618513	4.478969	-0.657272
115	8	0	-5.711813	1.774313	-1.548112
116	8	0	-5.860067	3.794835	-3.548131
117	1	0	5.535844	-1.185371	0.751345
118	1	0	-5.279153	1.478379	-0.726493
119	14	0	5.611720	-0.539997	2.947007
120	14	0	4.009467	-4.829938	0.432617
121	14	0	-6.325269	0.536873	-2.572880
122	14	0	-6.333474	5.096574	0.648136

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2) 32T with Si/Al = 31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.628134	-2.154535	-4.574794
2	14	0	1.808130	0.672008	-4.565812
3	14	0	2.395276	3.482547	-3.664359
4	14	0	5.019414	4.683668	-2.715010
5	14	0	4.828981	4.130780	0.324551
6	14	0	6.427044	2.474972	2.423414
7	14	0	2.570003	-4.180384	-2.215314
8	8	0	2.753416	-0.586916	-4.224430
9	8	0	2.130937	1.895855	-3.572395
10	8	0	3.971749	3.782389	-3.543214
11	8	0	5.246943	4.044747	-1.255828
12	8	0	5.553447	2.960607	1.161877
13	8	0	6.351226	0.844749	2.441228
14	8	0	3.777576	-4.284638	-1.107261
15	8	0	2.964666	-3.025273	-3.261880
16	14	0	1.679934	2.292886	3.485518
17	14	0	2.510348	-0.530496	3.513205
18	14	0	1.964555	-3.407148	2.539915
19	14	0	-0.675451	-4.630467	1.569883
20	14	0	-0.454471	-4.002806	-1.426622
21	14	0	-2.091396	-2.290198	-3.448547
22	14	0	-1.299254	0.635057	-4.020445
23	14	0	-2.022102	3.308491	-2.820010
24	14	0	0.407694	4.902640	-1.590392
25	14	0	1.785345	4.345428	1.109324
26	8	0	1.569605	0.722950	3.140543
27	8	0	2.218011	-1.760856	2.518401
28	8	0	0.387739	-3.705391	2.419290
29	8	0	-0.908871	-3.977844	0.117711
30	8	0	-1.192567	-2.809865	-2.218692
31	8	0	-2.058763	-0.681331	-3.488737
32	8	0	-1.281754	1.825741	-2.897283
33	8	0	-1.040618	4.375699	-2.090378
34	8	0	0.625055	4.496530	-0.048629
35	8	0	1.359004	3.203653	2.158097
36	1	0	3.580173	-2.493317	-5.652002
37	1	0	2.046538	1.097310	-5.960018
38	1	0	1.894522	3.986479	-4.959283
39	1	0	4.479361	6.050861	-2.571286
40	1	0	6.303889	4.735334	-3.442322
41	1	0	5.180487	5.442206	0.906045
42	1	0	7.822276	2.931840	2.261766
43	1	0	6.133270	-1.077966	4.063352
44	1	0	4.137688	-6.137372	0.559177
45	1	0	2.428409	-5.466899	-2.926903
46	1	0	0.698843	2.633391	4.535778
47	1	0	2.237336	-0.949266	4.903034
48	1	0	2.464935	-3.910973	3.835025
49	1	0	-0.139702	-5.997693	1.411158
50	8	0	-2.070993	-4.690310	2.369087
51	1	0	-0.822974	-5.298317	-2.032744
52	8	0	-3.610478	-2.787918	-3.251826

53	1	0	-1.976246	1.138668	-5.232710
54	1	0	-2.331933	3.795911	-4.240050
55	1	0	0.413200	6.374609	-1.712075
56	1	0	1.906474	5.640731	1.808642
57	8	0	1.126476	-2.468325	-5.058020
58	8	0	-1.506523	-2.875424	-4.829099
59	14	0	-0.225675	-3.042561	-5.791477
60	1	0	-0.467978	-2.322557	-7.058131
61	1	0	-0.001336	-4.475515	-6.070482
62	8	0	0.268634	0.238861	-4.391876
63	8	0	1.598885	4.286604	-2.479100
64	8	0	3.199649	3.961148	0.441653
65	8	0	3.167301	2.615336	4.005819
66	8	0	5.810608	3.092235	3.775998
67	14	0	4.508712	3.278609	4.706056
68	1	0	4.725755	2.591219	5.995209
69	1	0	4.273957	4.717236	4.944323
70	8	0	4.067764	-0.134633	3.207346
71	8	0	2.855426	-4.112675	1.366613
72	8	0	1.176106	-3.805333	-1.501101
73	14	0	-5.042742	-2.349022	-2.659928
74	14	0	-3.680289	-4.690338	2.372693
75	8	0	-5.188712	-2.889634	-1.150981
76	8	0	-5.192439	-0.707328	-2.602704
77	1	0	-6.119241	-2.918325	-3.495736
78	8	0	-4.212173	-3.830665	3.627424
79	8	0	-4.226616	-4.044034	1.003992
80	1	0	-4.172558	-6.078051	2.488685
81	1	0	-7.606334	-0.003669	-2.057949
82	1	0	-6.499786	1.128606	-3.878560
83	14	0	-5.389306	-4.101391	-0.108341
84	1	0	-6.705856	-3.972015	0.548535
85	1	0	-5.324409	-5.388157	-0.830525
86	8	0	-5.695363	4.476370	1.998102
87	1	0	-7.806962	4.661575	0.634738
88	1	0	-6.264736	6.516105	0.636552
89	14	0	-5.532225	-3.593973	4.516966
90	8	0	-5.851995	-2.017554	4.592569
91	1	0	-6.671013	-4.299393	3.894814
92	1	0	-5.309461	-4.116627	5.880321
93	14	0	-5.970553	4.312246	3.577019
94	8	0	-5.165565	3.034460	4.128923
95	1	0	-7.417264	4.119104	3.803406
96	1	0	-5.519096	5.526757	4.286017
97	14	0	-5.695294	-0.808387	5.644131
98	8	0	-5.086975	0.486906	4.904427
99	1	0	-7.015914	-0.467569	6.210996
100	1	0	-4.784175	-1.222651	6.730306
101	14	0	-4.755336	2.058569	5.343416
102	1	0	-5.562028	2.388356	6.535900
103	1	0	-3.292294	2.178500	5.506675
104	1	0	-6.131467	4.575893	-3.990064
105	1	0	8.239427	-2.202837	-0.468792
106	1	0	7.265615	-3.724361	3.541477
107	14	0	6.711205	-2.992243	1.312208
108	8	0	5.866987	-1.604656	1.623990
109	8	0	5.559673	-4.101499	0.924359

110	8	0	7.759829	-2.879862	0.050109
111	8	0	7.577035	-3.487160	2.642809
112	8	0	-3.417582	3.188817	-2.015308
113	13	0	-5.109785	3.533027	-2.050418
114	8	0	-5.656768	4.432694	-0.696828
115	8	0	-5.727090	1.724585	-1.575891
116	8	0	-5.888216	3.733142	-3.584997
117	1	0	-5.294773	1.436851	-0.751200
118	14	0	5.605340	-0.536120	2.840766
119	14	0	4.103106	-4.677820	0.451988
120	14	0	-6.326372	0.478319	-2.597148
121	14	0	-6.383963	5.052168	0.600931

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COMPLEXES :

1) 32T with Si/Al = 15

1.1) 44BPYH+/32T- open

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.697236	-2.277048	-4.501656
2	14	0	1.875418	0.548454	-4.556358
3	14	0	2.451428	3.376527	-3.703889
4	14	0	5.064814	4.598109	-2.750998
5	14	0	4.843160	4.104474	0.296636
6	14	0	6.420381	2.491255	2.443875
7	14	0	2.615852	-4.256517	-2.103810
8	8	0	2.817892	-0.702789	-4.180682
9	8	0	2.187122	1.791721	-3.583728
10	8	0	4.026372	3.679966	-3.572275
11	8	0	5.277572	3.987971	-1.277340
12	8	0	5.559629	2.951459	1.164106
13	8	0	6.350838	0.858464	2.499763
14	8	0	3.756119	-4.421390	-0.949289
15	8	0	3.020646	-3.121722	-3.168575
16	14	0	1.662549	2.324309	3.459475
17	14	0	2.495259	-0.497068	3.550398
18	14	0	1.962403	-3.392590	2.627185
19	14	0	-0.666119	-4.637411	1.653329
20	14	0	-0.414245	-4.067453	-1.352255
21	14	0	-2.031434	-2.396057	-3.423938
22	14	0	-1.236067	0.518512	-4.043899
23	14	0	-1.974909	3.232656	-2.904191
24	14	0	0.441673	4.852202	-1.681742
25	14	0	1.787826	4.353421	1.045155
26	8	0	1.557317	0.747883	3.143752
27	8	0	2.214542	-1.746737	2.576537
28	8	0	0.387222	-3.694900	2.495812
29	8	0	-0.884879	-4.013208	0.186456
30	8	0	-1.145096	-2.890862	-2.174913
31	8	0	-1.999890	-0.788229	-3.494848
32	8	0	-1.207934	1.744673	-2.951220
33	8	0	-0.987246	4.286519	-2.152327
34	8	0	0.641027	4.479714	-0.129095
35	8	0	1.348677	3.234977	2.113599
36	1	0	3.660627	-2.636001	-5.562108
37	1	0	2.128029	0.946664	-5.956053
38	1	0	1.963835	3.854692	-5.013523
39	1	0	4.522447	5.967400	-2.639600
40	1	0	6.356744	4.636631	-3.465814
41	1	0	5.187792	5.427284	0.856040
42	1	0	7.816930	2.946042	2.287829
43	1	0	6.124137	-1.026146	4.164838
44	1	0	3.957803	-6.302932	0.711567
45	1	0	2.482458	-5.556790	-2.791578
46	1	0	0.670165	2.683906	4.492622
47	1	0	2.208058	-0.889235	4.945120
48	1	0	2.449616	-3.870746	3.936964
49	1	0	-0.127456	-6.006838	1.526673

50	8	0	-2.069924	-4.683392	2.438864
51	1	0	-0.775145	-5.374839	-1.937083
52	8	0	-3.552033	-2.891619	-3.233599
53	1	0	-1.900755	0.997855	-5.272699
54	1	0	-2.268055	3.689125	-4.337993
55	1	0	0.449571	6.321165	-1.835412
56	1	0	1.901791	5.663621	1.717402
57	8	0	1.200874	-2.601446	-4.994220
58	8	0	-1.431526	-3.007155	-4.786714
59	14	0	-0.140469	-3.191373	-5.732183
60	1	0	-0.370110	-2.496224	-7.014977
61	1	0	0.088137	-4.629189	-5.981093
62	8	0	0.334468	0.117516	-4.389980
63	8	0	1.642582	4.216419	-2.543041
64	8	0	3.209451	3.954065	0.402342
65	8	0	3.144072	2.658426	3.989011
66	8	0	5.789535	3.134276	3.777684
67	14	0	4.477925	3.337671	4.690365
68	1	0	4.681998	2.675747	5.994873
69	1	0	4.239790	4.780476	4.898053
70	8	0	4.036504	-0.018167	3.337267
71	8	0	2.766547	-4.163873	1.447875
72	8	0	1.214373	-3.868756	-1.411561
73	14	0	-4.990856	-2.443017	-2.665357
74	14	0	-3.679168	-4.685180	2.425597
75	8	0	-5.152182	-2.954563	-1.147864
76	8	0	-5.121764	-0.819941	-2.621834
77	1	0	-6.057971	-3.029572	-3.501269
78	8	0	-4.225007	-3.802032	3.657829
79	8	0	-4.211691	-4.066061	1.039006
80	1	0	-4.171326	-6.070954	2.563221
81	1	0	-7.535773	-0.086454	-2.118504
82	1	0	-6.389475	1.021373	-3.929537
83	14	0	-5.362582	-4.146222	-0.084135
84	1	0	-6.686079	-4.005673	0.556279
85	1	0	-5.288900	-5.446630	-0.780583
86	8	0	-5.687660	4.475075	1.826274
87	1	0	-7.783889	4.630053	0.435694
88	1	0	-6.245728	6.487895	0.420681
89	14	0	-5.554553	-3.549704	4.528739
90	8	0	-5.876573	-1.972483	4.570500
91	1	0	-6.686085	-4.268304	3.908434
92	1	0	-5.345639	-4.045663	5.904206
93	14	0	-5.980578	4.339607	3.404720
94	8	0	-5.179263	3.074152	3.989408
95	1	0	-7.429375	4.147314	3.618123
96	1	0	-5.539855	5.568100	4.096165
97	14	0	-5.732056	-0.743054	5.600083
98	8	0	-5.117209	0.538398	4.841900
99	1	0	-7.058873	-0.392851	6.146382
100	1	0	-4.832016	-1.135226	6.703559
101	14	0	-4.780922	2.121907	5.226419
102	1	0	-5.601931	2.471867	6.403279
103	1	0	-3.320105	2.248255	5.404126
104	1	0	-5.981767	4.463624	-4.058239
105	1	0	8.280893	-2.249180	-0.317815
106	1	0	7.272419	-3.679304	3.717438

107	13	0	6.684150	-3.107900	1.396205
108	8	0	5.545429	-1.509668	1.634659
109	8	0	5.446138	-4.308804	1.170350
110	8	0	7.515452	-2.782095	-0.076874
111	8	0	7.432175	-3.081911	2.969801
112	8	0	-3.352526	3.132761	-2.091603
113	13	0	-5.121058	3.269294	-2.122793
114	8	0	-5.554972	4.385214	-0.849332
115	8	0	-5.650243	1.620391	-1.577471
116	8	0	-5.777636	3.588306	-3.708363
117	1	0	5.072012	-1.151721	0.837728
118	1	0	-4.521713	1.338097	-0.106739
119	14	0	5.553818	-0.462675	2.973330
120	14	0	4.042238	-4.844863	0.619412
121	14	0	-6.228872	0.461131	-2.579931
122	14	0	-6.354814	5.016551	0.389134
123	6	0	-0.843569	0.515615	0.094765
124	6	0	0.596917	0.221768	-0.119087
125	6	0	-1.813219	-0.493752	-0.057056
126	6	0	1.538509	1.213564	-0.433368
127	6	0	-1.306306	1.801255	0.427271
128	6	0	1.090698	-1.077833	-0.027915
129	6	0	-3.154896	-0.176182	-0.039232
130	6	0	2.891133	0.890527	-0.501779
131	6	0	-2.664338	2.074653	0.432680
132	6	0	2.458263	-1.309750	-0.147099
133	7	0	-3.549777	1.094517	0.168090
134	7	0	3.372633	-0.350488	-0.315451
135	1	0	-1.539519	-1.514074	-0.274247
136	1	0	1.226695	2.225289	-0.633705
137	1	0	-0.622114	2.614061	0.621068
138	1	0	0.445321	-1.905156	0.222180
139	1	0	-3.936090	-0.896084	-0.243311
140	1	0	3.624258	1.658067	-0.712844
141	1	0	-3.073059	3.063728	0.594671
142	1	0	2.838686	-2.312124	-0.039916

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1.2) 44BPYH<sup>+</sup>/32T<sup>-</sup> closed

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.728553	-2.284843	-4.485275
2	14	0	1.907857	0.540791	-4.549183
3	14	0	2.481337	3.370464	-3.700324
4	14	0	5.091265	4.593230	-2.739506
5	14	0	4.857225	4.106040	0.308240
6	14	0	6.425303	2.496831	2.465161
7	14	0	2.636918	-4.259266	-2.083641
8	8	0	2.848419	-0.709954	-4.167112
9	8	0	2.216049	1.785994	-3.577912
10	8	0	4.055837	3.673691	-3.563023
11	8	0	5.297913	3.986111	-1.263733
12	8	0	5.569840	2.954622	1.180987
13	8	0	6.350839	0.880438	2.515548
14	8	0	3.757783	-4.401223	-0.924413
15	8	0	3.046343	-3.126826	-3.149143
16	14	0	1.663326	2.331928	3.461484
17	14	0	2.495565	-0.489290	3.561196
18	14	0	1.966423	-3.386550	2.641302
19	14	0	-0.658108	-4.633157	1.659003
20	14	0	-0.393847	-4.068918	-1.346597
21	14	0	-2.002443	-2.401425	-3.428092
22	14	0	-1.204439	0.511942	-4.050312
23	14	0	-1.946693	3.225262	-2.926517
24	14	0	0.463826	4.847593	-1.695818
25	14	0	1.793936	4.357511	1.040512
26	8	0	1.559345	0.754908	3.148327
27	8	0	2.218819	-1.740802	2.588564
28	8	0	0.391786	-3.689072	2.504021
29	8	0	-0.870808	-4.011738	0.190058
30	8	0	-1.121268	-2.893876	-2.174491
31	8	0	-1.970557	-0.793735	-3.501927
32	8	0	-1.194919	1.736370	-2.955458
33	8	0	-0.966602	4.279287	-2.174512
34	8	0	0.653999	4.480404	-0.140759
35	8	0	1.347937	3.243071	2.110302
36	1	0	3.696079	-2.646311	-5.541099
37	1	0	2.166211	0.935994	-5.948682
38	1	0	1.999156	3.846038	-5.012901
39	1	0	4.548889	5.962918	-2.633149
40	1	0	6.386066	4.629858	-3.449209
41	1	0	5.200027	5.429911	0.866255
42	1	0	7.822611	2.950859	2.313771
43	1	0	6.109996	-1.008128	4.174142
44	1	0	3.967948	-6.272131	0.747368
45	1	0	2.505874	-5.560934	-2.769220
46	1	0	0.666709	2.693512	4.489852
47	1	0	2.202614	-0.878799	4.955467
48	1	0	2.448225	-3.862227	3.953981
49	1	0	-0.118972	-6.002835	1.537168
50	8	0	-2.065135	-4.677612	2.438838
51	1	0	-0.752377	-5.377405	-1.930419
52	8	0	-3.523828	-2.896589	-3.243072

53	1	0	-1.864048	0.988964	-5.282746
54	1	0	-2.231289	3.676903	-4.363568
55	1	0	0.473534	6.316006	-1.854560
56	1	0	1.904852	5.669980	1.708833
57	8	0	1.234078	-2.609809	-4.983162
58	8	0	-1.396950	-3.015126	-4.787224
59	14	0	-0.102017	-3.201172	-5.727018
60	1	0	-0.326354	-2.508456	-7.012066
61	1	0	0.127565	-4.639463	-5.972252
62	8	0	0.366115	0.110678	-4.388091
63	8	0	1.669275	4.208076	-2.547961
64	8	0	3.218988	3.955049	0.407298
65	8	0	3.142667	2.667016	3.996478
66	8	0	5.789312	3.142836	3.795080
67	14	0	4.474114	3.348544	4.702061
68	1	0	4.672740	2.689287	6.008758
69	1	0	4.235605	4.791854	4.905774
70	8	0	4.028021	-0.004434	3.333320
71	8	0	2.752691	-4.129463	1.432347
72	8	0	1.232795	-3.869626	-1.397837
73	14	0	-4.964963	-2.446873	-2.681610
74	14	0	-3.674311	-4.679387	2.418951
75	8	0	-5.132550	-2.955530	-1.163825
76	8	0	-5.108942	-0.810315	-2.643547
77	1	0	-6.028647	-3.034990	-3.520792
78	8	0	-4.225190	-3.793886	3.647246
79	8	0	-4.201103	-4.062891	1.029006
80	1	0	-4.167076	-6.064885	2.557182
81	1	0	-7.529631	-0.092587	-2.149670
82	1	0	-6.386048	1.017468	-3.961055
83	14	0	-5.347364	-4.145160	-0.098709
84	1	0	-6.673481	-4.003363	0.535985
85	1	0	-5.270857	-5.446891	-0.792374
86	8	0	-5.699045	4.473766	1.820410
87	1	0	-7.791788	4.620530	0.423699
88	1	0	-6.258642	6.482521	0.409617
89	14	0	-5.558302	-3.539871	4.512195
90	8	0	-5.880440	-1.962566	4.549633
91	1	0	-6.687293	-4.259623	3.888604
92	1	0	-5.355066	-4.033220	5.889450
93	14	0	-5.996012	4.340351	3.398274
94	8	0	-5.192902	3.078139	3.987491
95	1	0	-7.444873	4.144502	3.607976
96	1	0	-5.560564	5.571285	4.088719
97	14	0	-5.740124	-0.731186	5.577463
98	8	0	-5.122121	0.548808	4.819383
99	1	0	-7.069168	-0.379914	6.117629
100	1	0	-4.844646	-1.121281	6.685378
101	14	0	-4.795440	2.129215	5.227334
102	1	0	-5.620688	2.479064	6.401260
103	1	0	-3.335475	2.259858	5.408893
104	1	0	-6.002760	4.462123	-4.100054
105	1	0	8.283941	-2.225594	-0.301719
106	1	0	7.251594	-3.663809	3.724613
107	13	0	6.648559	-2.970413	1.433488
108	8	0	5.548287	-1.529010	1.674597
109	8	0	5.471075	-4.284803	1.189744

110	8	0	7.506284	-2.753941	-0.081863
111	8	0	7.568198	-3.219228	2.920106
112	8	0	-3.352335	3.150095	-2.154118
113	13	0	-5.074344	3.390450	-2.163089
114	8	0	-5.586448	4.383247	-0.856602
115	8	0	-5.608004	1.618835	-1.625425
116	8	0	-5.830154	3.594096	-3.711137
117	1	0	4.234653	-0.467771	-0.300415
118	1	0	-5.037393	1.335027	-0.818078
119	14	0	5.561014	-0.514141	2.921066
120	14	0	4.079618	-4.813827	0.655807
121	14	0	-6.230487	0.402303	-2.648152
122	14	0	-6.369740	5.016902	0.400590
123	6	0	-0.939857	0.450325	0.152267
124	6	0	0.506079	0.189760	-0.076044
125	6	0	-1.883795	-0.583331	0.053809
126	6	0	1.402325	1.212532	-0.444558
127	6	0	-1.435111	1.730547	0.441374
128	6	0	1.042603	-1.093769	0.049320
129	6	0	-3.238893	-0.278357	0.092828
130	6	0	2.754225	0.962292	-0.551699
131	6	0	-2.813532	1.943080	0.467135
132	6	0	2.402681	-1.311226	-0.081442
133	7	0	-3.711326	0.970379	0.234129
134	7	0	3.227434	-0.285758	-0.341108
135	1	0	-1.594872	-1.608977	-0.119762
136	1	0	1.045375	2.208943	-0.643522
137	1	0	-0.775760	2.572842	0.606982
138	1	0	0.425484	-1.928493	0.338497
139	1	0	-3.976018	-1.062417	-0.039166
140	1	0	3.481051	1.721637	-0.794739
141	1	0	-3.213548	2.937972	0.631927
142	1	0	2.867621	-2.270902	0.071297

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1.3) 44BPYH<sub>2</sub><sup>2+</sup>/32T<sup>2-</sup>

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.702106	-2.293957	-4.483684
2	14	0	1.890946	0.534475	-4.545553
3	14	0	2.474761	3.361785	-3.695867
4	14	0	5.089657	4.575237	-2.736751
5	14	0	4.856616	4.087407	0.310969
6	14	0	6.421101	2.471871	2.465769
7	14	0	2.605861	-4.269190	-2.082897
8	8	0	2.827591	-0.719634	-4.164887
9	8	0	2.204205	1.778167	-3.573967
10	8	0	4.050399	3.659605	-3.559797
11	8	0	5.295528	3.966724	-1.261443
12	8	0	5.566080	2.933166	1.182556
13	8	0	6.336800	0.855260	2.509568
14	8	0	3.726595	-4.416809	-0.922770
15	8	0	3.018199	-3.137643	-3.148224
16	14	0	1.659486	2.323309	3.466382
17	14	0	2.481898	-0.500854	3.564238
18	14	0	1.941738	-3.395877	2.643705
19	14	0	-0.688052	-4.632872	1.663322
20	14	0	-0.424555	-4.068389	-1.342299
21	14	0	-2.029182	-2.394440	-3.421674
22	14	0	-1.221514	0.516348	-4.043494
23	14	0	-1.953858	3.229077	-2.915676
24	14	0	0.463128	4.842670	-1.686174
25	14	0	1.795534	4.345079	1.047683
26	8	0	1.549678	0.746787	3.152709
27	8	0	2.199868	-1.751005	2.591375
28	8	0	0.365923	-3.692811	2.507747
29	8	0	-0.899909	-4.010134	0.194814
30	8	0	-1.148598	-2.890474	-2.169072
31	8	0	-1.991714	-0.786844	-3.494915
32	8	0	-1.183515	1.739180	-2.946633
33	8	0	-0.962746	4.275690	-2.160585
34	8	0	0.654347	4.472884	-0.131859
35	8	0	1.347712	3.230559	2.116628
36	1	0	3.667481	-2.658207	-5.540519
37	1	0	2.149422	0.929459	-5.945091
38	1	0	1.993056	3.839612	-5.007801
39	1	0	4.552025	5.946707	-2.629280
40	1	0	6.383958	4.607808	-3.447564
41	1	0	5.204394	5.409844	0.869306
42	1	0	7.819809	2.921227	2.313375
43	1	0	6.085347	-1.038611	4.160522
44	1	0	3.929129	-6.290329	0.747025
45	1	0	2.469805	-5.570083	-2.768970
46	1	0	0.665085	2.687990	4.495802
47	1	0	2.188852	-0.889877	4.958625
48	1	0	2.423065	-3.873758	3.955758
49	1	0	-0.153844	-6.004387	1.540463
50	8	0	-2.094515	-4.672687	2.444427
51	1	0	-0.788214	-5.375379	-1.926300
52	8	0	-3.552128	-2.884328	-3.235456

53	1	0	-1.880568	0.996167	-5.275139
54	1	0	-2.239089	3.683437	-4.351743
55	1	0	0.476956	6.311254	-1.843012
56	1	0	1.911242	5.656338	1.717564
57	8	0	1.206104	-2.613616	-4.980421
58	8	0	-1.427090	-3.009733	-4.781597
59	14	0	-0.133678	-3.199959	-5.722648
60	1	0	-0.356753	-2.505957	-7.007221
61	1	0	0.090626	-4.638952	-5.968649
62	8	0	0.347894	0.109519	-4.383319
63	8	0	1.665513	4.200714	-2.540808
64	8	0	3.218522	3.939241	0.411985
65	8	0	3.140482	2.652989	4.000153
66	8	0	5.788462	3.119401	3.796544
67	14	0	4.474759	3.329142	4.704767
68	1	0	4.672283	2.668600	6.010981
69	1	0	4.241325	4.773157	4.909364
70	8	0	4.011838	-0.015895	3.328794
71	8	0	2.725133	-4.139429	1.433566
72	8	0	1.203665	-3.875112	-1.395686
73	14	0	-4.991161	-2.429771	-2.672502
74	14	0	-3.703705	-4.668801	2.426011
75	8	0	-5.159147	-2.938430	-1.154761
76	8	0	-5.114576	-0.805275	-2.630205
77	1	0	-6.057670	-3.013819	-3.510939
78	8	0	-4.250346	-3.781850	3.655152
79	8	0	-4.229595	-4.049915	1.036787
80	1	0	-4.201208	-6.052613	2.564154
81	1	0	-7.526876	-0.060088	-2.135951
82	1	0	-6.368798	1.041390	-3.943358
83	14	0	-5.377168	-4.127715	-0.089910
84	1	0	-6.702198	-3.981507	0.546050
85	1	0	-5.305869	-5.429435	-0.784151
86	8	0	-5.679255	4.493922	1.804206
87	1	0	-7.771027	4.651381	0.407206
88	1	0	-6.227675	6.504915	0.392214
89	14	0	-5.581767	-3.523492	4.521418
90	8	0	-5.898327	-1.945080	4.559762
91	1	0	-6.713849	-4.239028	3.898581
92	1	0	-5.379009	-4.018090	5.898295
93	14	0	-5.977100	4.363040	3.382117
94	8	0	-5.180991	3.096772	3.972132
95	1	0	-7.427034	4.175272	3.591788
96	1	0	-5.534963	5.591958	4.071904
97	14	0	-5.752746	-0.714602	5.587942
98	8	0	-5.130943	0.563510	4.829793
99	1	0	-7.080054	-0.358874	6.129459
100	1	0	-4.857633	-1.108274	6.694886
101	14	0	-4.788865	2.146387	5.212555
102	1	0	-5.612290	2.501433	6.386200
103	1	0	-3.328222	2.269113	5.394183
104	1	0	-5.944285	4.481603	-4.072228
105	1	0	8.249465	-2.250864	-0.321511
106	1	0	7.210520	-3.699318	3.699449
107	13	0	6.610317	-2.982628	1.417919
108	8	0	5.507158	-1.534405	1.649239
109	8	0	5.438099	-4.301885	1.187157



110	8	0	7.454024	-2.751455	-0.101077
111	8	0	7.516894	-3.215584	2.913407
112	8	0	-3.327428	3.127521	-2.097044
113	13	0	-5.097336	3.284906	-2.136893
114	8	0	-5.534748	4.399137	-0.867830
115	8	0	-5.623090	1.632349	-1.589176
116	8	0	-5.723881	3.606126	-3.732055
117	1	0	4.334519	-0.554256	-0.190518
118	1	0	-4.493337	1.319853	-0.189209
119	14	0	5.540283	-0.533995	2.911381
120	14	0	4.046756	-4.834030	0.654908
121	14	0	-6.216613	0.478889	-2.594234
122	14	0	-6.341294	5.035150	0.366608
123	6	0	-0.823765	0.492394	0.095794
124	6	0	0.622813	0.197202	-0.105155
125	6	0	-1.785535	-0.519674	-0.064937
126	6	0	1.548982	1.198039	-0.456561
127	6	0	-1.283748	1.780770	0.412790
128	6	0	1.117192	-1.099149	0.034238
129	6	0	-3.128874	-0.198369	-0.074380
130	6	0	2.898280	0.912634	-0.524093
131	6	0	-2.644110	2.054629	0.393061
132	6	0	2.477081	-1.348625	-0.057950
133	7	0	-3.522726	1.074203	0.112017
134	7	0	3.332634	-0.344729	-0.289879
135	1	0	-1.512056	-1.542726	-0.269260
136	1	0	1.222710	2.199940	-0.680674
137	1	0	-0.602984	2.594084	0.619211
138	1	0	0.474395	-1.919982	0.308175
139	1	0	-3.907334	-0.919432	-0.285436
140	1	0	3.651008	1.650890	-0.753907
141	1	0	-3.054443	3.044446	0.546101
142	1	0	2.912220	-2.319531	0.107543

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1.4) PYH<sup>+</sup>/32T<sup>+</sup> open

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-2.787131	-2.325315	4.541662
2	14	0	-1.964261	0.499288	4.621278
3	14	0	-2.543011	3.335923	3.799671
4	14	0	-5.160014	4.567669	2.870072
5	14	0	-4.951293	4.104604	-0.183268
6	14	0	-6.537984	2.513424	-2.339954
7	14	0	-2.716390	-4.280628	2.123743
8	8	0	-2.908670	-0.747882	4.237019
9	8	0	-2.279677	1.752337	3.662496
10	8	0	-4.118405	3.641065	3.677723
11	8	0	-5.379132	3.972412	1.391269
12	8	0	-5.671734	2.960537	-1.059254
13	8	0	-6.490068	0.872079	-2.443035
14	8	0	-3.876540	-4.414653	0.979871
15	8	0	-3.116380	-3.156480	3.201537
16	14	0	-1.784490	2.355107	-3.377023
17	14	0	-2.618596	-0.464952	-3.492658
18	14	0	-2.082945	-3.369728	-2.600657
19	14	0	0.549163	-4.625065	-1.650269
20	14	0	0.310034	-4.085092	1.361886
21	14	0	1.936457	-2.435004	3.443398
22	14	0	1.144740	0.473479	4.095767
23	14	0	1.880109	3.174948	2.978616
24	14	0	-0.538157	4.809084	1.779129
25	14	0	-1.898952	4.332446	-0.944459
26	8	0	-1.678514	0.775571	-3.077510
27	8	0	-2.334273	-1.724382	-2.532513
28	8	0	-0.507339	-3.673842	-2.478888
29	8	0	0.774266	-4.015623	-0.178158
30	8	0	1.044737	-2.917016	2.193202
31	8	0	1.905792	-0.827955	3.530503
32	8	0	1.114230	1.694431	3.004154
33	8	0	0.895940	4.259064	2.264697
34	8	0	-0.746089	4.447732	0.224975
35	8	0	-1.467985	3.220190	-2.022651
36	1	0	-3.746171	-2.694655	5.602493
37	1	0	-2.210881	0.883488	6.025948
38	1	0	-2.049788	3.800792	5.111980
39	1	0	-4.617716	5.937873	2.770151
40	1	0	-6.448922	4.599338	3.590656
41	1	0	-5.297880	5.433051	-0.727911
42	1	0	-7.933731	2.966972	-2.173488
43	1	0	-6.298378	-0.967381	-4.162124
44	1	0	-4.119897	-6.265267	-0.709898
45	1	0	-2.580494	-5.587775	2.797857
46	1	0	-0.796293	2.724693	-4.410658
47	1	0	-2.337356	-0.843254	-4.892416
48	1	0	-2.575790	-3.834614	-3.913103
49	1	0	0.010537	-5.995516	-1.535056
50	8	0	1.949663	-4.663644	-2.442077
51	1	0	0.672895	-5.398373	1.932108
52	8	0	3.456068	-2.929128	3.241772

53	1	0	1.814721	0.940304	5.326511
54	1	0	2.181472	3.620846	4.414040
55	1	0	-0.541435	6.276979	1.942849
56	1	0	-2.012757	5.647500	-1.607187
57	8	0	-1.288812	-2.655019	5.024658
58	8	0	1.342015	-3.059498	4.802493
59	14	0	0.054846	-3.252742	5.751454
60	1	0	0.290087	-2.570521	7.040161
61	1	0	-0.173242	-4.692899	5.986935
62	8	0	-0.424149	0.069655	4.444114
63	8	0	-1.736504	4.170554	2.641962
64	8	0	-3.318459	3.932404	-0.297407
65	8	0	-3.268086	2.694976	-3.897005
66	8	0	-5.912550	3.169646	-3.669877
67	14	0	-4.604721	3.381864	-4.585969
68	1	0	-4.814460	2.733123	-5.896188
69	1	0	-4.367035	4.826622	-4.780159
70	8	0	-4.173374	-0.002443	-3.322315
71	8	0	-2.918807	-4.136212	-1.443107
72	8	0	-1.317714	-3.886289	1.429545
73	14	0	4.892672	-2.475331	2.672040
74	14	0	3.558948	-4.666081	-2.435546
75	8	0	5.047481	-2.971738	1.148850
76	8	0	5.026966	-0.851215	2.661421
77	1	0	5.963050	-3.070554	3.497588
78	8	0	4.099964	-3.770838	-3.661159
79	8	0	4.097474	-4.061022	-1.045072
80	1	0	4.050025	-6.050569	-2.589064
81	1	0	7.438899	-0.112435	2.155882
82	1	0	6.308267	0.959743	3.997953
83	14	0	5.253010	-4.152774	0.072398
84	1	0	6.573875	-4.006256	-0.572099
85	1	0	5.181761	-5.460053	0.756118
86	8	0	5.569661	4.484951	-1.741592
87	1	0	7.669695	4.629452	-0.355630
88	1	0	6.125881	6.482175	-0.313203
89	14	0	5.425958	-3.510246	-4.535046
90	8	0	5.748372	-1.932790	-4.562389
91	1	0	6.559805	-4.235373	-3.926681
92	1	0	5.211128	-3.992366	-5.914516
93	14	0	5.858113	4.369692	-3.322464
94	8	0	5.058889	3.108987	-3.920131
95	1	0	7.306827	4.184532	-3.542626
96	1	0	5.411477	5.605164	-3.997485
97	14	0	5.600009	-0.693086	-5.579023
98	8	0	4.988795	0.580923	-4.805512
99	1	0	6.924664	-0.337867	-6.127328
100	1	0	4.695233	-1.073921	-6.682596
101	14	0	4.659655	2.170692	-5.167471
102	1	0	5.475940	2.537559	-6.342467
103	1	0	3.197914	2.294653	-5.339157
104	1	0	5.909233	4.399403	4.201401
105	1	0	-8.443916	-2.288742	0.297950
106	1	0	-7.478885	-3.616957	-3.782504
107	13	0	-6.840442	-3.112219	-1.454274
108	8	0	-5.733426	-1.500998	-1.668147
109	8	0	-5.606605	-4.282324	-1.125619

110	8	0	-7.554733	-2.359124	-0.062091
111	8	0	-7.702683	-3.169557	-2.955325
112	8	0	3.257619	3.082145	2.157047
113	13	0	5.014428	3.257155	2.222773
114	8	0	5.457593	4.358308	0.938172
115	8	0	5.549054	1.601056	1.679401
116	8	0	5.689035	3.549227	3.803369
117	1	0	-5.951566	-1.065976	-0.814922
118	1	0	4.457882	1.206791	0.517663
119	14	0	-5.696397	-0.422701	-2.977649
120	14	0	-4.178688	-4.804056	-0.592337
121	14	0	6.139889	0.419037	2.648928
122	14	0	6.241987	5.011641	-0.297999
123	6	0	1.423083	0.544706	-1.649913
124	6	0	2.051969	-0.512062	-0.985871
125	6	0	1.947679	1.836271	-1.554195
126	6	0	3.179220	-0.243966	-0.226961
127	6	0	3.077864	2.051429	-0.778552
128	7	0	3.651976	1.013146	-0.143285
129	1	0	1.666298	-1.523566	-1.032165
130	1	0	1.474932	2.677063	-2.048327
131	1	0	3.720856	-0.994904	0.332586
132	1	0	3.538245	3.020534	-0.630519
133	1	0	0.521360	0.362703	-2.224717

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1.5) PYH<sup>+</sup>/32T<sup>+</sup> closed

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.525433	-2.101717	-4.566195
2	14	0	1.719952	0.728683	-4.522864
3	14	0	2.316079	3.523336	-3.578920
4	14	0	4.940544	4.697428	-2.597216
5	14	0	4.728777	4.103448	0.433168
6	14	0	6.305510	2.410357	2.518376
7	14	0	2.442509	-4.159752	-2.235487
8	8	0	2.656649	-0.539785	-4.193337
9	8	0	2.043003	1.936935	-3.510617
10	8	0	3.893311	3.813204	-3.444148
11	8	0	5.155899	4.037155	-1.145711
12	8	0	5.442112	2.918000	1.258482
13	8	0	6.244984	0.784415	2.546105
14	8	0	3.579635	-4.352933	-1.091029
15	8	0	2.849476	-2.992323	-3.263509
16	14	0	1.551123	2.237708	3.549046
17	14	0	2.367164	-0.589989	3.542295
18	14	0	1.812911	-3.449960	2.525596
19	14	0	-0.827201	-4.646140	1.522567
20	14	0	-0.584688	-3.977869	-1.463473
21	14	0	-2.200562	-2.228889	-3.471147
22	14	0	-1.390259	0.699977	-3.997288
23	14	0	-2.107639	3.363481	-2.767648
24	14	0	0.321730	4.928279	-1.500071
25	14	0	1.676238	4.329222	1.202393
26	8	0	1.435033	0.673323	3.181497
27	8	0	2.074763	-1.804847	2.528637
28	8	0	0.235388	-3.738440	2.391253
29	8	0	-1.048431	-3.972140	0.078273
30	8	0	-1.311917	-2.770241	-2.243247
31	8	0	-2.159613	-0.619805	-3.488640
32	8	0	-1.354223	1.877536	-2.853421
33	8	0	-1.118972	4.406473	-2.015581
34	8	0	0.525416	4.501463	0.037961
35	8	0	1.235838	3.176674	2.233423
36	1	0	3.482254	-2.430510	-5.642261
37	1	0	1.969023	1.172018	-5.909568
38	1	0	1.825810	4.047798	-4.869697
39	1	0	4.406675	6.065305	-2.437756
40	1	0	6.229670	4.752448	-3.316002
41	1	0	5.083490	5.404824	1.034937
42	1	0	7.704031	2.862122	2.371489
43	1	0	6.038116	-1.130013	4.179444
44	1	0	3.792430	-6.283654	0.510955
45	1	0	2.298623	-5.435520	-2.965721
46	1	0	0.565336	2.568531	4.598002
47	1	0	2.083540	-1.026700	4.924456
48	1	0	2.302800	-3.974345	3.816549
49	1	0	-0.297360	-6.013738	1.347999
50	8	0	-2.227901	-4.709990	2.312382
51	1	0	-0.955960	-5.262898	-2.089880
52	8	0	-3.723301	-2.721549	-3.290636

53	1	0	-2.057266	1.223896	-5.206478
54	1	0	-2.404231	3.870572	-4.183622
55	1	0	0.336251	6.401617	-1.602998
56	1	0	1.799326	5.614874	1.918967
57	8	0	1.025146	-2.400912	-5.062757
58	8	0	-1.610161	-2.797775	-4.856169
59	14	0	-0.324276	-2.958000	-5.812989
60	1	0	-0.555174	-2.219163	-7.070898
61	1	0	-0.105416	-4.388047	-6.110636
62	8	0	0.177216	0.301232	-4.364222
63	8	0	1.516059	4.316870	-2.387761
64	8	0	3.093313	3.945498	0.540301
65	8	0	3.036877	2.545265	4.082803
66	8	0	5.684034	3.012016	3.875676
67	14	0	4.377474	3.192271	4.800385
68	1	0	4.583133	2.485946	6.081142
69	1	0	4.148664	4.628662	5.057202
70	8	0	3.922405	-0.142464	3.336054
71	8	0	2.603943	-4.159564	1.295426
72	8	0	1.046238	-3.787354	-1.524532
73	14	0	-5.156957	-2.283655	-2.701370
74	14	0	-3.837168	-4.701854	2.306234
75	8	0	-5.314906	-2.844508	-1.201042
76	8	0	-5.301299	-0.641398	-2.620275
77	1	0	-6.231142	-2.835740	-3.551581
78	8	0	-4.372415	-3.857043	3.569600
79	8	0	-4.371841	-4.033760	0.943406
80	1	0	-4.337094	-6.088519	2.399847
81	1	0	-7.716060	0.062740	-2.079996
82	1	0	-6.594110	1.218278	-3.876404
83	14	0	-5.527966	-4.069680	-0.176642
84	1	0	-6.847852	-3.942747	0.473987
85	1	0	-5.465103	-5.346578	-0.916310
86	8	0	-5.806578	4.477902	2.045089
87	1	0	-7.909219	4.689725	0.671791
88	1	0	-6.360451	6.538428	0.708661
89	14	0	-5.696694	-3.626037	4.454342
90	8	0	-6.009004	-2.049213	4.550014
91	1	0	-6.835173	-4.316895	3.815509
92	1	0	-5.484924	-4.168763	5.811593
93	14	0	-6.091904	4.292859	3.619888
94	8	0	-5.294826	3.004605	4.158783
95	1	0	-7.540636	4.101853	3.834879
96	1	0	-5.640433	5.495748	4.348421
97	14	0	-5.852686	-0.855636	5.619295
98	8	0	-5.233347	0.446716	4.901454
99	1	0	-7.175027	-0.516014	6.182855
100	1	0	-4.950340	-1.289646	6.705084
101	14	0	-4.895441	2.010451	5.362026
102	1	0	-5.708166	2.326580	6.554112
103	1	0	-3.432998	2.122772	5.535725
104	1	0	-6.212891	4.665492	-3.933609
105	1	0	8.173741	-2.263635	-0.336705
106	1	0	7.197249	-3.768944	3.679021
107	13	0	6.563663	-3.106419	1.375249
108	8	0	5.495667	-1.645459	1.707981
109	8	0	5.308855	-4.313802	1.017308

110	8	0	7.389055	-2.788317	-0.136214
111	8	0	7.506444	-3.438077	2.820435
112	8	0	-3.501965	3.225951	-1.970219
113	13	0	-5.194454	3.586738	-2.008931
114	8	0	-5.747224	4.464244	-0.644208
115	8	0	-5.856414	1.788502	-1.564303
116	8	0	-5.924828	3.822689	-3.559953
117	1	0	4.441228	-1.347571	0.394488
118	1	0	-5.560699	1.522717	-0.675152
119	14	0	5.465624	-0.613501	2.952371
120	14	0	3.909887	-4.823543	0.471319
121	14	0	-6.432823	0.546294	-2.604683
122	14	0	-6.484946	5.076070	0.653916
123	7	0	3.673801	-0.824634	-0.099857
124	6	0	2.454994	-1.370580	-0.223026
125	6	0	3.910824	0.468810	-0.389522
126	6	0	1.372753	-0.599482	-0.617253
127	6	0	2.868812	1.272612	-0.800773
128	6	0	1.576479	0.747542	-0.883164
129	1	0	2.376407	-2.413667	0.021603
130	1	0	4.928402	0.812312	-0.253456
131	1	0	0.392392	-1.053050	-0.694694
132	1	0	3.057778	2.304813	-1.031438
133	1	0	0.744689	1.380429	-1.172178

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2) 32T with Si/Al = 31

2.1) 44BPYH<sup>+</sup>/32T<sup>-</sup> open

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.736543	-2.208245	-4.524245
2	14	0	1.883924	0.608510	-4.551955
3	14	0	2.428540	3.434275	-3.671651
4	14	0	5.027927	4.674996	-2.705289
5	14	0	4.810113	4.149316	0.337259
6	14	0	6.403750	2.532588	2.469686
7	14	0	2.675571	-4.211745	-2.145830
8	8	0	2.839823	-0.635961	-4.187886
9	8	0	2.181524	1.845573	-3.567074
10	8	0	4.000004	3.753615	-3.536108
11	8	0	5.246581	4.052894	-1.237508
12	8	0	5.538683	2.995805	1.193919
13	8	0	6.346013	0.901644	2.502563
14	8	0	3.866157	-4.293836	-1.016168
15	8	0	3.068487	-3.062279	-3.199247
16	14	0	1.647573	2.306605	3.481611
17	14	0	2.509584	-0.506681	3.546396
18	14	0	2.007212	-3.398793	2.595806
19	14	0	-0.607887	-4.661694	1.609177
20	14	0	-0.360971	-4.060947	-1.390818
21	14	0	-1.994785	-2.387085	-3.447410
22	14	0	-1.229590	0.541297	-4.039629
23	14	0	-1.997938	3.235786	-2.874991
24	14	0	0.400385	4.869286	-1.635273
25	14	0	1.749907	4.358912	1.087811
26	8	0	1.558863	0.732203	3.151053
27	8	0	2.242213	-1.749998	2.560721
28	8	0	0.435307	-3.716230	2.460925
29	8	0	-0.832645	-4.026051	0.148134
30	8	0	-1.103754	-2.884352	-2.202709
31	8	0	-1.979951	-0.778421	-3.503210
32	8	0	-1.214693	1.757946	-2.937620
33	8	0	-1.024965	4.293436	-2.109803
34	8	0	0.602631	4.484171	-0.086084
35	8	0	1.321989	3.225714	2.145208
36	1	0	3.704343	-2.546304	-5.587546
37	1	0	2.132891	1.023072	-5.947549
38	1	0	1.936429	3.919807	-4.976876
39	1	0	4.470568	6.037130	-2.580906
40	1	0	6.319725	4.734591	-3.418895
41	1	0	5.139976	5.470303	0.909720
42	1	0	7.795326	3.004094	2.318934
43	1	0	6.131828	-1.007718	4.140881
44	1	0	4.219433	-6.129975	0.669983
45	1	0	2.556753	-5.506636	-2.846307
46	1	0	0.651152	2.646138	4.517657
47	1	0	2.226010	-0.914905	4.937248
48	1	0	2.498945	-3.884139	3.901243
49	1	0	-0.054954	-6.024189	1.469895
50	8	0	-2.011399	-4.729667	2.393639



51	1	0	-0.708051	-5.366469	-1.988040
52	8	0	-3.510206	-2.900205	-3.262368
53	1	0	-1.898824	1.025221	-5.264159
54	1	0	-2.294964	3.702745	-4.304612
55	1	0	0.392720	6.339647	-1.774947
56	1	0	1.849420	5.663782	1.772605
57	8	0	1.244070	-2.544158	-5.020870
58	8	0	-1.388111	-2.979084	-4.815611
59	14	0	-0.094905	-3.140976	-5.762229
60	1	0	-0.331358	-2.436242	-7.038541
61	1	0	0.148729	-4.573934	-6.024529
62	8	0	0.347692	0.159161	-4.390737
63	8	0	1.608602	4.254584	-2.501640
64	8	0	3.176152	3.980884	0.442344
65	8	0	3.125356	2.651140	4.014907
66	8	0	5.765235	3.155666	3.809298
67	14	0	4.451016	3.335840	4.723106
68	1	0	4.661635	2.663510	6.021237
69	1	0	4.197041	4.773869	4.944683
70	8	0	4.063316	-0.095632	3.257003
71	8	0	2.911664	-4.102217	1.432193
72	8	0	1.269587	-3.846073	-1.450703
73	14	0	-4.953801	-2.471949	-2.690542
74	14	0	-3.620533	-4.748078	2.379661
75	8	0	-5.110281	-2.999380	-1.177987
76	8	0	-5.111002	-0.851722	-2.635661
77	1	0	-6.014485	-3.061699	-3.532369
78	8	0	-4.175946	-3.882291	3.619909
79	8	0	-4.159008	-4.121515	0.998723
80	1	0	-4.098289	-6.140130	2.504037
81	1	0	-7.536124	-0.161070	-2.125203
82	1	0	-6.409725	0.977742	-3.929492
83	14	0	-5.308623	-4.203075	-0.125623
84	1	0	-6.633726	-4.082342	0.515511
85	1	0	-5.221175	-5.496031	-0.834246
86	8	0	-5.722856	4.395385	1.861758
87	1	0	-7.820078	4.540970	0.471659
88	1	0	-6.301500	6.414911	0.474238
89	14	0	-5.508336	-3.652014	4.492581
90	8	0	-5.846771	-2.078692	4.549033
91	1	0	-6.632117	-4.376484	3.865056
92	1	0	-5.294725	-4.158696	5.863410
93	14	0	-6.014917	4.242518	3.438773
94	8	0	-5.200570	2.980287	4.012317
95	1	0	-7.461695	4.033103	3.649744
96	1	0	-5.587372	5.469241	4.141542
97	14	0	-5.715405	-0.857562	5.590189
98	8	0	-5.113679	0.437296	4.844354
99	1	0	-7.045980	-0.526339	6.139178
100	1	0	-4.811694	-1.250705	6.690313
101	14	0	-4.792698	2.021075	5.240810
102	1	0	-5.617764	2.351687	6.420425
103	1	0	-3.333353	2.161133	5.420329
104	1	0	-6.058140	4.426974	-4.034682
105	1	0	8.300097	-2.152237	-0.356924
106	1	0	7.299430	-3.646029	3.657158
107	14	0	6.763187	-2.944201	1.415946

108	8	0	5.893223	-1.571221	1.713396
109	8	0	5.625693	-4.073957	1.029790
110	8	0	7.823317	-2.829250	0.165893
111	8	0	7.619028	-3.422780	2.757991
112	8	0	-3.380945	3.102201	-2.072508
113	13	0	-5.148838	3.228704	-2.105913
114	8	0	-5.589134	4.323699	-0.812229
115	8	0	-5.703453	1.581438	-1.577202
116	8	0	-5.809882	3.562339	-3.687101
117	1	0	-4.753221	1.286723	0.022421
118	14	0	5.611165	-0.484364	2.905867
119	14	0	4.185880	-4.673834	0.546857
120	14	0	-6.240823	0.411276	-2.586434
121	14	0	-6.395362	4.942791	0.427247
122	6	0	-1.082123	0.510323	0.220807
123	6	0	0.350243	0.270225	-0.058954
124	6	0	-2.033133	-0.518024	0.072011
125	6	0	1.182250	1.313275	-0.479130
126	6	0	-1.559072	1.787555	0.570270
127	6	0	0.932233	-0.994851	0.028643
128	6	0	-3.377955	-0.218474	0.099005
129	6	0	2.528361	1.066416	-0.724343
130	6	0	-2.918707	2.042044	0.579672
131	6	0	2.288464	-1.141229	-0.258873
132	7	0	-3.788288	1.047835	0.314221
133	7	0	3.094985	-0.138986	-0.612881
134	1	0	-1.735880	-1.531497	-0.157100
135	1	0	0.781999	2.298654	-0.640090
136	1	0	-0.879899	2.607065	0.762932
137	1	0	0.363179	-1.846765	0.371551
138	1	0	-4.149317	-0.946818	-0.111526
139	1	0	3.183112	1.870964	-1.032593
140	1	0	-3.344780	3.024315	0.741669
141	1	0	2.757553	-2.109213	-0.167677

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2.2) 44BPYH<sup>+</sup>/32T<sup>-</sup> closed

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.705392	-2.194460	-4.540001
2	14	0	1.892115	0.634040	-4.542253
3	14	0	2.472197	3.442795	-3.630723
4	14	0	5.084445	4.637228	-2.641007
5	14	0	4.846439	4.083565	0.395058
6	14	0	6.408396	2.423074	2.517273
7	14	0	2.606498	-4.221121	-2.182575
8	8	0	2.829078	-0.627289	-4.187077
9	8	0	2.202690	1.856704	-3.543496
10	8	0	4.047355	3.738802	-3.485462
11	8	0	5.288205	3.997170	-1.178813
12	8	0	5.555271	2.911317	1.242798
13	8	0	6.330620	0.806683	2.533042
14	8	0	3.728229	-4.393354	-1.027404
15	8	0	3.019812	-3.066536	-3.222502
16	14	0	1.645109	2.248400	3.505638
17	14	0	2.470084	-0.576455	3.543683
18	14	0	1.934415	-3.451314	2.559531
19	14	0	-0.692387	-4.669175	1.547689
20	14	0	-0.423974	-4.039344	-1.444483
21	14	0	-2.026435	-2.322143	-3.489984
22	14	0	-1.220452	0.602206	-4.046980
23	14	0	-1.958148	3.291122	-2.859007
24	14	0	0.455349	4.879736	-1.590734
25	14	0	1.784712	4.323060	1.133194
26	8	0	1.537402	0.678955	3.157615
27	8	0	2.191037	-1.805451	2.543391
28	8	0	0.359139	-3.746690	2.414260
29	8	0	-0.902173	-4.014905	0.092655
30	8	0	-1.147650	-2.844435	-2.246828
31	8	0	-1.990386	-0.713302	-3.528246
32	8	0	-1.255164	1.798277	-2.912331
33	8	0	-0.987020	4.325434	-2.081036
34	8	0	0.644936	4.475755	-0.044752
35	8	0	1.336768	3.184576	2.176526
36	1	0	3.672906	-2.535089	-5.602742
37	1	0	2.152738	1.059334	-5.932479
38	1	0	1.992422	3.948453	-4.932896
39	1	0	4.545542	6.005655	-2.504916
40	1	0	6.379964	4.686105	-3.348659
41	1	0	5.192190	5.393907	0.982415
42	1	0	7.807016	2.876658	2.377084
43	1	0	6.084501	-1.116394	4.150702
44	1	0	3.931877	-6.301409	0.602679
45	1	0	2.472674	-5.507004	-2.896807
46	1	0	0.648478	2.589727	4.540893
47	1	0	2.174871	-0.995934	4.928751
48	1	0	2.413819	-3.957121	3.861783
49	1	0	-0.156625	-6.037203	1.396068
50	8	0	-2.100231	-4.727256	2.325152
51	1	0	-0.785306	-5.333689	-2.057376
52	8	0	-3.549242	-2.817368	-3.317229

53	1	0	-1.877729	1.108038	-5.269130
54	1	0	-2.242015	3.776932	-4.285014
55	1	0	0.467696	6.351455	-1.714916
56	1	0	1.898018	5.619247	1.832186
57	8	0	1.210517	-2.504449	-5.046170
58	8	0	-1.421288	-2.907214	-4.861837
59	14	0	-0.125994	-3.075773	-5.804428
60	1	0	-0.347416	-2.354264	-7.074045
61	1	0	0.100143	-4.508879	-6.081192
62	8	0	0.349117	0.204519	-4.391964
63	8	0	1.659603	4.258268	-2.457790
64	8	0	3.209004	3.933036	0.490557
65	8	0	3.124806	2.567798	4.049175
66	8	0	5.772919	3.041266	3.860589
67	14	0	4.457465	3.230387	4.770803
68	1	0	4.653212	2.541955	6.062807
69	1	0	4.222555	4.669477	5.006105
70	8	0	4.005725	-0.092029	3.328958
71	8	0	2.722996	-4.172037	1.337593
72	8	0	1.202792	-3.843015	-1.489499
73	14	0	-4.989729	-2.376469	-2.747177
74	14	0	-3.709388	-4.724467	2.303858
75	8	0	-5.159971	-2.918113	-1.241146
76	8	0	-5.054373	-0.738828	-2.647492
77	1	0	-6.054154	-2.943170	-3.600042
78	8	0	-4.259128	-3.864935	3.550966
79	8	0	-4.233345	-4.076037	0.927437
80	1	0	-4.205805	-6.111413	2.410996
81	1	0	-7.442321	0.077200	-2.146902
82	1	0	-6.227502	1.198008	-3.904494
83	14	0	-5.378781	-4.130407	-0.202802
84	1	0	-6.705111	-3.999285	0.433739
85	1	0	-5.304955	-5.416667	-0.925029
86	8	0	-5.627335	4.452627	1.765590
87	1	0	-7.710532	4.645762	0.360277
88	1	0	-6.160069	6.493165	0.390480
89	14	0	-5.592373	-3.626690	4.420185
90	8	0	-5.910533	-2.049778	4.492220
91	1	0	-6.722623	-4.329582	3.779866
92	1	0	-5.391642	-4.150898	5.786363
93	14	0	-5.934618	4.291859	3.338922
94	8	0	-5.146692	3.011107	3.908296
95	1	0	-7.386424	4.105686	3.536732
96	1	0	-5.491722	5.505212	4.055265
97	14	0	-5.768020	-0.841786	5.547146
98	8	0	-5.146076	0.453070	4.818085
99	1	0	-7.096659	-0.499138	6.093810
100	1	0	-4.874540	-1.258574	6.646923
101	14	0	-4.765216	2.034941	5.131905
102	1	0	-5.593919	2.370017	6.307705
103	1	0	-3.305169	2.148343	5.324079
104	1	0	-5.675946	4.622574	-3.907637
105	1	0	8.259802	-2.242413	-0.348377
106	1	0	7.221072	-3.764206	3.645467
107	13	0	6.622843	-3.025673	1.367437
108	8	0	5.532062	-1.584072	1.640667
109	8	0	5.439732	-4.327299	1.088815

110	8	0	7.482035	-2.776528	-0.143354
111	8	0	7.544709	-3.316562	2.845397
112	8	0	-3.384698	3.268134	-2.065925
113	14	0	-5.023168	3.321186	-2.044401
114	8	0	-5.489121	4.409103	-0.923174
115	8	0	-5.568413	1.815389	-1.671962
116	8	0	-5.623800	3.726512	-3.535491
117	14	0	5.537103	-0.595548	2.907693
118	14	0	4.045938	-4.841518	0.545024
119	14	0	-6.112614	0.551944	-2.604918
120	14	0	-6.289086	5.025478	0.373429
121	6	0	-0.870387	0.437463	0.242818
122	6	0	0.547918	0.175431	-0.107112
123	6	0	-1.827508	-0.589542	0.264821
124	6	0	1.447872	1.201253	-0.463662
125	6	0	-1.302875	1.710760	0.643653
126	6	0	1.083832	-1.113275	-0.023270
127	6	0	-3.128181	-0.304619	0.679812
128	6	0	2.798021	0.950630	-0.581040
129	6	0	-2.627534	1.888729	1.045328
130	6	0	2.442000	-1.330356	-0.158056
131	7	0	-3.537478	0.907986	1.072576
132	7	0	3.270928	-0.301545	-0.394384
133	1	0	-1.591104	-1.598807	-0.041902
134	1	0	1.096158	2.205330	-0.630186
135	1	0	-0.629173	2.554855	0.680779
136	1	0	0.465813	-1.950323	0.255773
137	1	0	-3.874107	-1.094758	0.698116
138	1	0	3.526716	1.713086	-0.809248
139	1	0	-2.973332	2.869862	1.363451
140	1	0	2.905424	-2.292276	-0.016944
141	1	0	4.277058	-0.484794	-0.348347

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### 2.3) PYH<sup>+</sup>/32T<sup>+</sup> open

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-2.827237	-2.298074	4.517371
2	14	0	-1.971562	0.516494	4.606061
3	14	0	-2.513120	3.361253	3.787191
4	14	0	-5.111167	4.625433	2.848015
5	14	0	-4.893949	4.165546	-0.205213
6	14	0	-6.489357	2.597118	-2.372110
7	14	0	-2.768459	-4.249650	2.096113
8	8	0	-2.928813	-0.718763	4.215151
9	8	0	-2.267828	1.774922	3.648217
10	8	0	-4.084237	3.685158	3.658648
11	8	0	-5.330508	4.035509	1.367109
12	8	0	-5.623777	3.031653	-1.086636
13	8	0	-6.432826	0.966942	-2.438977
14	8	0	-3.962126	-4.302985	0.968810
15	8	0	-3.160118	-3.122847	3.174195
16	14	0	-1.733415	2.387088	-3.388567
17	14	0	-2.598917	-0.423075	-3.513995
18	14	0	-2.100185	-3.335626	-2.625953
19	14	0	0.513296	-4.622750	-1.666717
20	14	0	0.266980	-4.086500	1.345524
21	14	0	1.902773	-2.459388	3.437753
22	14	0	1.141187	0.456498	4.092939
23	14	0	1.912146	3.151646	2.986714
24	14	0	-0.481648	4.815882	1.779550
25	14	0	-1.834179	4.361451	-0.951939
26	8	0	-1.646677	0.805817	-3.092020
27	8	0	-2.333138	-1.687680	-2.555342
28	8	0	-0.528681	-3.657851	-2.497911
29	8	0	0.738772	-4.019027	-0.192308
30	8	0	1.011185	-2.928603	2.182604
31	8	0	1.889934	-0.852284	3.528214
32	8	0	1.130216	1.679009	3.003761
33	8	0	0.944770	4.248089	2.270098
34	8	0	-0.685908	4.460831	0.223459
35	8	0	-1.410385	3.247152	-2.030864
36	1	0	-3.795394	-2.658037	5.573130
37	1	0	-2.220068	0.900997	6.010316
38	1	0	-2.020471	3.817864	5.102612
39	1	0	-4.552331	5.989337	2.753148
40	1	0	-6.402894	4.670958	3.562786
41	1	0	-5.222383	5.498981	-0.748915
42	1	0	-7.880420	3.066757	-2.211135
43	1	0	-6.219789	-0.908016	-4.116705
44	1	0	-4.324276	-6.098695	-0.758497
45	1	0	-2.651039	-5.559538	2.768373
46	1	0	-0.736523	2.747634	-4.417032
47	1	0	-2.315783	-0.801578	-4.913316
48	1	0	-2.592457	-3.792111	-3.941559
49	1	0	-0.041336	-5.987243	-1.556848
50	8	0	1.916760	-4.675544	-2.452432
51	1	0	0.612409	-5.405023	1.914475
52	8	0	3.417564	-2.970284	3.241727

53	1	0	1.810963	0.913083	5.327629
54	1	0	2.211382	3.590493	4.424754
55	1	0	-0.469269	6.283301	1.947055
56	1	0	-1.929925	5.679369	-1.611827
57	8	0	-1.335125	-2.646285	5.006555
58	8	0	1.295297	-3.079986	4.792863
59	14	0	0.001845	-3.260636	5.735744
60	1	0	0.239111	-2.583872	7.026954
61	1	0	-0.243582	-4.698612	5.967090
62	8	0	-0.435819	0.069077	4.435099
63	8	0	-1.691352	4.188679	2.634810
64	8	0	-3.261277	3.975748	-0.312929
65	8	0	-3.210743	2.744874	-3.914345
66	8	0	-5.850177	3.248375	-3.697931
67	14	0	-4.535772	3.446875	-4.607664
68	1	0	-4.747131	2.803052	-5.920047
69	1	0	-4.280239	4.889091	-4.798047
70	8	0	-4.149958	-0.010430	-3.212562
71	8	0	-3.009794	-4.061932	-1.484458
72	8	0	-1.362084	-3.870532	1.409025
73	14	0	4.861717	-2.531597	2.679296
74	14	0	3.525869	-4.696252	-2.438818
75	8	0	5.017616	-3.026496	1.155728
76	8	0	5.014788	-0.909608	2.673420
77	1	0	5.921627	-3.140673	3.508239
78	8	0	4.082417	-3.804624	-3.660105
79	8	0	4.065055	-4.100269	-1.044685
80	1	0	4.001901	-6.085892	-2.593161
81	1	0	7.437251	-0.197537	2.180050
82	1	0	6.311215	0.883017	4.020041
83	14	0	5.214513	-4.207474	0.077668
84	1	0	6.539797	-4.074597	-0.560687
85	1	0	5.125425	-5.515294	0.758255
86	8	0	5.637578	4.429186	-1.714482
87	1	0	7.733088	4.545701	-0.319069
88	1	0	6.211002	6.416367	-0.278926
89	14	0	5.415135	-3.557246	-4.527581
90	8	0	5.755527	-1.983495	-4.550100
91	1	0	6.537984	-4.296471	-3.915793
92	1	0	5.200962	-4.033997	-5.909018
93	14	0	5.931554	4.314233	-3.294357
94	8	0	5.120167	3.064429	-3.898495
95	1	0	7.378938	4.112547	-3.508670
96	1	0	5.502435	5.556455	-3.968353
97	14	0	5.625729	-0.740045	-5.564696
98	8	0	5.025576	0.539182	-4.791138
99	1	0	6.956741	-0.398720	-6.106390
100	1	0	4.721583	-1.108261	-6.673059
101	14	0	4.715362	2.133814	-5.149787
102	1	0	5.541024	2.493782	-6.320356
103	1	0	3.255943	2.275383	-5.327510
104	1	0	5.951147	4.326545	4.230628
105	1	0	-8.389681	-2.144413	0.355928
106	1	0	-7.389446	-3.554959	-3.688265
107	14	0	-6.848329	-2.894098	-1.433460
108	8	0	-5.973830	-1.511746	-1.691565
109	8	0	-5.717817	-4.034819	-1.076611

110	8	0	-7.902133	-2.805146	-0.176443
111	8	0	-7.706685	-3.324025	-2.790061
112	8	0	3.294519	3.044013	2.175007
113	13	0	5.052941	3.199795	2.245417
114	8	0	5.510866	4.298359	0.964017
115	8	0	5.570743	1.539192	1.698828
116	8	0	5.729002	3.479178	3.827725
117	1	0	4.478094	1.170100	0.525110
118	14	0	-5.699346	-0.409242	-2.872668
119	14	0	-4.276481	-4.644832	-0.602311
120	14	0	6.142441	0.348387	2.668405
121	14	0	6.309437	4.944587	-0.267045
122	7	0	3.665166	0.988320	-0.129596
123	6	0	3.184535	-0.265297	-0.220911
124	6	0	3.086801	2.036959	-0.743884
125	6	0	2.044576	-0.518152	-0.965764
126	6	0	1.942854	1.837267	-1.503295
127	6	0	1.409887	0.549720	-1.606376
128	1	0	3.729767	-1.025395	0.322743
129	1	0	3.554173	3.001837	-0.590908
130	1	0	1.653155	-1.527070	-1.018855
131	1	0	1.465069	2.686379	-1.977802
132	1	0	0.497588	0.380051	-2.168236

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## 2.4) PYH<sup>+</sup>/32T<sup>-</sup> closed

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.491845	-2.012917	-4.614224
2	14	0	1.694511	0.818088	-4.506962
3	14	0	2.301730	3.590044	-3.504947
4	14	0	4.932831	4.735429	-2.507224
5	14	0	4.729731	4.076681	0.510339
6	14	0	6.308769	2.334592	2.553008
7	14	0	2.411074	-4.120611	-2.328247
8	8	0	2.628742	-0.459774	-4.208165
9	8	0	2.024427	2.003284	-3.469973
10	8	0	3.880221	3.872607	-3.369419
11	8	0	5.151273	4.043349	-1.071079
12	8	0	5.442518	2.871719	1.307378
13	8	0	6.243054	0.709339	2.544567
14	8	0	3.553115	-4.340831	-1.193508
15	8	0	2.817823	-2.932358	-3.332215
16	14	0	1.557437	2.152414	3.596050
17	14	0	2.365657	-0.676651	3.525258
18	14	0	1.800089	-3.512429	2.448782
19	14	0	-0.846693	-4.679508	1.429186
20	14	0	-0.612458	-3.947370	-1.542503
21	14	0	-2.230292	-2.150979	-3.506256
22	14	0	-1.413697	0.786412	-3.971634
23	14	0	-2.120755	3.424647	-2.679887
24	14	0	0.316759	4.955324	-1.386545
25	14	0	1.679429	4.293165	1.297026
26	8	0	1.435791	0.596673	3.195112
27	8	0	2.066477	-1.868473	2.486542
28	8	0	0.221331	-3.793696	2.313660
29	8	0	-1.070951	-3.973789	0.000595
30	8	0	-1.338988	-2.721188	-2.293438
31	8	0	-2.184961	-0.542010	-3.489045
32	8	0	-1.420468	1.930688	-2.783887
33	8	0	-1.133582	4.437008	-1.897302
34	8	0	0.524892	4.493914	0.140867
35	8	0	1.239988	3.118944	2.303723
36	1	0	3.444053	-2.321002	-5.700462
37	1	0	1.940101	1.290608	-5.884619
38	1	0	1.808545	4.143616	-4.782388
39	1	0	4.403371	6.101001	-2.316397
40	1	0	6.219646	4.802431	-3.229128
41	1	0	5.090164	5.363771	1.138842
42	1	0	7.708052	2.785575	2.411053
43	1	0	6.035290	-1.240496	4.135354
44	1	0	3.768268	-6.305437	0.366412
45	1	0	2.261099	-5.379896	-3.085371
46	1	0	0.576118	2.463082	4.655307
47	1	0	2.085504	-1.142445	4.898604
48	1	0	2.292901	-4.065974	3.726379
49	1	0	-0.321217	-6.044419	1.223217
50	8	0	-2.244883	-4.756705	2.222252
51	1	0	-0.989394	-5.217530	-2.195297
52	8	0	-3.753764	-2.643342	-3.331193

53	1	0	-2.083348	1.338193	-5.166889
54	1	0	-2.421186	3.963809	-4.083145
55	1	0	0.334379	6.430551	-1.456712
56	1	0	1.808069	5.562255	2.041600
57	8	0	0.989034	-2.297188	-5.111919
58	8	0	-1.646170	-2.691314	-4.905302
59	14	0	-0.363991	-2.834230	-5.869807
60	1	0	-0.597123	-2.067706	-7.110622
61	1	0	-0.150094	-4.258077	-6.199101
62	8	0	0.151126	0.391546	-4.352236
63	8	0	1.506496	4.361127	-2.291914
64	8	0	3.093242	3.921067	0.621462
65	8	0	3.045826	2.444355	4.131231
66	8	0	5.693637	2.908489	3.925140
67	14	0	4.390761	3.072323	4.858064
68	1	0	4.598790	2.337920	6.122542
69	1	0	4.166905	4.503454	5.146649
70	8	0	3.920189	-0.225721	3.321443
71	8	0	2.587076	-4.194721	1.200486
72	8	0	1.018299	-3.759827	-1.604561
73	14	0	-5.184195	-2.214463	-2.727634
74	14	0	-3.854133	-4.744120	2.221820
75	8	0	-5.338595	-2.807263	-1.239266
76	8	0	-5.237701	-0.580453	-2.563165
77	1	0	-6.262781	-2.745117	-3.585880
78	8	0	-4.382770	-3.925463	3.505031
79	8	0	-4.391570	-4.045207	0.875637
80	1	0	-4.357565	-6.131141	2.287087
81	1	0	-7.614719	0.228890	-2.003227
82	1	0	-6.413251	1.410727	-3.729742
83	14	0	-5.551568	-4.053733	-0.240944
84	1	0	-6.868891	-3.937397	0.416820
85	1	0	-5.494727	-5.314455	-1.008328
86	8	0	-5.724047	4.453514	2.037774
87	1	0	-7.824599	4.707863	0.668504
88	1	0	-6.261036	6.543045	0.740073
89	14	0	-5.703404	-3.710135	4.399126
90	8	0	-6.011041	-2.134923	4.530016
91	1	0	-6.845938	-4.383927	3.749395
92	1	0	-5.488537	-4.282727	5.743558
93	14	0	-6.011208	4.241351	3.608814
94	8	0	-5.224622	2.936882	4.123581
95	1	0	-7.461478	4.058009	3.820079
96	1	0	-5.550254	5.426741	4.359748
97	14	0	-5.847816	-0.965226	5.624360
98	8	0	-5.227322	0.350716	4.932779
99	1	0	-7.167304	-0.634352	6.199690
100	1	0	-4.942997	-1.425085	6.697375
101	14	0	-4.833499	1.917219	5.308045
102	1	0	-5.643924	2.217512	6.505778
103	1	0	-3.370240	2.014522	5.483922
104	1	0	-5.840801	4.829608	-3.605505
105	1	0	8.152385	-2.279571	-0.412150
106	1	0	7.184158	-3.871252	3.572156
107	13	0	6.545665	-3.152543	1.287368
108	8	0	5.481080	-1.696544	1.652737
109	8	0	5.288729	-4.350174	0.910083

110	8	0	7.365871	-2.804509	-0.220351
111	8	0	7.491324	-3.512324	2.724100
112	8	0	-3.532615	3.366509	-1.860623
113	14	0	-5.168808	3.447688	-1.812045
114	8	0	-5.618759	4.499480	-0.651022
115	8	0	-5.723644	1.933277	-1.477387
116	8	0	-5.782063	3.915595	-3.279897
117	1	0	4.404549	-1.386284	0.352263
118	14	0	5.459941	-0.695133	2.921733
119	14	0	3.886849	-4.845151	0.357525
120	14	0	-6.286626	0.711173	-2.458540
121	14	0	-6.398512	5.078536	0.675078
122	7	0	3.637402	-0.846899	-0.123886
123	6	0	2.412196	-1.377822	-0.250528
124	6	0	3.886124	0.450373	-0.385278
125	6	0	1.334589	-0.586789	-0.617732
126	6	0	2.849436	1.274122	-0.769556
127	6	0	1.551244	0.763831	-0.852574
128	1	0	2.323643	-2.425877	-0.031271
129	1	0	4.908485	0.779794	-0.249698
130	1	0	0.348359	-1.027666	-0.696332
131	1	0	3.047210	2.309573	-0.977321
132	1	0	0.723256	1.411986	-1.117450

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