Electronic Supplementary Material (ESI) for Nanoscale.

Activation of deposition reactions at surface through cooperative effect

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Supporting Information

The Supporting Information (SI) contains six figures (1 to 6). Modelling coordinates are also included. The dimensions of simulation box are given in Å and atomic positions are represented in Cartesian coordinates.

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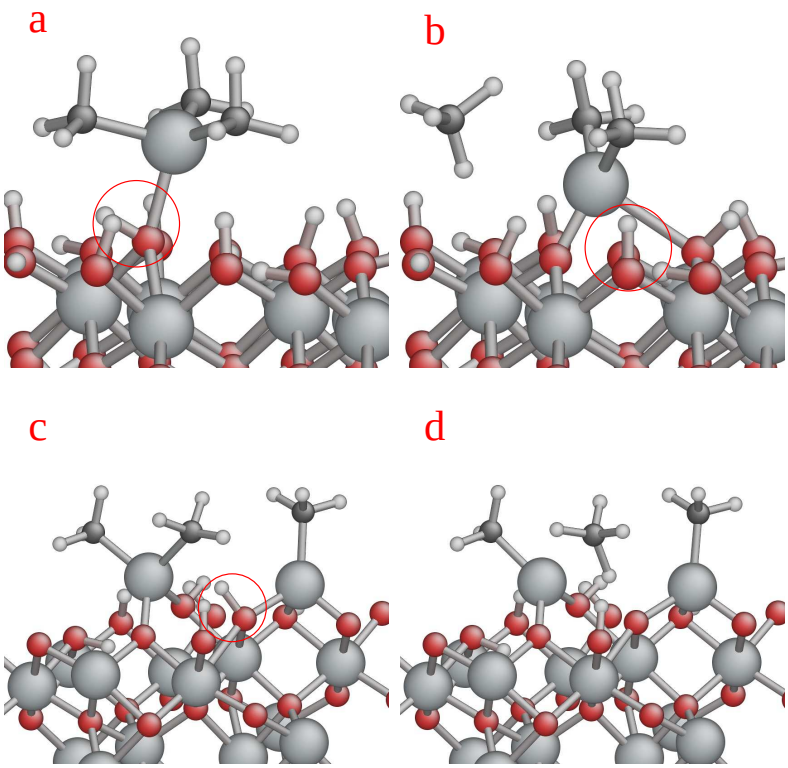
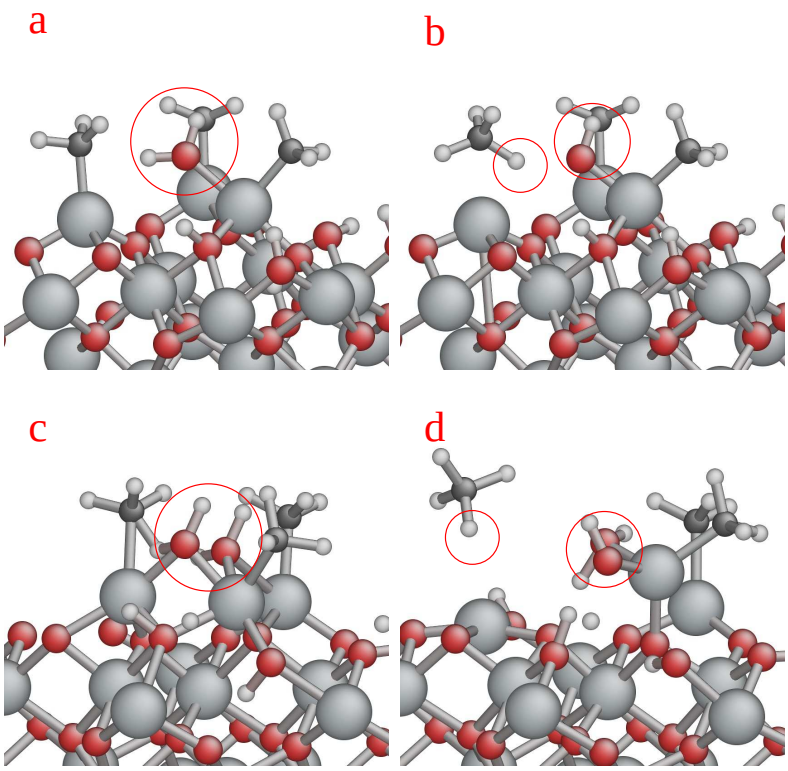
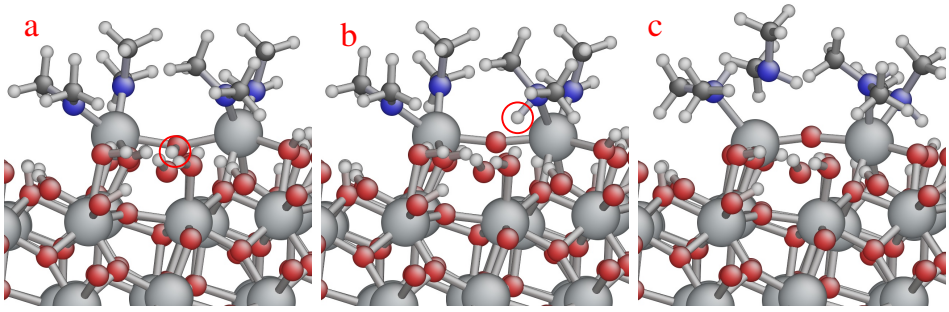


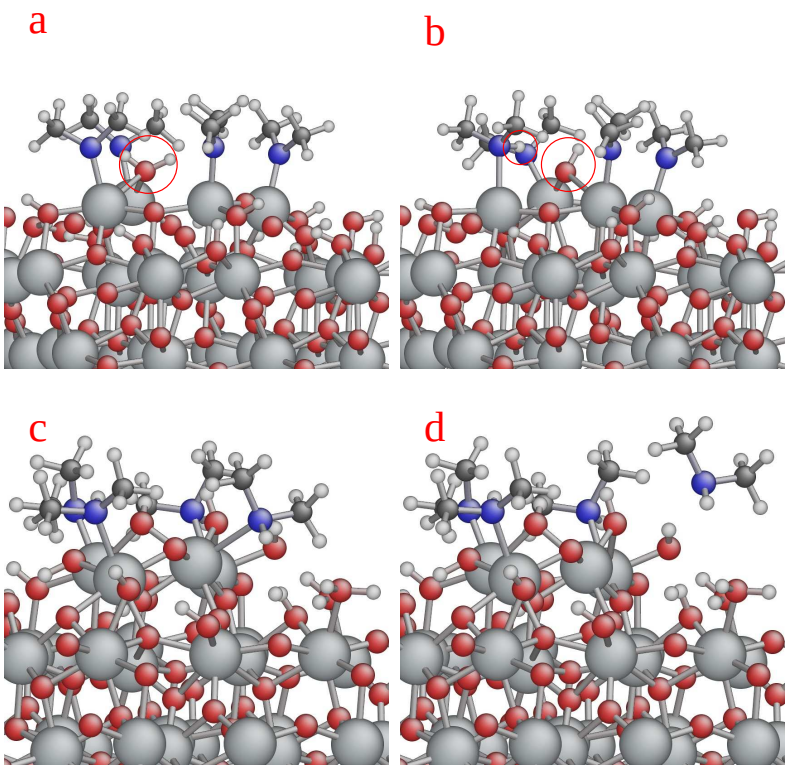
SI Figure 1. Through multiple adsorptions of AlX_3 (X=CH_3), the surface oxygen becomes coordinatively saturated. The rate of proton diffusion from this oxygen therefore increases and facilitates the desorption of HX and bonding of the metal of the precursor to another surface oxygen. (a) Adsorption of AlX_3. Circle shows the OH group to which AlX_3 is anchored. (b) Desorption of HX due to proton transfer from the anchor OH group. Circle shows an OH group that is low coordinated because of the absence of neighbouring adsorbates. (c) Co-existence of remaining precursor fragments, resulting in coordinative saturation of the OH group (circle). (d) Desorption of second HX due to proton diffusion from coordinatively saturated OH group. (red = O, white = H, large gray = Al, small gray = C).



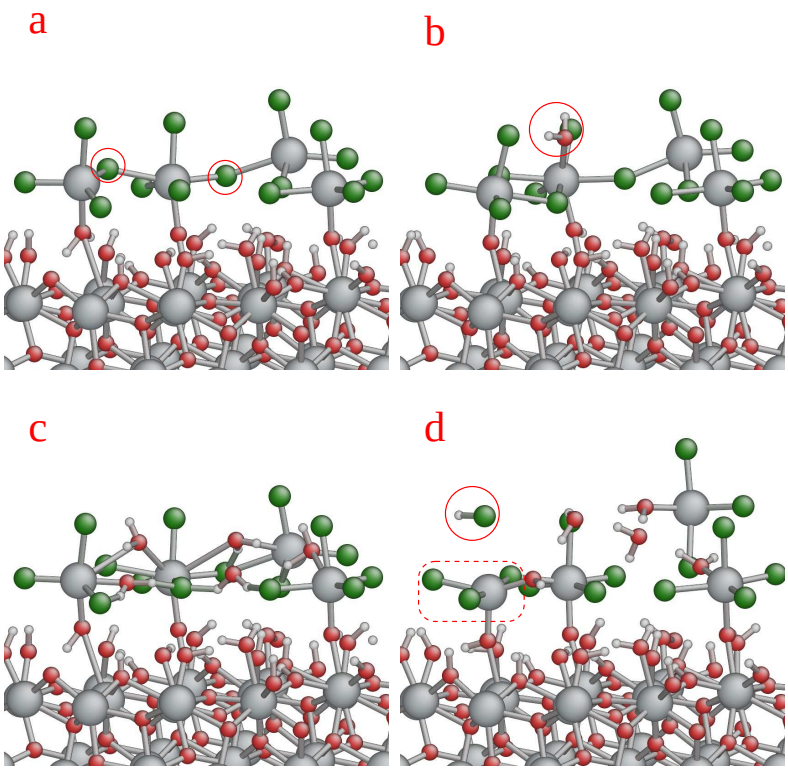
SI Figure 2. Effect of multiple adsorptions of H_2O molecules in a cluster of 3 AlX. By including more H_2O molecules, the proton diffusion from H_2O and associated desorption of HX become barrierless. Overall, by this process, the remaining ligand is replaced with an OH group. (a) Cluster of 3 AlX. Circle shows an incoming H_2O molecule. (b) Dissociation of the incoming H_2O molecule. Circles show the dissociated parts of the original H_2O molecule. (c) Arrival of two H_2O molecules into the cluster. (d) An H_2O molecule from (c) is barrierlessly dissociated leading to desorption of HX from cluster.



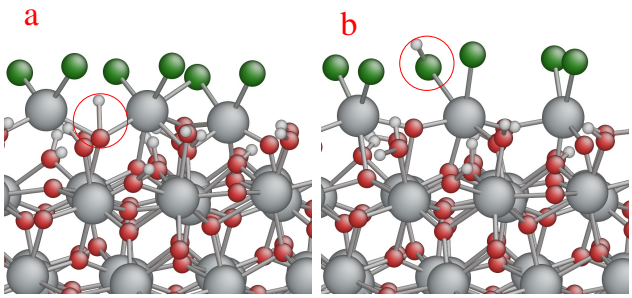
SI Figure 3. The bonding of adjacent precursor fragments (here $2HfX_2$ with $X{=}N(CH_3)_2$) to a shared oxygen atom (circled) on the surface increases the c.n. of the shared atom. The rate of proton donation from oxygen is significantly higher when coordinatively saturated. Due to repulsion between the remaining ligands, the rate of desorption of HX is also increased. (red = O, blue = N, white = H, large gray = Hf, small gray = C).



SI Figure 4. The incoming H_2O molecule is readily dissociated in the cluster of remaining precursor fragments (here 4 HfX). Due to multiple adsorptions of H_2O molecules, dissociation of the remaining ligands becomes energetically possible. (a) Cluster of 4 HfX. Circle shows an incoming H_2O molecule. (b) The incoming H_2O molecule is barrierlessly dissociated. (c) Multiple adsorptions of H_2O molecules into the cluster. (d) Desorption of the remaining ligands is facilitated through multiple adsorptions of H_2O molecules.



SI Figure 5. Considering the multiple adsorptions of $HfCl_4$ and H_2O molecules, the relevant activation energies for proton diffusion and dissociative reactions decrease significantly. (a) Chemisorption and physisorption of multiple precursors (here 4 $HfCl_4$) due to the bonding to the surface oxygen and bridging chloride. Circles show bridging Cl. (b) An incoming H_2O molecule adsorbing into the cluster. (c) Multiple adsorptions of H_2O molecules into the cluster. (d) Dissociation of the H_2O molecules and desorption of HCl. Circle shows the desorbed HCl and dashed rectangle shows the remaining $HfCl_3$. (red = O, green = Cl, white = H, large gray = Hf).



SI Figure 6. Proton diffusion from the coordinatively saturated oxygen to the remaining chloride in the clusters. These oxygen atoms can be either from the oxygen pulse (H_2O) or from the surface. (a) 3 $HfCl_2$ cluster. Circle shows the coordinatively saturated OH group. (b) Proton diffusion from the OH group to the remaining Cl.

Fig. 1a					
Simulation box:					
a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99
127 atoms					
Atomic id	element	x	y	z	
1	Al	0.069	0.040	6.077	
2	Al	-2.309	4.109	6.133	
3	Al	4.834	0.006	6.127	
4	Al	2.458	4.107	6.098	
5	Al	0.108	2.808	1.535	
6	Al	-2.372	6.876	1.620	
7	Al	4.885	2.786	1.792	
8	Al	2.467	6.800	1.536	
9	Al	0.061	0.008	3.376	
10	Al	-2.263	4.125	3.420	
11	Al	0.064	8.224	3.394	
12	Al	2.433	4.111	3.395	
13	Al	2.403	1.391	7.927	
14	Al	0.044	5.473	7.907	
15	Al	7.237	1.362	7.950	
16	Al	4.856	5.611	7.786	
17	Al	2.365	1.477	1.204	
18	Al	0.061	5.561	1.294	
19	Al	7.257	1.328	1.229	
20	Al	4.807	5.393	1.210	
21	Al	0.071	2.761	5.615	

22	Al	-2.301	6.866	5.582
23	Al	4.834	2.716	5.614
24	Al	2.456	6.870	5.580
25	Al	2.442	1.366	3.886
26	Al	0.088	5.494	3.922
27	Al	7.212	1.374	3.898
28	Al	4.828	5.494	3.905
29	Al	0.105	2.740	8.303
30	Al	-2.259	6.875	8.250
31	Al	4.851	2.759	8.294
32	Al	2.393	6.867	8.221
33	Al	2.469	3.298	10.654
34	Al	5.829	1.089	10.190
35	O	1.540	0.003	4.739
36	O	-0.850	4.126	4.757
37	O	6.284	0.010	4.742
38	O	3.927	4.092	4.773
39	O	4.094	1.345	9.454
40	O	1.564	5.461	9.027
41	O	-0.772	1.404	9.125
42	O	6.268	5.552	9.136
43	O	1.616	2.860	0.422
44	O	-0.858	6.889	0.337
45	O	6.142	2.471	0.332
46	O	3.957	6.698	0.313
47	O	-0.650	1.279	4.744
48	O	-3.043	5.379	4.777

49	O	4.085	1.261	4.760
50	O	1.740	5.380	4.744
51	O	1.727	2.693	9.154
52	O	-0.716	6.713	9.174
53	O	6.360	2.530	9.227
54	O	3.981	6.619	9.147
55	O	-0.752	4.176	0.357
56	O	-3.187	8.222	0.354
57	O	4.142	3.874	0.448
58	O	1.774	8.122	0.366
59	O	1.737	2.850	4.758
60	O	-0.662	6.978	4.745
61	O	6.472	2.853	4.768
62	O	4.103	6.975	4.735
63	O	1.716	0.061	9.124
64	O	-0.661	4.142	9.140
65	O	6.535	-0.000	9.096
66	O	4.059	3.943	9.698
67	O	-0.739	1.614	0.291
68	O	-3.084	5.572	0.368
69	O	3.916	1.177	0.046
70	O	1.598	5.560	0.358
71	O	0.968	1.388	2.544
72	O	-1.408	5.527	2.547
73	O	5.726	1.357	2.533
74	O	3.364	5.453	2.540
75	O	-1.408	2.739	6.965

76	O	-3.751	6.915	6.936
77	O	3.375	2.757	7.082
78	O	0.972	6.837	6.913
79	O	3.171	0.114	2.476
80	O	0.768	4.237	2.586
81	O	7.939	0.091	2.518
82	O	5.600	4.227	2.582
83	O	0.832	1.493	6.943
84	O	-1.586	5.609	6.957
85	O	5.549	1.493	6.968
86	O	3.221	5.569	6.932
87	O	3.226	2.607	2.569
88	O	0.813	6.779	2.536
89	O	7.929	2.654	2.511
90	O	5.548	6.757	2.541
91	O	0.801	4.018	6.936
92	O	-1.543	8.165	7.020
93	O	5.533	4.054	7.049
94	O	3.204	8.114	6.941
95	C	1.759	4.656	11.878
96	C	2.760	1.681	11.896
97	C	6.074	1.088	12.114
98	H	1.952	0.269	10.043
99	H	-1.626	3.988	9.252
100	H	1.968	4.596	8.806
101	H	3.555	1.545	10.316
102	H	-0.278	0.567	9.231

103	H	-0.700	6.153	9.969
104	H	3.731	6.064	9.909
105	H	-0.056	0.971	0.024
106	H	6.403	3.214	23.242
107	H	3.172	3.670	0.313
108	H	-0.316	3.901	22.997
109	H	-2.391	4.865	0.339
110	H	-1.150	6.511	22.960
111	H	2.096	7.880	22.952
112	H	1.794	4.584	0.268
113	H	4.202	0.202	0.141
114	H	-2.867	8.072	22.918
115	H	5.889	6.011	9.908
116	H	4.874	4.064	10.230
117	H	4.708	1.717	23.233
118	H	4.609	7.427	0.261
119	H	1.864	4.361	12.930
120	H	2.182	5.664	11.762
121	H	0.684	4.749	11.662
122	H	1.730	1.701	12.314
123	H	3.432	2.017	12.697
124	H	2.993	0.618	11.773
125	H	5.860	2.067	12.563
126	H	5.506	0.335	12.669
127	H	7.143	0.892	12.287

Fig. 1b

Simulation box:					
a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78
322 atoms					
Atomic id	element	x	y	z	
1	Hf	2.364	3.806	1.287	
2	Hf	-1.171	10.521	1.297	
3	Hf	9.839	3.813	1.310	
4	Hf	6.302	10.525	1.311	
5	Hf	-1.550	6.013	4.016	
6	Hf	-5.085	12.730	4.048	
7	Hf	5.932	6.032	4.016	
8	Hf	2.399	12.738	4.039	
9	Hf	5.597	1.622	6.890	
10	Hf	2.051	8.328	6.867	
11	Hf	13.059	1.614	6.894	
12	Hf	9.508	8.311	6.895	
13	Hf	1.667	4.003	9.675	
14	Hf	-1.757	10.524	9.606	
15	Hf	9.279	3.855	9.634	
16	Hf	5.620	10.527	9.698	
17	Hf	-1.521	3.227	1.315	
18	Hf	-5.067	9.947	1.318	
19	Hf	5.954	3.239	1.323	
20	Hf	2.410	9.952	1.319	
21	Hf	1.982	5.593	4.140	
22	Hf	-1.543	12.304	4.159	

23	Hf	9.483	5.575	4.172
24	Hf	5.944	12.286	4.176
25	Hf	1.658	1.159	6.973
26	Hf	-1.857	7.822	6.946
27	Hf	9.132	1.145	6.966
28	Hf	5.589	7.839	6.956
29	Hf	5.166	3.447	9.755
30	Hf	1.717	10.060	9.776
31	Hf	12.684	3.341	9.871
32	Hf	9.040	10.039	9.814
33	Hf	-6.602	13.303	1.118
34	Hf	-3.082	6.592	1.088
35	Hf	0.869	13.307	1.111
36	Hf	4.394	6.594	1.088
37	Hf	4.088	2.043	3.892
38	Hf	0.548	8.753	3.886
39	Hf	11.570	2.041	3.896
40	Hf	8.023	8.748	3.897
41	Hf	0.160	4.312	6.727
42	Hf	-3.378	11.004	6.693
43	Hf	7.648	4.347	6.738
44	Hf	4.111	11.031	6.742
45	Hf	3.728	6.554	9.459
46	Hf	0.249	13.320	9.492
47	Hf	11.280	6.653	9.513
48	Hf	7.736	13.301	9.502
49	Hf	4.363	0.295	0.982

50	Hf	0.819	7.005	0.964
51	Hf	11.828	0.296	0.981
52	Hf	8.288	7.008	0.975
53	Hf	0.561	2.502	3.857
54	Hf	-2.980	9.203	3.833
55	Hf	8.035	2.504	3.863
56	Hf	4.490	9.210	3.845
57	Hf	4.112	4.780	6.575
58	Hf	0.578	11.491	6.606
59	Hf	11.610	4.764	6.642
60	Hf	8.075	11.472	6.643
61	Hf	3.763	0.280	9.442
62	Hf	0.257	7.112	9.510
63	Hf	11.251	0.387	9.479
64	Hf	7.656	7.074	9.499
65	Hf	3.140	5.485	12.437
66	Hf	3.770	9.537	12.491
67	H	0.018	2.442	10.753
68	H	-3.675	9.328	10.700
69	H	7.226	3.718	11.222
70	H	3.155	2.359	10.976
71	H	-0.817	9.510	11.928
72	H	9.936	2.935	12.027
73	H	6.499	10.018	12.345
74	H	-1.726	12.563	11.529
75	H	9.509	5.819	11.573
76	H	5.799	12.557	11.509

77	H	5.063	2.753	12.406
78	H	1.213	8.288	12.000
79	H	12.053	1.728	11.891
80	H	8.470	8.520	11.900
81	H	1.428	3.408	12.440
82	H	-2.342	9.107	11.900
83	H	8.183	1.796	11.462
84	H	2.314	0.516	11.677
85	H	-1.314	7.336	11.580
86	H	9.956	0.672	11.779
87	H	7.130	6.187	11.985
88	H	5.068	1.824	19.758
89	H	1.529	8.535	19.745
90	H	12.532	1.833	19.756
91	H	9.000	8.533	19.750
92	H	1.659	0.376	19.993
93	H	-1.884	7.097	19.985
94	H	9.125	0.376	19.983
95	H	5.587	7.097	19.962
96	H	0.436	4.703	20.580
97	H	-3.094	11.416	20.593
98	H	7.918	4.705	20.596
99	H	4.391	11.417	20.597
100	H	3.693	4.509	20.221
101	H	0.183	11.207	20.244
102	H	11.132	4.505	20.234
103	H	7.644	11.209	20.255

104	H	1.511	2.695	19.903
105	H	-2.016	9.437	19.898
106	H	8.975	2.707	19.921
107	H	5.456	9.442	19.908
108	H	3.412	2.007	20.040
109	H	-0.129	8.727	20.035
110	H	10.875	2.012	20.050
111	H	7.341	8.728	20.044
112	H	-3.051	6.651	18.937
113	H	-6.584	13.361	18.946
114	H	4.410	6.690	18.909
115	H	0.878	13.362	18.941
116	H	-1.479	4.363	19.918
117	H	-4.989	11.070	19.904
118	H	6.018	4.370	19.920
119	H	2.502	11.081	19.906
120	H	-1.840	5.568	11.298
121	H	-5.368	12.230	11.233
122	H	1.970	12.145	11.428
123	H	5.120	7.236	11.664
124	H	6.567	1.569	11.554
125	H	-4.273	8.081	11.669
126	H	14.256	1.285	11.678
127	H	1.733	6.317	15.785
128	H	1.162	7.642	14.735
129	H	2.874	7.140	14.688
130	H	-0.050	4.578	13.059

131	H	-0.551	6.016	13.945
132	H	0.169	4.649	14.839
133	H	6.414	5.481	14.447
134	H	6.227	4.883	12.768
135	H	6.306	3.736	14.127
136	H	2.967	4.347	15.332
137	H	4.473	5.020	16.028
138	H	4.435	3.337	15.450
139	H	3.573	11.879	15.344
140	H	3.359	13.051	14.012
141	H	4.707	11.897	13.968
142	H	0.785	10.480	13.430
143	H	1.036	12.210	13.786
144	H	1.325	10.994	15.053
145	H	6.720	9.330	14.845
146	H	6.564	8.234	13.430
147	H	6.249	7.635	15.068
148	H	3.125	9.423	15.558
149	H	4.749	9.852	16.173
150	H	4.210	8.160	16.197
151	N	4.464	4.797	13.904
152	N	1.550	5.804	13.720
153	N	4.721	8.892	14.265
154	N	2.809	11.050	13.533
155	C	1.838	6.764	14.774
156	C	0.230	5.234	13.896
157	C	5.914	4.725	13.809

158	C	4.060	4.359	15.236
159	C	3.648	12.009	14.245
160	C	1.431	11.188	13.963
161	C	6.116	8.508	14.397
162	C	4.174	9.097	15.598
163	O	0.481	3.279	1.831
164	O	-3.060	9.996	1.828
165	O	7.949	3.299	1.847
166	O	4.411	10.013	1.840
167	O	4.000	5.660	4.669
168	O	0.470	12.379	4.698
169	O	11.491	5.651	4.710
170	O	7.953	12.342	4.709
171	O	3.668	1.224	7.513
172	O	0.152	7.864	7.466
173	O	11.125	1.157	7.444
174	O	7.562	7.908	7.473
175	O	-0.167	3.401	10.348
176	O	-3.766	10.186	10.186
177	O	7.147	3.924	10.268
178	O	3.693	10.154	10.419
179	O	4.074	4.686	0.132
180	O	0.559	11.390	0.156
181	O	11.537	4.691	0.132
182	O	8.032	11.392	0.162
183	O	3.862	0.102	3.031
184	O	0.321	6.806	3.012

185	O	11.323	0.103	3.025
186	O	7.782	6.812	3.019
187	O	-0.032	2.367	5.880
188	O	-3.578	9.060	5.856
189	O	7.446	2.364	5.878
190	O	3.897	9.073	5.865
191	O	3.537	4.632	8.607
192	O	0.003	11.416	8.679
193	O	11.017	4.721	8.713
194	O	7.455	11.364	8.698
195	O	-2.040	5.000	2.286
196	O	-5.565	11.713	2.311
197	O	5.434	5.007	2.292
198	O	1.900	11.718	2.310
199	O	5.152	0.604	5.168
200	O	1.626	7.323	5.132
201	O	12.644	0.601	5.147
202	O	9.079	7.293	5.162
203	O	1.286	2.902	7.966
204	O	-2.229	9.577	7.910
205	O	8.647	2.851	8.011
206	O	5.114	9.535	7.995
207	O	-2.583	5.176	10.776
208	O	-6.159	11.848	10.768
209	O	4.469	4.975	10.864
210	O	1.299	11.846	10.772
211	O	6.293	1.193	0.795

212	O	2.751	7.905	0.785
213	O	13.767	1.184	0.795
214	O	10.224	7.898	0.785
215	O	2.441	3.453	3.479
216	O	-1.097	10.164	3.476
217	O	9.920	3.448	3.482
218	O	6.378	10.156	3.485
219	O	-1.445	5.711	6.263
220	O	-4.970	12.420	6.258
221	O	6.014	5.724	6.248
222	O	2.477	12.432	6.271
223	O	5.676	1.296	9.096
224	O	2.199	8.026	9.067
225	O	13.176	1.252	9.038
226	O	9.601	7.965	9.054
227	O	2.386	0.202	0.538
228	O	-1.157	6.907	0.513
229	O	9.858	0.191	0.521
230	O	6.317	6.902	0.511
231	O	6.020	2.456	3.338
232	O	2.481	9.170	3.325
233	O	13.500	2.460	3.332
234	O	9.957	9.153	3.326
235	O	2.083	4.716	6.091
236	O	-1.438	11.404	6.086
237	O	9.598	4.640	6.099
238	O	6.043	11.381	6.123

239	O	1.763	0.237	8.886
240	O	-1.773	7.038	8.941
241	O	9.208	0.306	8.961
242	O	5.661	6.891	8.944
243	O	2.562	5.701	2.114
244	O	-0.970	12.415	2.128
245	O	10.041	5.704	2.140
246	O	6.509	12.412	2.146
247	O	2.216	1.287	4.932
248	O	-1.315	7.985	4.908
249	O	9.686	1.288	4.929
250	O	6.136	7.996	4.922
251	O	-1.704	3.565	7.777
252	O	-5.247	10.270	7.751
253	O	5.803	3.588	7.754
254	O	2.223	10.291	7.758
255	O	1.979	5.923	10.512
256	O	-1.575	12.497	10.567
257	O	9.453	5.840	10.602
258	O	5.894	12.551	10.539
259	O	1.188	5.210	0.042
260	O	-2.338	11.926	0.051
261	O	8.670	5.215	0.056
262	O	5.144	11.928	0.054
263	O	0.893	0.749	2.882
264	O	-2.641	7.456	2.853
265	O	8.375	0.761	2.866

266	O	4.837	7.471	2.847
267	O	4.503	3.039	5.637
268	O	0.959	9.757	5.631
269	O	11.984	3.041	5.640
270	O	8.435	9.742	5.634
271	O	0.549	5.316	8.493
272	O	-2.856	12.002	8.434
273	O	8.197	5.387	8.405
274	O	4.542	12.006	8.488
275	O	3.996	2.421	1.692
276	O	0.454	9.128	1.689
277	O	11.472	2.422	1.693
278	O	7.929	9.130	1.695
279	O	0.096	4.626	4.483
280	O	-3.432	11.332	4.485
281	O	7.583	4.635	4.503
282	O	4.043	11.345	4.506
283	O	7.224	0.201	7.332
284	O	3.670	6.885	7.306
285	O	14.722	0.186	7.306
286	O	11.190	6.912	7.323
287	O	3.241	2.416	9.991
288	O	-0.139	9.190	9.895
289	O	10.857	2.463	9.810
290	O	7.203	9.132	9.882
291	O	2.177	3.676	11.878
292	O	-1.715	9.898	11.855

293	O	9.074	3.159	11.630
294	O	5.670	10.231	11.883
295	O	5.396	2.366	11.577
296	O	1.831	9.018	11.785
297	O	12.794	2.332	11.680
298	O	9.250	9.052	11.644
299	O	3.079	-0.001	11.352
300	O	-0.460	6.887	11.418
301	O	10.718	0.169	11.445
302	O	6.971	6.992	11.464
303	O	4.252	1.330	19.979
304	O	0.711	8.045	19.967
305	O	11.718	1.338	19.982
306	O	8.181	8.046	19.976
307	O	2.358	2.885	20.347
308	O	-1.170	9.606	20.350
309	O	9.823	2.886	20.367
310	O	6.302	9.606	20.363
311	O	-0.912	3.702	20.349
312	O	-4.428	10.419	20.357
313	O	6.576	3.706	20.358
314	O	3.053	10.421	20.357
315	O	0.690	0.488	19.724
316	O	-2.854	7.207	19.709
317	O	8.155	0.489	19.718
318	O	4.615	7.207	19.707
319	O	4.123	7.394	11.616

320	O	7.487	1.065	11.319
321	O	-3.384	7.814	11.268
322	O	0.156	1.060	11.195

Fig. 2

Simulation box:

a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

319 atoms

Atomic id	element	x	y	z
1	Hf	2.362	3.809	1.262
2	Hf	-1.168	10.513	1.260
3	Hf	9.842	3.802	1.264
4	Hf	6.305	10.519	1.266
5	Hf	-1.539	6.015	4.001
6	Hf	-5.091	12.729	3.999
7	Hf	5.929	6.012	3.979
8	Hf	2.391	12.725	4.011
9	Hf	5.585	1.602	6.821
10	Hf	2.024	8.335	6.815
11	Hf	13.050	1.631	6.867
12	Hf	9.484	8.346	6.844
13	Hf	1.523	3.609	9.872
14	Hf	-1.867	10.593	9.594
15	Hf	9.040	3.810	9.713
16	Hf	5.617	10.518	9.649
17	Hf	-1.523	3.236	1.290
18	Hf	-5.056	9.946	1.281

19	Hf	5.956	3.229	1.285
20	Hf	2.419	9.947	1.281
21	Hf	1.997	5.578	4.135
22	Hf	-1.531	12.285	4.129
23	Hf	9.476	5.593	4.124
24	Hf	5.931	12.304	4.139
25	Hf	1.657	1.157	6.910
26	Hf	-1.970	7.829	6.875
27	Hf	9.123	1.149	6.930
28	Hf	5.588	7.848	6.864
29	Hf	5.209	3.317	9.687
30	Hf	1.571	10.079	9.765
31	Hf	12.495	3.445	9.720
32	Hf	9.003	10.160	9.793
33	Hf	-6.615	13.299	1.077
34	Hf	-3.080	6.589	1.069
35	Hf	0.861	13.299	1.079
36	Hf	4.395	6.592	1.067
37	Hf	4.076	2.032	3.845
38	Hf	0.554	8.755	3.870
39	Hf	11.562	2.047	3.878
40	Hf	8.024	8.758	3.852
41	Hf	0.210	4.328	6.765
42	Hf	-3.390	11.029	6.683
43	Hf	7.658	4.321	6.679
44	Hf	4.100	11.043	6.722
45	Hf	3.736	6.617	9.306

46	Hf	0.259	13.373	9.512
47	Hf	11.167	6.622	9.521
48	Hf	7.748	13.414	9.452
49	Hf	4.352	0.296	0.946
50	Hf	0.821	7.003	0.960
51	Hf	11.833	0.296	0.961
52	Hf	8.292	7.007	0.944
53	Hf	0.550	2.511	3.827
54	Hf	-2.982	9.210	3.797
55	Hf	8.030	2.499	3.812
56	Hf	4.492	9.217	3.802
57	Hf	4.144	4.743	6.577
58	Hf	0.577	11.480	6.606
59	Hf	11.584	4.788	6.602
60	Hf	8.060	11.493	6.611
61	Hf	3.726	0.387	9.436
62	Hf	0.255	6.995	9.480
63	Hf	11.216	0.398	9.472
64	Hf	7.686	7.094	9.372
65	Hf	3.588	9.231	12.113
66	Hf	-0.270	8.715	12.239
67	Hf	3.577	5.678	12.296
68	Hf	-1.366	5.037	12.122
69	H	-3.704	9.290	10.654
70	H	9.971	2.978	11.995
71	H	6.351	9.826	12.295
72	H	-1.656	12.588	11.464

73	H	9.218	5.835	11.481
74	H	5.752	12.598	11.526
75	H	4.621	1.726	11.931
76	H	12.386	2.303	12.243
77	H	8.369	8.628	11.882
78	H	-2.550	10.379	12.250
79	H	8.099	1.802	11.452
80	H	2.454	0.718	11.647
81	H	9.983	0.627	11.801
82	H	5.045	1.834	19.718
83	H	1.526	8.522	19.720
84	H	12.542	1.817	19.730
85	H	8.996	8.533	19.713
86	H	1.643	0.375	19.964
87	H	-1.878	7.082	19.964
88	H	9.133	0.378	19.960
89	H	5.592	7.093	19.913
90	H	0.443	4.710	20.556
91	H	-3.084	11.421	20.552
92	H	7.914	4.708	20.558
93	H	4.387	11.424	20.555
94	H	3.680	4.546	20.192
95	H	0.176	11.217	20.205
96	H	11.178	4.489	20.207
97	H	7.627	11.212	20.206
98	H	1.480	2.700	19.893
99	H	-2.028	9.421	19.874

100	H	8.989	2.707	19.876
101	H	5.445	9.423	19.877
102	H	3.388	2.005	20.014
103	H	-0.128	8.710	20.009
104	H	10.887	2.004	20.013
105	H	7.339	8.724	20.010
106	H	-3.053	6.651	18.913
107	H	-6.606	13.358	18.921
108	H	4.409	6.729	18.848
109	H	0.888	13.386	18.901
110	H	-1.456	4.353	19.875
111	H	-4.991	11.082	19.878
112	H	6.007	4.361	19.872
113	H	2.493	11.065	19.854
114	H	-5.353	12.380	11.201
115	H	2.119	12.333	11.188
116	H	6.252	1.733	11.627
117	H	10.454	8.152	11.569
118	H	-0.209	2.072	11.178
119	H	5.485	10.831	15.323
120	H	6.179	9.582	14.251
121	H	5.412	9.109	15.780
122	H	1.982	9.726	14.699
123	H	2.977	10.860	15.647
124	H	3.019	9.120	16.037
125	H	0.510	8.333	16.012
126	H	-0.253	7.182	14.857

127	H	-1.254	8.090	16.011
128	H	-0.872	11.304	14.259
129	H	0.113	10.801	15.655
130	H	-1.639	10.484	15.649
131	H	5.084	6.322	15.997
132	H	6.201	5.706	14.743
133	H	5.494	4.581	15.932
134	H	2.085	4.836	14.402
135	H	2.663	5.679	15.867
136	H	2.989	3.932	15.626
137	H	-0.577	4.146	15.914
138	H	-0.295	3.060	14.526
139	H	13.150	2.927	15.474
140	H	-3.158	6.116	14.109
141	H	-2.341	5.951	15.676
142	H	11.393	4.738	15.168
143	H	5.929	5.662	11.054
144	H	6.270	7.484	11.476
145	H	3.328	7.549	13.962
146	H	1.711	7.215	13.853
147	N	4.043	9.606	14.215
148	N	-0.494	9.208	14.311
149	N	4.141	5.286	14.333
150	N	-1.673	4.610	14.138
151	C	5.327	9.803	14.913
152	C	2.961	9.840	15.190
153	C	-0.364	8.168	15.342

154	C	-0.734	10.499	14.993
155	C	5.270	5.473	15.282
156	C	2.943	4.916	15.094
157	C	-1.066	3.646	15.047
158	C	-2.724	5.379	14.803
159	O	0.471	3.301	1.812
160	O	-3.060	10.007	1.796
161	O	7.954	3.277	1.793
162	O	4.416	9.994	1.796
163	O	4.010	5.634	4.659
164	O	0.473	12.355	4.682
165	O	11.487	5.685	4.672
166	O	7.934	12.381	4.687
167	O	3.647	1.207	7.404
168	O	0.078	7.918	7.387
169	O	11.145	1.159	7.437
170	O	7.547	7.941	7.385
171	O	-0.328	4.236	10.584
172	O	-3.839	10.207	10.204
173	O	7.109	3.596	10.045
174	O	3.607	10.069	10.322
175	O	4.060	4.693	0.105
176	O	0.553	11.387	0.117
177	O	11.559	4.675	0.115
178	O	8.015	11.393	0.112
179	O	3.842	0.089	2.981
180	O	0.308	6.815	2.999

181	O	11.332	0.104	3.009
182	O	7.785	6.810	2.981
183	O	-0.018	2.378	5.860
184	O	-3.595	9.071	5.826
185	O	7.431	2.338	5.820
186	O	3.894	9.087	5.834
187	O	3.624	4.684	8.728
188	O	-0.004	11.332	8.710
189	O	11.004	4.652	8.639
190	O	7.455	11.426	8.698
191	O	-2.042	5.001	2.277
192	O	-5.590	11.706	2.274
193	O	5.428	4.997	2.257
194	O	1.906	11.707	2.277
195	O	5.146	0.590	5.103
196	O	1.619	7.306	5.115
197	O	12.643	0.616	5.133
198	O	9.071	7.321	5.108
199	O	1.199	2.834	8.015
200	O	-2.296	9.556	7.927
201	O	8.726	2.869	7.901
202	O	5.105	9.544	7.967
203	O	12.010	5.130	10.891
204	O	-6.190	12.008	10.788
205	O	5.026	5.131	10.910
206	O	1.366	11.890	10.692
207	O	6.287	1.183	0.754

208	O	2.755	7.900	0.751
209	O	13.764	1.191	0.768
210	O	10.226	7.902	0.755
211	O	2.437	3.451	3.444
212	O	-1.092	10.160	3.440
213	O	9.916	3.449	3.442
214	O	6.375	10.170	3.444
215	O	-1.459	5.728	6.256
216	O	-4.994	12.430	6.208
217	O	6.021	5.725	6.194
218	O	2.484	12.411	6.245
219	O	5.661	1.294	9.002
220	O	2.145	7.965	8.927
221	O	13.142	1.324	9.101
222	O	9.554	8.021	9.005
223	O	2.378	0.181	0.488
224	O	-1.150	6.893	0.491
225	O	9.856	0.195	0.504
226	O	6.314	6.913	0.490
227	O	6.018	2.448	3.290
228	O	2.483	9.161	3.292
229	O	13.492	2.463	3.309
230	O	9.958	9.162	3.289
231	O	2.123	4.657	6.085
232	O	-1.440	11.382	6.072
233	O	9.584	4.666	6.028
234	O	6.026	11.400	6.104

235	O	1.767	0.165	8.792
236	O	-1.852	6.948	8.901
237	O	9.217	0.317	8.896
238	O	5.633	6.910	8.815
239	O	2.547	5.708	2.103
240	O	-0.966	12.407	2.101
241	O	10.043	5.700	2.093
242	O	6.494	12.415	2.105
243	O	2.206	1.285	4.875
244	O	-1.359	8.005	4.863
245	O	9.695	1.278	4.892
246	O	6.136	8.005	4.855
247	O	-1.679	3.590	7.757
248	O	-5.278	10.307	7.718
249	O	5.746	3.564	7.654
250	O	2.215	10.280	7.767
251	O	1.237	6.756	11.061
252	O	-1.616	12.594	10.492
253	O	9.275	5.836	10.507
254	O	5.930	12.527	10.569
255	O	1.197	5.218	0.014
256	O	-2.330	11.927	0.014
257	O	8.667	5.215	0.020
258	O	5.138	11.929	0.022
259	O	0.886	0.757	2.833
260	O	-2.637	7.467	2.813
261	O	8.362	0.742	2.843

262	O	4.817	7.458	2.831
263	O	4.491	3.033	5.570
264	O	0.982	9.771	5.593
265	O	11.982	3.051	5.623
266	O	8.422	9.781	5.582
267	O	0.797	5.293	8.487
268	O	-2.880	12.018	8.408
269	O	8.150	5.393	8.331
270	O	4.524	11.992	8.510
271	O	3.992	2.417	1.653
272	O	0.462	9.126	1.657
273	O	11.470	2.415	1.666
274	O	7.931	9.131	1.656
275	O	0.109	4.637	4.490
276	O	-3.433	11.335	4.459
277	O	7.577	4.624	4.444
278	O	4.043	11.343	4.469
279	O	7.229	0.172	7.299
280	O	3.685	6.880	7.222
281	O	14.673	0.216	7.312
282	O	11.079	6.902	7.260
283	O	3.298	2.368	9.930
284	O	-0.254	9.109	10.077
285	O	10.814	2.422	9.917
286	O	7.181	9.179	9.815
287	O	2.475	4.305	11.499
288	O	-1.698	10.243	11.793

289	O	9.072	3.227	11.714
290	O	5.534	9.904	11.785
291	O	5.373	2.311	11.700
292	O	1.619	9.526	11.900
293	O	13.051	2.784	11.724
294	O	9.123	9.199	11.650
295	O	3.100	0.025	11.397
296	O	-1.095	6.963	12.302
297	O	3.538	13.405	11.418
298	O	6.965	6.807	11.330
299	O	4.233	1.334	19.942
300	O	0.709	8.031	19.940
301	O	11.724	1.325	19.950
302	O	8.179	8.043	19.940
303	O	2.330	2.873	20.335
304	O	-1.181	9.591	20.323
305	O	9.836	2.889	20.319
306	O	6.295	9.604	20.316
307	O	-0.897	3.697	20.322
308	O	-4.432	10.419	20.316
309	O	6.567	3.707	20.317
310	O	3.049	10.413	20.310
311	O	0.672	0.493	19.691
312	O	-2.849	7.198	19.690
313	O	8.162	0.491	19.692
314	O	4.619	7.206	19.665
315	O	4.129	7.442	11.334

316	O	7.503	1.017	11.242
317	O	-3.636	7.820	11.153
318	O	0.557	1.736	10.644
319	O	2.622	7.342	13.408

Fig. 3

Simulation box:

a=14.949	b=15.168	c=25.974	α=90.00	β90.00	γ=117.78

323 atoms

Atomic id	element	x	y	z
1	Hf	2.291	3.818	1.295
2	Hf	-1.245	10.525	1.304
3	Hf	9.766	3.815	1.293
4	Hf	6.226	10.527	1.304
5	Hf	-1.609	6.039	4.029
6	Hf	-5.153	12.741	4.042
7	Hf	5.855	6.038	4.017
8	Hf	2.319	12.735	4.040
9	Hf	5.512	1.582	6.889
10	Hf	1.945	8.312	6.904
11	Hf	12.979	1.642	6.885
12	Hf	9.433	8.333	6.865
13	Hf	1.713	3.804	9.608
14	Hf	-1.855	10.510	9.667
15	Hf	9.056	3.848	9.524
16	Hf	5.571	10.544	9.655
17	Hf	-1.601	3.248	1.315

18	Hf	-5.135	9.961	1.316
19	Hf	5.869	3.246	1.308
20	Hf	2.334	9.958	1.314
21	Hf	1.935	5.601	4.156
22	Hf	-1.610	12.298	4.167
23	Hf	9.407	5.601	4.150
24	Hf	5.860	12.307	4.171
25	Hf	1.562	1.128	6.934
26	Hf	-1.967	7.837	6.944
27	Hf	9.050	1.103	6.944
28	Hf	5.490	7.847	6.937
29	Hf	5.154	3.293	9.785
30	Hf	1.582	10.047	9.808
31	Hf	12.511	3.398	9.762
32	Hf	8.961	10.082	9.797
33	Hf	-6.669	13.308	1.119
34	Hf	-3.132	6.602	1.105
35	Hf	0.803	13.308	1.107
36	Hf	4.346	6.607	1.093
37	Hf	4.008	2.058	3.897
38	Hf	0.471	8.771	3.905
39	Hf	11.481	2.057	3.900
40	Hf	7.940	8.766	3.883
41	Hf	0.094	4.348	6.709
42	Hf	-3.455	11.028	6.742
43	Hf	7.532	4.317	6.652
44	Hf	4.015	11.021	6.733

45	Hf	3.702	6.579	9.463
46	Hf	0.205	13.273	9.548
47	Hf	11.158	6.626	9.507
48	Hf	7.637	13.327	9.470
49	Hf	4.287	0.305	0.990
50	Hf	0.751	7.018	0.990
51	Hf	11.758	0.307	0.992
52	Hf	8.226	7.021	0.980
53	Hf	0.479	2.523	3.845
54	Hf	-3.065	9.225	3.851
55	Hf	7.946	2.505	3.827
56	Hf	4.409	9.225	3.849
57	Hf	4.035	4.761	6.612
58	Hf	0.491	11.475	6.637
59	Hf	11.511	4.794	6.607
60	Hf	7.974	11.474	6.624
61	Hf	3.656	0.351	9.453
62	Hf	0.128	7.032	9.470
63	Hf	11.148	0.358	9.495
64	Hf	7.574	7.094	9.434
65	Hf	1.612	9.547	14.229
66	Hf	9.762	2.873	14.430
67	Hf	5.429	2.023	14.412
68	Hf	0.648	4.038	15.277
69	H	-0.325	3.742	11.138
70	H	-3.816	9.262	10.614
71	H	7.296	2.401	10.920

72	H	3.809	9.134	10.845
73	H	2.169	2.865	12.088
74	H	-1.319	9.798	12.480
75	H	10.249	2.341	11.471
76	H	6.849	9.940	12.147
77	H	1.793	5.746	11.496
78	H	-1.764	12.521	11.570
79	H	9.380	5.857	11.519
80	H	5.868	12.538	11.493
81	H	4.506	1.569	11.911
82	H	0.866	8.432	11.976
83	H	12.448	2.413	12.466
84	H	8.367	8.416	11.850
85	H	0.646	1.751	11.394
86	H	-2.579	9.064	11.853
87	H	8.844	1.840	12.045
88	H	5.290	10.031	12.558
89	H	2.641	0.535	12.026
90	H	-0.925	7.246	12.057
91	H	10.651	0.125	12.254
92	H	6.144	7.395	11.534
93	H	4.982	1.814	24.737
94	H	1.452	8.534	24.743
95	H	12.465	1.822	24.746
96	H	8.929	8.547	24.742
97	H	1.571	0.391	24.950
98	H	-1.959	7.106	24.945

99	H	9.049	0.394	24.936
100	H	5.513	7.109	24.912
101	H	0.375	4.723	25.591
102	H	-3.153	11.431	25.593
103	H	7.846	4.723	25.592
104	H	4.316	11.432	25.598
105	H	3.657	4.515	25.240
106	H	0.126	11.216	25.252
107	H	11.141	4.508	25.244
108	H	7.606	11.219	25.256
109	H	1.432	2.748	24.903
110	H	-2.098	9.467	24.903
111	H	8.915	2.756	24.896
112	H	5.377	9.476	24.900
113	H	3.331	2.012	25.046
114	H	-0.201	8.727	25.047
115	H	10.814	2.015	25.042
116	H	7.275	8.734	25.042
117	H	-3.172	6.721	23.928
118	H	0.358	0.012	23.931
119	H	4.291	6.731	23.905
120	H	7.832	0.020	23.919
121	H	-1.503	4.341	24.869
122	H	-5.030	11.066	24.876
123	H	5.972	4.337	24.855
124	H	2.440	11.058	24.869
125	H	-2.082	5.567	11.330

126	H	-5.440	12.301	11.214
127	H	5.641	5.640	11.050
128	H	2.126	12.338	11.187
129	H	3.742	7.581	12.028
130	H	7.039	0.700	12.056
131	H	10.501	8.072	11.643
132	H	13.978	1.549	11.494
133	H	7.505	2.908	17.530
134	H	7.559	3.939	16.316
135	H	1.567	7.417	16.231
136	H	2.379	6.786	15.033
137	H	3.315	5.203	15.514
138	H	3.335	3.632	15.337
139	H	4.353	7.540	14.356
140	H	4.411	5.981	14.167
141	H	6.868	4.986	15.101
142	H	9.372	5.390	13.537
143	O	0.399	3.310	1.840
144	O	-3.137	10.025	1.849
145	O	7.874	3.298	1.831
146	O	4.332	10.020	1.847
147	O	3.935	5.670	4.698
148	O	0.400	12.361	4.719
149	O	11.410	5.666	4.697
150	O	7.869	12.374	4.714
151	O	3.582	1.163	7.446
152	O	0.028	7.906	7.489

153	O	11.046	1.201	7.485
154	O	7.503	7.877	7.414
155	O	-0.424	3.882	10.171
156	O	-3.899	10.141	10.136
157	O	7.249	3.313	10.395
158	O	3.653	10.048	10.374
159	O	4.021	4.685	0.158
160	O	0.492	11.387	0.169
161	O	11.501	4.682	0.163
162	O	7.968	11.389	0.175
163	O	3.779	0.113	3.040
164	O	0.243	6.831	3.036
165	O	11.253	0.109	3.037
166	O	7.713	6.819	3.021
167	O	-0.122	2.366	5.860
168	O	-3.658	9.077	5.879
169	O	7.336	2.356	5.849
170	O	3.803	9.075	5.875
171	O	3.473	4.637	8.653
172	O	-0.076	11.357	8.708
173	O	10.924	4.651	8.682
174	O	7.380	11.392	8.684
175	O	-2.103	5.023	2.307
176	O	-5.642	11.728	2.318
177	O	5.367	5.023	2.296
178	O	1.834	11.725	2.313
179	O	5.095	0.610	5.148

180	O	1.535	7.312	5.171
181	O	12.550	0.620	5.162
182	O	9.027	7.331	5.131
183	O	1.105	2.839	7.961
184	O	-2.327	9.571	7.945
185	O	8.654	2.882	7.880
186	O	5.086	9.579	7.950
187	O	12.143	5.181	10.790
188	O	-6.207	11.897	10.726
189	O	4.891	5.136	10.625
190	O	1.357	11.842	10.722
191	O	6.217	1.198	0.806
192	O	2.683	7.915	0.801
193	O	13.692	1.201	0.813
194	O	10.158	7.915	0.807
195	O	2.370	3.463	3.479
196	O	-1.173	10.171	3.496
197	O	9.832	3.459	3.487
198	O	6.295	10.173	3.491
199	O	-1.532	5.728	6.255
200	O	-5.074	12.434	6.277
201	O	5.933	5.705	6.247
202	O	2.401	12.420	6.289
203	O	5.627	1.228	9.123
204	O	2.063	7.985	9.135
205	O	13.043	1.318	9.065
206	O	9.507	7.956	9.032

207	O	2.312	0.206	0.547
208	O	-1.219	6.923	0.541
209	O	9.787	0.215	0.547
210	O	6.255	6.933	0.531
211	O	5.937	2.483	3.329
212	O	2.399	9.180	3.342
213	O	13.414	2.483	3.340
214	O	9.879	9.189	3.335
215	O	2.041	4.640	6.069
216	O	-1.519	11.408	6.118
217	O	9.483	4.725	6.105
218	O	5.944	11.414	6.126
219	O	1.659	0.306	8.909
220	O	-1.889	6.967	8.933
221	O	9.141	0.323	8.930
222	O	5.600	6.973	8.852
223	O	2.487	5.713	2.133
224	O	-1.043	12.415	2.145
225	O	9.972	5.708	2.133
226	O	6.431	12.417	2.146
227	O	2.145	1.297	4.924
228	O	-1.402	8.008	4.931
229	O	9.611	1.282	4.927
230	O	6.064	8.000	4.911
231	O	-1.786	3.604	7.756
232	O	-5.348	10.280	7.739
233	O	5.724	3.533	7.786

234	O	2.145	10.271	7.804
235	O	1.949	5.759	10.518
236	O	-1.554	12.420	10.615
237	O	9.309	5.773	10.551
238	O	5.860	12.558	10.518
239	O	1.128	5.231	0.053
240	O	-2.400	11.938	0.056
241	O	8.601	5.231	0.055
242	O	5.069	11.940	0.059
243	O	0.817	0.767	2.882
244	O	-2.714	7.482	2.870
245	O	8.286	0.754	2.877
246	O	4.754	7.480	2.862
247	O	4.448	3.039	5.648
248	O	0.889	9.752	5.660
249	O	11.877	3.060	5.646
250	O	8.336	9.759	5.627
251	O	0.664	5.382	8.356
252	O	-2.953	12.002	8.483
253	O	7.971	5.285	8.454
254	O	4.441	12.004	8.512
255	O	3.919	2.430	1.696
256	O	0.381	9.141	1.704
257	O	11.392	2.432	1.701
258	O	7.855	9.143	1.699
259	O	0.031	4.651	4.496
260	O	-3.511	11.352	4.517

261	O	7.501	4.641	4.481
262	O	3.960	11.348	4.512
263	O	7.151	0.181	7.340
264	O	3.580	6.900	7.311
265	O	14.607	0.203	7.319
266	O	11.085	6.900	7.321
267	O	3.368	2.421	9.873
268	O	-0.232	9.139	9.957
269	O	10.608	2.484	10.039
270	O	7.115	9.148	9.818
271	O	1.427	2.952	11.461
272	O	-2.040	9.903	11.817
273	O	9.665	2.401	12.295
274	O	5.986	10.335	11.900
275	O	5.182	2.256	12.064
276	O	1.555	9.111	12.159
277	O	12.848	2.417	11.581
278	O	9.046	9.087	11.639
279	O	3.096	-0.024	11.369
280	O	-0.385	6.744	11.421
281	O	3.414	13.273	11.341
282	O	6.933	6.829	11.372
283	O	4.167	1.334	24.989
284	O	0.637	8.050	24.988
285	O	11.650	1.338	24.989
286	O	8.115	8.059	24.982
287	O	2.278	2.893	25.365

288	O	-1.253	9.606	25.369
289	O	9.760	2.899	25.359
290	O	6.222	9.612	25.366
291	O	-0.956	3.705	25.358
292	O	-4.487	10.421	25.358
293	O	6.521	3.713	25.356
294	O	2.987	10.424	25.360
295	O	0.593	0.487	24.746
296	O	-2.937	7.203	24.740
297	O	8.069	0.484	24.741
298	O	4.533	7.201	24.723
299	O	4.194	7.702	11.170
300	O	7.607	0.987	11.310
301	O	-3.591	7.844	11.185
302	O	-0.094	1.008	11.254
303	O	6.749	4.202	15.702
304	O	1.457	7.090	15.304
305	O	2.980	4.370	15.949
306	O	4.056	6.665	14.717
307	O	8.398	4.263	13.720
308	Cl	1.905	9.703	16.621
309	Cl	4.127	9.491	14.053
310	Cl	-0.731	9.024	14.330
311	Cl	1.707	11.829	13.956
312	Cl	10.021	3.824	16.527
313	Cl	10.612	5.925	13.553
314	Cl	11.634	1.397	14.443

315	Cl	8.016	1.328	14.989
316	Cl	4.753	1.601	16.608
317	Cl	5.561	4.589	13.206
318	Cl	5.490	-0.247	13.814
319	Cl	3.016	2.015	14.046
320	Cl	0.587	4.077	17.595
321	Cl	1.758	5.045	13.363
322	Cl	-0.067	1.866	14.852
323	Cl	-1.409	5.043	14.816

SI Fig. 1a

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

129 atoms

Atomic id	element	x	y	z
1	Al	0.110	0.020	6.080
2	Al	-2.269	4.102	6.121
3	Al	0.131	8.223	6.102
4	Al	2.492	4.107	6.099
5	Al	0.146	2.801	1.523
6	Al	-2.338	6.867	1.611
7	Al	4.921	2.781	1.786
8	Al	2.504	6.791	1.525
9	Al	0.099	0.002	3.369
10	Al	-2.226	4.117	3.409
11	Al	0.098	8.212	3.381
12	Al	2.474	4.105	3.390

13	Al	2.501	1.394	7.913
14	Al	0.101	5.440	7.916
15	Al	7.269	1.310	7.928
16	Al	4.882	5.595	7.820
17	Al	2.405	1.470	1.192
18	Al	0.098	5.554	1.285
19	Al	7.294	1.317	1.220
20	Al	4.842	5.387	1.200
21	Al	0.117	2.745	5.589
22	Al	-2.259	6.858	5.570
23	Al	4.857	2.718	5.590
24	Al	2.498	6.860	5.587
25	Al	2.478	1.357	3.875
26	Al	0.129	5.482	3.913
27	Al	7.247	1.364	3.888
28	Al	4.867	5.491	3.896
29	Al	0.085	2.712	8.235
30	Al	-2.206	6.886	8.210
31	Al	4.911	2.727	8.260
32	Al	2.429	6.812	8.244
33	Al	4.146	4.005	11.552
34	O	-3.174	8.223	4.727
35	O	-0.811	4.117	4.748
36	O	1.576	8.227	4.739
37	O	3.966	4.102	4.752
38	O	4.019	1.401	9.140
39	O	1.572	5.478	9.112

40	O	-0.751	1.371	9.110
41	O	-3.155	5.614	9.188
42	O	1.657	2.854	0.411
43	O	-0.828	6.882	0.334
44	O	6.171	2.462	0.332
45	O	3.994	6.699	0.307
46	O	-0.612	1.262	4.730
47	O	-3.001	5.371	4.766
48	O	4.123	1.243	4.742
49	O	1.779	5.376	4.745
50	O	1.717	2.722	9.091
51	O	-0.649	6.761	9.140
52	O	6.550	2.639	9.094
53	O	4.033	6.699	9.112
54	O	-0.704	4.168	0.347
55	O	-3.150	8.216	0.342
56	O	4.176	3.873	0.436
57	O	1.803	8.114	0.354
58	O	1.775	2.846	4.740
59	O	-0.617	6.962	4.734
60	O	6.505	2.846	4.752
61	O	4.145	6.965	4.742
62	O	1.779	0.058	9.144
63	O	-0.627	4.134	9.110
64	O	6.514	0.018	9.111
65	O	4.429	4.023	9.597
66	O	-0.705	1.607	0.279

67	O	-3.052	5.564	0.350
68	O	3.953	1.160	0.039
69	O	1.634	5.556	0.343
70	O	1.007	1.381	2.523
71	O	-1.374	5.520	2.534
72	O	5.765	1.345	2.524
73	O	3.398	5.451	2.529
74	O	-1.364	2.704	6.925
75	O	-3.712	6.899	6.945
76	O	3.420	2.766	6.998
77	O	1.009	6.820	6.928
78	O	3.204	0.104	2.469
79	O	0.803	4.230	2.583
80	O	7.976	0.074	2.508
81	O	5.638	4.222	2.572
82	O	0.883	1.470	6.939
83	O	-1.540	5.593	6.957
84	O	5.609	1.486	6.946
85	O	3.251	5.557	6.954
86	O	3.266	2.601	2.561
87	O	0.850	6.768	2.521
88	O	7.968	2.644	2.501
89	O	5.582	6.748	2.532
90	O	0.838	3.998	6.929
91	O	-1.507	8.146	6.966
92	O	5.598	4.058	7.051
93	O	3.231	8.095	6.940

94	C	3.814	5.898	12.105
95	C	5.916	3.396	12.231
96	C	2.675	2.762	12.081
97	H	2.187	0.185	10.016
98	H	-1.600	4.015	9.188
99	H	1.951	4.575	9.195
100	H	6.615	2.276	9.997
101	H	3.796	1.674	10.051
102	H	-0.263	0.530	9.226
103	H	5.536	-0.011	9.211
104	H	-0.608	6.253	9.969
105	H	3.902	6.354	10.020
106	H	-0.021	0.970	0.000
107	H	6.416	3.195	23.219
108	H	3.207	3.664	0.297
109	H	-0.271	3.898	22.984
110	H	-2.363	4.853	0.331
111	H	-1.128	6.505	22.958
112	H	2.122	7.867	22.941
113	H	1.829	4.578	0.254
114	H	4.227	0.179	0.131
115	H	-2.836	8.062	22.904
116	H	-3.504	6.132	9.939
117	H	5.374	4.337	9.700
118	H	1.675	2.535	10.047
119	H	4.753	1.694	23.236
120	H	4.642	7.431	0.258

121	H	3.710	5.822	13.200
122	H	4.648	6.607	11.965
123	H	2.895	6.392	11.758
124	H	5.912	3.523	13.326
125	H	6.779	3.977	11.869
126	H	6.152	2.331	12.065
127	H	2.734	2.762	13.183
128	H	2.746	1.692	11.821
129	H	1.653	3.107	11.857

SI Fig. 1b

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

129 atoms

Atomic id	element	x	y	z
1	Al	-4.666	8.207	6.129
2	Al	-2.297	4.086	6.130
3	Al	0.091	8.219	6.113
4	Al	2.471	4.084	6.113
5	Al	0.117	2.766	1.566
6	Al	-2.369	6.836	1.651
7	Al	4.896	2.751	1.819
8	Al	2.474	6.762	1.571
9	Al	-4.684	8.205	3.405
10	Al	-2.254	4.093	3.436
11	Al	0.069	8.192	3.402
12	Al	2.440	4.073	3.415

13	Al	2.443	1.330	7.968
14	Al	0.128	5.446	7.893
15	Al	7.208	1.354	7.992
16	Al	4.823	5.505	7.911
17	Al	2.377	1.435	1.234
18	Al	0.068	5.521	1.330
19	Al	7.264	1.285	1.255
20	Al	4.809	5.348	1.241
21	Al	0.084	2.713	5.631
22	Al	-2.285	6.838	5.607
23	Al	4.837	2.707	5.595
24	Al	2.462	6.847	5.595
25	Al	2.439	1.335	3.913
26	Al	0.100	5.463	3.940
27	Al	7.222	1.344	3.912
28	Al	4.837	5.468	3.929
29	Al	0.085	2.693	8.293
30	Al	-2.234	6.820	8.254
31	Al	4.818	2.701	8.214
32	Al	2.442	6.887	8.239
33	Al	2.254	3.219	10.700
34	O	-3.206	8.194	4.769
35	O	-0.837	4.095	4.780
36	O	1.543	8.215	4.753
37	O	3.925	4.081	4.778
38	O	4.011	1.339	9.074
39	O	1.627	5.495	9.069

40	O	-0.816	1.373	9.107
41	O	-3.104	5.452	9.239
42	O	1.629	2.823	0.451
43	O	-0.850	6.847	0.371
44	O	6.156	2.444	0.368
45	O	3.968	6.665	0.340
46	O	-0.642	1.238	4.754
47	O	-3.029	5.357	4.804
48	O	4.091	1.231	4.760
49	O	1.747	5.353	4.769
50	O	1.663	2.586	9.202
51	O	-0.644	6.736	9.147
52	O	6.356	2.609	9.173
53	O	4.047	6.740	9.175
54	O	-0.739	4.128	0.385
55	O	-3.174	8.177	0.383
56	O	4.141	3.833	0.468
57	O	1.779	8.081	0.392
58	O	1.733	2.816	4.761
59	O	-0.651	6.947	4.757
60	O	6.482	2.831	4.763
61	O	4.111	6.943	4.777
62	O	-3.000	8.184	9.176
63	O	-0.596	4.167	9.142
64	O	6.495	0.032	9.137
65	O	4.101	4.092	9.330
66	O	-0.721	1.561	0.319

67	O	-3.080	5.528	0.387
68	O	3.927	1.135	0.070
69	O	1.611	5.528	0.387
70	O	0.978	1.346	2.557
71	O	-1.405	5.494	2.561
72	O	5.736	1.318	2.540
73	O	3.367	5.423	2.561
74	O	-1.391	2.713	6.970
75	O	-3.747	6.834	7.017
76	O	3.363	2.722	6.995
77	O	0.986	6.833	6.921
78	O	3.173	0.075	2.492
79	O	0.773	4.202	2.607
80	O	7.945	0.043	2.544
81	O	5.601	4.192	2.600
82	O	0.839	1.427	6.972
83	O	-1.544	5.555	6.978
84	O	5.579	1.472	6.940
85	O	3.221	5.554	6.973
86	O	3.236	2.568	2.590
87	O	0.819	6.735	2.557
88	O	7.941	2.613	2.527
89	O	5.553	6.724	2.568
90	O	0.827	3.973	6.965
91	O	-1.550	8.093	6.975
92	O	5.566	4.027	7.018
93	O	3.201	8.108	6.962

94	C	1.371	4.454	11.890
95	C	3.429	2.149	11.843
96	C	0.051	1.128	12.068
97	H	2.101	0.187	10.050
98	H	-1.470	4.357	9.358
99	H	2.129	4.670	8.895
100	H	6.719	3.507	9.263
101	H	3.963	1.427	10.045
102	H	-0.323	0.538	9.206
103	H	5.524	0.015	9.236
104	H	-0.563	6.287	10.008
105	H	3.794	6.364	10.038
106	H	-0.042	0.915	0.063
107	H	6.413	3.185	23.270
108	H	3.167	3.616	0.355
109	H	-0.298	3.854	23.033
110	H	-2.390	4.822	0.380
111	H	-1.154	6.462	23.000
112	H	2.119	7.833	22.986
113	H	1.814	4.549	0.302
114	H	4.211	0.157	0.170
115	H	-2.856	8.024	22.947
116	H	6.087	5.915	10.033
117	H	4.824	4.136	10.000
118	H	0.202	1.430	11.059
119	H	4.717	1.674	23.256
120	H	4.631	7.387	0.309

121	H	1.363	4.039	12.931
122	H	1.947	5.411	11.967
123	H	0.328	4.718	11.624
124	H	3.066	2.406	12.857
125	H	4.464	2.538	11.799
126	H	3.497	1.049	11.811
127	H	0.735	1.697	12.714
128	H	0.247	0.071	12.191
129	H	-0.983	1.343	12.327

SI Fig. 1c is a duplicate of Fig. 1a.

SI Fig. 1d

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

127 atoms

Atomic id	element	x	y	z
1	Al	0.079	0.050	6.094
2	Al	-2.306	4.102	6.131
3	Al	4.839	0.000	6.130
4	Al	2.462	4.102	6.090
5	Al	0.107	2.808	1.537
6	Al	-2.373	6.875	1.621
7	Al	4.885	2.788	1.792
8	Al	2.466	6.800	1.536
9	Al	0.061	0.008	3.381
10	Al	-2.265	4.127	3.419

11	Al	0.065	8.222	3.390
12	Al	2.433	4.113	3.394
13	Al	2.480	1.391	8.002
14	Al	0.039	5.474	7.908
15	Al	7.234	1.363	7.973
16	Al	4.857	5.604	7.787
17	Al	2.365	1.476	1.207
18	Al	0.061	5.560	1.294
19	Al	7.257	1.328	1.231
20	Al	4.807	5.393	1.210
21	Al	0.078	2.759	5.617
22	Al	-2.301	6.868	5.582
23	Al	4.834	2.717	5.606
24	Al	2.463	6.869	5.581
25	Al	2.440	1.368	3.886
26	Al	0.090	5.494	3.921
27	Al	7.215	1.375	3.899
28	Al	4.829	5.494	3.905
29	Al	0.101	2.724	8.285
30	Al	-2.263	6.872	8.241
31	Al	4.847	2.732	8.276
32	Al	2.393	6.878	8.227
33	Al	2.499	3.454	10.513
34	Al	5.689	1.083	10.141
35	O	1.542	0.004	4.742
36	O	-0.848	4.125	4.759
37	O	6.286	0.005	4.741

38	O	3.927	4.094	4.769
39	O	4.029	1.444	9.354
40	O	1.582	5.443	9.057
41	O	-0.767	1.402	9.130
42	O	6.273	5.554	9.138
43	O	1.617	2.861	0.421
44	O	-0.858	6.889	0.338
45	O	6.141	2.468	0.330
46	O	3.956	6.698	0.313
47	O	-0.649	1.280	4.749
48	O	-3.041	5.380	4.778
49	O	4.087	1.259	4.758
50	O	1.740	5.381	4.746
51	O	1.700	2.701	9.168
52	O	-0.713	6.716	9.182
53	O	6.350	2.534	9.234
54	O	3.980	6.635	9.141
55	O	-0.754	4.176	0.359
56	O	-3.187	8.221	0.354
57	O	4.143	3.874	0.447
58	O	1.773	8.123	0.366
59	O	1.737	2.852	4.757
60	O	-0.660	6.979	4.748
61	O	6.473	2.853	4.767
62	O	4.104	6.977	4.738
63	O	1.703	0.047	9.139
64	O	-0.658	4.139	9.139

65	O	6.514	0.004	9.110
66	O	4.075	4.025	9.715
67	O	-0.741	1.615	0.290
68	O	-3.084	5.572	0.366
69	O	3.916	1.175	0.042
70	O	1.596	5.562	0.357
71	O	0.968	1.388	2.545
72	O	-1.410	5.526	2.548
73	O	5.726	1.355	2.533
74	O	3.363	5.455	2.538
75	O	-1.402	2.736	6.971
76	O	-3.751	6.908	6.936
77	O	3.374	2.772	7.067
78	O	0.976	6.830	6.921
79	O	3.171	0.114	2.476
80	O	0.768	4.237	2.586
81	O	7.940	0.090	2.519
82	O	5.602	4.228	2.581
83	O	0.860	1.495	6.968
84	O	-1.582	5.604	6.962
85	O	5.564	1.489	6.946
86	O	3.216	5.564	6.943
87	O	3.227	2.606	2.569
88	O	0.813	6.780	2.534
89	O	7.930	2.655	2.513
90	O	5.547	6.758	2.542
91	O	0.808	4.025	6.946

92	O	-1.538	8.152	7.019
93	O	5.537	4.049	7.046
94	O	3.206	8.115	6.951
95	C	1.773	4.619	11.897
96	C	2.871	1.560	11.814
97	C	6.039	1.085	12.080
98	H	1.994	0.245	10.039
99	H	-1.621	3.979	9.249
100	H	1.961	4.615	8.692
101	H	3.361	1.641	10.670
102	H	-0.273	0.566	9.226
103	H	-0.715	6.140	9.963
104	H	3.748	6.068	9.898
105	H	-0.054	0.969	0.026
106	H	6.403	3.216	23.244
107	H	3.172	3.670	0.313
108	H	-0.315	3.899	22.997
109	H	-2.391	4.866	0.340
110	H	-1.152	6.510	22.961
111	H	2.099	7.878	22.951
112	H	1.794	4.583	0.267
113	H	4.201	0.203	0.140
114	H	-2.867	8.072	22.918
115	H	5.884	6.019	9.895
116	H	4.904	4.063	10.235
117	H	4.709	1.716	23.236
118	H	4.609	7.428	0.262

119	H	1.872	4.331	12.947
120	H	2.190	5.632	11.772
121	H	0.698	4.713	11.662
122	H	1.800	1.754	12.060
123	H	3.486	2.006	12.611
124	H	3.010	0.470	11.938
125	H	5.851	2.070	12.554
126	H	5.500	0.333	12.679
127	H	7.122	0.892	12.226

SI Fig. 2a

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

128 atoms

Atomic id	element	x	y	z
1	Al	0.139	0.056	6.130
2	Al	-2.257	4.136	6.122
3	Al	4.897	0.027	6.121
4	Al	2.522	4.117	6.042
5	Al	0.159	2.819	1.535
6	Al	-2.320	6.886	1.624
7	Al	4.941	2.799	1.785
8	Al	2.523	6.819	1.536
9	Al	0.116	0.024	3.394
10	Al	-2.209	4.139	3.413
11	Al	4.867	0.005	3.391
12	Al	2.492	4.126	3.371

13	Al	2.556	1.366	8.005
14	Al	0.090	5.516	7.879
15	Al	7.304	1.417	8.064
16	Al	4.934	5.583	7.869
17	Al	2.425	1.480	1.204
18	Al	0.117	5.576	1.288
19	Al	7.312	1.344	1.229
20	Al	4.856	5.405	1.208
21	Al	0.136	2.760	5.593
22	Al	-2.244	6.886	5.603
23	Al	4.893	2.733	5.573
24	Al	2.518	6.899	5.583
25	Al	2.492	1.375	3.884
26	Al	0.144	5.509	3.920
27	Al	7.268	1.385	3.897
28	Al	4.891	5.520	3.904
29	Al	0.090	2.801	8.214
30	Al	-2.216	6.944	8.271
31	Al	4.887	2.745	8.181
32	Al	2.507	6.967	8.229
33	Al	2.386	3.905	10.280
34	Al	5.461	0.997	9.995
35	Al	0.648	0.960	10.056
36	O	1.590	0.017	4.742
37	O	-0.783	4.135	4.754
38	O	6.339	0.019	4.737
39	O	3.985	4.117	4.743

40	O	4.004	1.481	9.131
41	O	1.791	5.322	8.991
42	O	-0.714	1.488	9.130
43	O	-3.107	5.546	9.150
44	O	1.677	2.868	0.414
45	O	-0.808	6.900	0.337
46	O	6.195	2.487	0.323
47	O	4.013	6.717	0.311
48	O	-0.598	1.288	4.745
49	O	-2.975	5.396	4.763
50	O	4.138	1.272	4.734
51	O	1.799	5.403	4.750
52	O	1.579	2.593	9.356
53	O	-0.589	6.782	9.151
54	O	6.297	2.506	9.275
55	O	4.106	6.765	9.142
56	O	-0.690	4.187	0.351
57	O	1.622	0.011	0.341
58	O	4.187	3.886	0.446
59	O	1.829	8.138	0.368
60	O	1.783	2.875	4.726
61	O	-0.602	6.986	4.743
62	O	6.531	2.876	4.737
63	O	4.153	6.985	4.749
64	O	1.810	0.056	9.154
65	O	-0.580	4.237	9.112
66	O	6.584	0.008	9.162

67	O	4.105	4.145	9.439
68	O	-0.680	1.625	0.291
69	O	-3.032	5.585	0.365
70	O	3.975	1.186	0.037
71	O	1.650	5.589	0.344
72	O	1.022	1.400	2.532
73	O	-1.352	5.537	2.538
74	O	5.781	1.366	2.524
75	O	3.416	5.473	2.531
76	O	-1.359	2.764	6.958
77	O	-3.708	6.894	6.943
78	O	3.391	2.795	7.003
79	O	1.049	6.850	6.949
80	O	3.224	0.124	2.472
81	O	0.829	4.255	2.574
82	O	7.994	0.100	2.525
83	O	5.655	4.243	2.571
84	O	0.913	1.528	6.951
85	O	-1.526	5.625	6.958
86	O	5.638	1.517	6.905
87	O	3.282	5.573	6.973
88	O	3.280	2.620	2.555
89	O	0.867	6.792	2.532
90	O	-1.523	2.668	2.502
91	O	5.599	6.776	2.546
92	O	0.870	4.050	6.939
93	O	-1.493	8.148	6.970

94	O	5.602	4.068	7.022
95	O	3.247	8.148	6.953
96	O	3.312	2.671	11.617
97	C	1.701	4.966	11.810
98	C	5.364	0.698	11.967
99	C	0.529	0.780	12.002
100	H	-1.551	4.192	9.248
101	H	2.271	4.880	8.242
102	H	-0.629	6.281	9.984
103	H	3.924	6.356	10.003
104	H	-0.003	0.978	0.019
105	H	6.446	3.238	23.237
106	H	3.216	3.673	0.318
107	H	-0.259	3.916	22.987
108	H	-2.341	4.876	0.347
109	H	-1.114	6.519	22.964
110	H	2.142	7.895	22.952
111	H	1.856	4.619	0.244
112	H	4.258	0.210	0.133
113	H	-2.810	8.081	22.906
114	H	-3.387	5.918	10.004
115	H	4.860	4.004	10.051
116	H	4.767	1.728	23.230
117	H	4.667	7.446	0.267
118	H	1.824	4.590	12.837
119	H	2.113	5.987	11.809
120	H	0.619	5.094	11.658

121	H	5.513	1.562	12.629
122	H	4.524	0.104	12.357
123	H	6.258	0.073	12.129
124	H	3.928	1.900	11.555
125	H	2.927	2.702	12.523
126	H	0.338	1.759	12.467
127	H	9.206	0.134	12.314
128	H	1.444	0.371	12.453

SI Fig. 2b

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

128 atoms

Atomic id	element	x	y	z
1	Al	0.136	0.049	6.124
2	Al	-2.248	4.143	6.122
3	Al	4.895	0.028	6.114
4	Al	2.521	4.129	6.042
5	Al	0.170	2.820	1.525
6	Al	-2.321	6.889	1.622
7	Al	4.940	2.798	1.786
8	Al	2.522	6.819	1.535
9	Al	0.115	0.024	3.393
10	Al	-2.208	4.138	3.411
11	Al	4.866	0.004	3.389
12	Al	2.491	4.124	3.366
13	Al	2.532	1.369	7.973

14	Al	0.110	5.522	7.892
15	Al	7.333	1.412	8.031
16	Al	4.929	5.589	7.876
17	Al	2.422	1.485	1.196
18	Al	0.116	5.574	1.288
19	Al	7.313	1.345	1.229
20	Al	4.856	5.405	1.207
21	Al	0.138	2.760	5.591
22	Al	-2.241	6.886	5.603
23	Al	4.895	2.737	5.561
24	Al	2.514	6.895	5.588
25	Al	2.493	1.372	3.881
26	Al	0.143	5.509	3.918
27	Al	7.268	1.385	3.893
28	Al	4.890	5.521	3.905
29	Al	0.103	2.819	8.227
30	Al	-2.214	6.940	8.269
31	Al	4.871	2.783	8.163
32	Al	2.505	6.938	8.237
33	Al	2.462	3.773	10.429
34	Al	5.430	0.988	9.836
35	Al	0.663	0.972	10.062
36	O	1.591	0.019	4.743
37	O	-0.785	4.138	4.756
38	O	6.343	0.022	4.741
39	O	3.987	4.121	4.742
40	O	3.983	1.460	9.078

41	O	1.760	5.359	8.983
42	O	-0.713	1.498	9.130
43	O	-3.100	5.544	9.155
44	O	1.677	2.874	0.413
45	O	-0.808	6.899	0.338
46	O	6.194	2.487	0.324
47	O	4.013	6.717	0.312
48	O	-0.603	1.287	4.750
49	O	-2.975	5.397	4.766
50	O	4.140	1.270	4.740
51	O	1.795	5.403	4.751
52	O	1.579	2.586	9.345
53	O	-0.585	6.805	9.175
54	O	6.285	2.476	9.280
55	O	4.108	6.762	9.149
56	O	-0.692	4.188	0.352
57	O	1.622	0.005	0.344
58	O	4.186	3.888	0.447
59	O	1.829	8.138	0.368
60	O	1.785	2.874	4.725
61	O	-0.599	6.986	4.742
62	O	6.533	2.874	4.741
63	O	4.153	6.989	4.752
64	O	1.812	0.056	9.146
65	O	-0.588	4.246	9.117
66	O	6.610	-0.031	9.227
67	O	4.111	4.138	9.412

68	O	-0.684	1.622	0.293
69	O	-3.033	5.585	0.368
70	O	3.975	1.186	0.039
71	O	1.651	5.590	0.344
72	O	1.023	1.399	2.538
73	O	-1.353	5.538	2.540
74	O	5.781	1.367	2.525
75	O	3.417	5.476	2.534
76	O	-1.360	2.771	6.964
77	O	-3.706	6.896	6.946
78	O	3.392	2.797	6.991
79	O	1.048	6.870	6.950
80	O	3.223	0.124	2.474
81	O	0.825	4.256	2.579
82	O	7.992	0.100	2.526
83	O	5.652	4.243	2.571
84	O	0.905	1.523	6.949
85	O	-1.515	5.629	6.967
86	O	5.646	1.516	6.915
87	O	3.285	5.583	6.961
88	O	3.285	2.617	2.565
89	O	0.868	6.790	2.532
90	O	-1.523	2.668	2.503
91	O	5.599	6.774	2.546
92	O	0.873	4.048	6.938
93	O	-1.496	8.151	6.961
94	O	5.609	4.077	7.023

95	O	3.249	8.151	6.978
96	O	3.372	2.684	11.549
97	C	1.674	4.989	11.805
98	C	5.239	0.760	12.131
99	C	0.519	0.777	12.005
100	H	-1.560	4.205	9.240
101	H	2.256	4.821	8.324
102	H	-0.629	6.253	9.978
103	H	3.915	6.344	10.004
104	H	-0.002	0.980	0.022
105	H	6.445	3.238	23.239
106	H	3.213	3.671	0.319
107	H	-0.259	3.915	22.989
108	H	-2.342	4.876	0.347
109	H	-1.115	6.519	22.966
110	H	2.143	7.895	22.952
111	H	1.857	4.617	0.244
112	H	4.259	0.210	0.133
113	H	-2.810	8.082	22.908
114	H	-3.386	5.917	10.007
115	H	4.844	4.014	10.055
116	H	4.767	1.728	23.231
117	H	4.667	7.446	0.267
118	H	1.798	4.626	12.839
119	H	2.104	6.004	11.797
120	H	0.593	5.129	11.653
121	H	5.558	1.474	12.895

122	H	4.562	0.038	12.590
123	H	6.133	0.225	11.775
124	H	4.559	1.437	11.506
125	H	2.990	2.744	12.439
126	H	0.337	1.757	12.471
127	H	9.199	0.127	12.317
128	H	1.441	0.376	12.450

SI Fig. 2c

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

131 atoms

Atomic id	element	x	y	z
1	Al	0.142	0.054	6.125
2	Al	-2.258	4.138	6.121
3	Al	4.901	0.025	6.120
4	Al	2.521	4.116	6.043
5	Al	0.165	2.817	1.527
6	Al	-2.324	6.884	1.615
7	Al	4.939	2.797	1.787
8	Al	2.519	6.819	1.530
9	Al	0.117	0.017	3.390
10	Al	-2.207	4.136	3.413
11	Al	4.866	0.003	3.391
12	Al	2.491	4.123	3.371
13	Al	2.552	1.371	8.001
14	Al	0.088	5.523	7.880

15	Al	7.300	1.421	8.059
16	Al	4.934	5.582	7.871
17	Al	2.421	1.481	1.205
18	Al	0.112	5.573	1.287
19	Al	7.313	1.343	1.227
20	Al	4.852	5.403	1.204
21	Al	0.134	2.759	5.592
22	Al	-2.242	6.885	5.601
23	Al	4.896	2.731	5.575
24	Al	2.522	6.895	5.582
25	Al	2.494	1.372	3.885
26	Al	0.147	5.507	3.918
27	Al	7.271	1.382	3.894
28	Al	4.890	5.514	3.902
29	Al	0.090	2.809	8.215
30	Al	-2.218	6.947	8.265
31	Al	4.881	2.747	8.189
32	Al	2.511	6.976	8.226
33	Al	2.358	3.950	10.273
34	Al	0.647	0.969	10.058
35	Al	4.677	2.754	10.296
36	O	1.591	0.015	4.739
37	O	-0.784	4.138	4.756
38	O	6.344	0.017	4.738
39	O	3.983	4.116	4.747
40	O	3.997	1.477	9.152
41	O	1.793	5.335	8.989

42	O	-0.716	1.495	9.135
43	O	-3.102	5.547	9.145
44	O	1.678	2.867	0.426
45	O	-0.812	6.899	0.336
46	O	6.193	2.492	0.337
47	O	4.009	6.718	0.311
48	O	-0.598	1.285	4.746
49	O	-2.976	5.394	4.763
50	O	4.144	1.267	4.738
51	O	1.798	5.399	4.750
52	O	1.578	2.606	9.360
53	O	-0.590	6.793	9.145
54	O	6.293	2.515	9.283
55	O	4.108	6.769	9.144
56	O	-0.692	4.181	0.349
57	O	1.617	0.003	0.349
58	O	4.181	3.886	0.442
59	O	1.821	8.143	0.359
60	O	1.784	2.866	4.734
61	O	-0.595	6.981	4.743
62	O	6.537	2.868	4.742
63	O	4.160	6.980	4.747
64	O	1.800	0.061	9.145
65	O	-0.579	4.243	9.123
66	O	6.586	0.019	9.148
67	O	4.102	4.149	9.434
68	O	-0.686	1.623	0.283

69	O	-3.040	5.579	0.352
70	O	3.972	1.188	0.044
71	O	1.646	5.586	0.341
72	O	1.022	1.398	2.536
73	O	-1.357	5.535	2.534
74	O	5.783	1.365	2.526
75	O	3.412	5.471	2.530
76	O	-1.361	2.773	6.964
77	O	-3.707	6.895	6.944
78	O	3.386	2.795	7.008
79	O	1.053	6.850	6.949
80	O	3.221	0.123	2.474
81	O	0.826	4.254	2.581
82	O	7.996	0.098	2.519
83	O	5.649	4.237	2.577
84	O	0.907	1.529	6.956
85	O	-1.525	5.627	6.956
86	O	5.636	1.515	6.912
87	O	3.280	5.573	6.974
88	O	3.283	2.616	2.566
89	O	0.868	6.790	2.528
90	O	-1.521	2.665	2.504
91	O	5.593	6.765	2.533
92	O	0.872	4.052	6.947
93	O	-1.489	8.155	6.964
94	O	5.602	4.068	7.021
95	O	3.258	8.153	6.953

96	O	3.528	3.548	11.573
97	O	2.323	2.368	11.320
98	C	1.678	5.000	11.810
99	C	0.538	0.785	12.007
100	C	4.579	2.447	12.250
101	H	-1.552	4.196	9.253
102	H	2.269	4.892	8.238
103	H	-0.625	6.295	9.981
104	H	3.926	6.355	10.004
105	H	-0.005	0.978	0.015
106	H	6.443	3.239	23.242
107	H	3.208	3.669	0.321
108	H	-0.258	3.913	22.987
109	H	-2.348	4.872	0.338
110	H	-1.121	6.519	22.963
111	H	2.142	7.899	22.945
112	H	1.854	4.615	0.244
113	H	4.258	0.212	0.134
114	H	-2.819	8.080	22.912
115	H	-3.381	5.909	10.004
116	H	4.896	4.132	10.040
117	H	4.762	1.731	23.232
118	H	4.662	7.447	0.271
119	H	1.815	4.601	12.826
120	H	2.096	6.019	11.820
121	H	0.593	5.126	11.668
122	H	3.972	2.689	11.365

123	H	3.136	3.514	12.464
124	H	0.344	1.765	12.470
125	H	9.212	0.141	12.317
126	H	1.450	0.375	12.462
127	H	4.695	3.334	12.888
128	H	3.728	1.860	12.629
129	H	5.469	1.829	12.443
130	H	2.768	1.509	11.112
131	H	1.932	2.334	12.211

SI Fig. 2d

Simulation box:

a=9.510	b=9.502	c=23.470	α=90.00	β90.00	γ=119.99

131 atoms

Atomic id	element	x	y	z
1	Al	0.146	0.188	6.110
2	Al	-2.223	4.276	6.107
3	Al	4.879	0.169	6.069
4	Al	2.550	4.274	6.075
5	Al	0.190	2.960	1.527
6	Al	-2.293	7.029	1.613
7	Al	4.966	2.943	1.779
8	Al	2.549	6.955	1.525
9	Al	0.140	0.165	3.380
10	Al	-2.187	4.275	3.408
11	Al	4.890	0.154	3.368
12	Al	2.514	4.267	3.381

13	Al	2.419	1.628	8.011
14	Al	0.177	5.630	7.764
15	Al	7.310	1.525	8.040
16	Al	4.977	5.632	7.860
17	Al	2.448	1.630	1.200
18	Al	0.146	5.712	1.284
19	Al	7.340	1.478	1.215
20	Al	4.886	5.550	1.202
21	Al	0.162	2.901	5.603
22	Al	-2.237	7.030	5.611
23	Al	4.906	2.881	5.605
24	Al	2.540	7.045	5.546
25	Al	2.514	1.525	3.884
26	Al	0.160	5.653	3.910
27	Al	7.290	1.531	3.882
28	Al	4.912	5.657	3.899
29	Al	0.059	2.973	8.293
30	Al	-2.211	7.159	8.282
31	Al	4.860	2.959	8.256
32	Al	2.536	6.967	8.148
33	Al	1.731	3.510	10.938
34	Al	0.120	0.314	9.879
35	Al	5.232	0.715	9.427
36	O	1.610	0.164	4.751
37	O	-0.774	4.281	4.760
38	O	6.362	0.168	4.720
39	O	4.005	4.264	4.744

40	O	3.816	1.680	9.249
41	O	1.637	5.645	9.007
42	O	-0.731	1.628	9.155
43	O	-2.970	5.706	9.105
44	O	1.699	3.013	0.419
45	O	-0.775	7.043	0.337
46	O	6.232	2.632	0.329
47	O	4.040	6.860	0.307
48	O	-0.586	1.432	4.746
49	O	-2.955	5.542	4.766
50	O	4.164	1.419	4.733
51	O	1.812	5.550	4.739
52	O	1.614	3.002	9.226
53	O	-0.555	7.254	9.318
54	O	6.191	2.369	9.269
55	O	4.154	6.917	9.252
56	O	-0.659	4.325	0.346
57	O	1.641	0.146	0.346
58	O	4.222	4.031	0.435
59	O	6.599	0.042	0.351
60	O	1.802	3.016	4.727
61	O	-0.593	7.139	4.738
62	O	6.550	2.996	4.743
63	O	4.180	7.140	4.732
64	O	1.700	0.256	9.137
65	O	-0.611	4.506	9.073
66	O	6.716	-0.004	9.191

67	O	4.268	4.419	9.049
68	O	-0.657	1.762	0.279
69	O	-3.004	5.727	0.352
70	O	4.005	1.335	0.043
71	O	1.683	5.717	0.344
72	O	1.047	1.539	2.533
73	O	-1.330	5.677	2.536
74	O	5.806	1.508	2.507
75	O	3.442	5.615	2.529
76	O	-1.363	2.918	6.996
77	O	-3.705	7.025	6.967
78	O	3.416	2.912	6.971
79	O	1.044	7.010	6.898
80	O	3.247	0.268	2.469
81	O	0.846	4.396	2.582
82	O	8.021	0.237	2.507
83	O	5.679	4.384	2.572
84	O	0.873	1.677	6.954
85	O	-1.485	5.813	6.970
86	O	5.603	1.574	6.983
87	O	3.315	5.766	6.920
88	O	3.309	2.762	2.559
89	O	0.890	6.933	2.526
90	O	-1.493	2.805	2.502
91	O	-3.880	6.913	2.538
92	O	0.878	4.182	6.893
93	O	3.258	0.107	7.005

94	O	5.659	4.159	6.960
95	O	8.024	0.058	6.968
96	O	3.110	4.638	11.272
97	O	2.633	1.909	11.488
98	C	0.214	3.917	12.102
99	C	0.119	0.102	11.851
100	C	5.834	1.214	12.627
101	H	-1.594	4.579	9.124
102	H	2.004	4.730	8.911
103	H	-0.329	6.533	9.943
104	H	3.826	6.382	10.012
105	H	0.029	1.120	0.016
106	H	6.487	3.367	23.220
107	H	3.251	3.822	0.307
108	H	-0.219	4.051	22.988
109	H	-2.317	5.016	0.337
110	H	-1.078	6.663	22.962
111	H	2.176	8.022	22.941
112	H	1.881	4.741	0.260
113	H	4.287	0.358	0.133
114	H	-2.792	8.219	22.909
115	H	-3.253	5.704	10.032
116	H	3.972	4.465	10.008
117	H	4.797	1.872	23.227
118	H	4.695	7.589	0.266
119	H	0.446	3.734	13.162
120	H	-0.009	4.991	12.011

121	H	-0.705	3.375	11.851
122	H	5.842	1.932	11.796
123	H	3.533	4.526	12.140
124	H	0.016	1.051	12.397
125	H	8.752	-0.492	12.153
126	H	0.986	-0.433	12.277
127	H	6.477	1.614	13.418
128	H	4.819	1.084	13.011
129	H	6.248	0.252	12.303
130	H	3.138	1.714	10.581
131	H	2.030	1.150	11.648

SI Fig. 3a is a duplicate of Fig. 1b.

SI Fig. 3b					
Simulation box:					
a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78
322 atoms					
Atomic id	element	x	y	z	
1	Hf	2.367	3.804	1.282	
2	Hf	-1.174	10.514	1.290	
3	Hf	9.841	3.805	1.292	
4	Hf	6.302	10.513	1.303	
5	Hf	-1.549	6.006	4.015	
6	Hf	-5.088	12.723	4.038	
7	Hf	5.947	6.023	4.010	
8	Hf	2.405	12.735	4.033	

9	Hf	5.598	1.617	6.881
10	Hf	2.042	8.334	6.861
11	Hf	13.054	1.592	6.894
12	Hf	9.508	8.300	6.888
13	Hf	1.620	3.950	9.660
14	Hf	-1.748	10.531	9.581
15	Hf	9.277	3.844	9.633
16	Hf	5.602	10.463	9.690
17	Hf	-1.520	3.226	1.307
18	Hf	-5.063	9.944	1.312
19	Hf	5.959	3.237	1.318
20	Hf	2.413	9.956	1.314
21	Hf	1.979	5.594	4.134
22	Hf	-1.537	12.302	4.151
23	Hf	9.492	5.569	4.164
24	Hf	5.946	12.282	4.172
25	Hf	1.653	1.138	6.949
26	Hf	-1.863	7.814	6.936
27	Hf	9.131	1.135	6.952
28	Hf	5.601	7.817	6.952
29	Hf	5.189	3.445	9.738
30	Hf	1.682	10.105	9.812
31	Hf	12.664	3.303	9.867
32	Hf	9.085	10.032	9.818
33	Hf	-6.604	13.296	1.097
34	Hf	-3.073	6.594	1.091
35	Hf	0.873	13.301	1.102

36	Hf	4.406	6.597	1.094
37	Hf	4.078	2.030	3.871
38	Hf	0.540	8.753	3.881
39	Hf	11.562	2.040	3.896
40	Hf	8.019	8.748	3.901
41	Hf	0.148	4.293	6.700
42	Hf	-3.384	11.002	6.683
43	Hf	7.661	4.333	6.733
44	Hf	4.098	11.021	6.740
45	Hf	3.682	6.533	9.375
46	Hf	0.242	13.352	9.490
47	Hf	11.290	6.628	9.516
48	Hf	7.728	13.275	9.506
49	Hf	4.361	0.294	0.970
50	Hf	0.825	7.005	0.966
51	Hf	11.828	0.294	0.978
52	Hf	8.292	7.006	0.974
53	Hf	0.554	2.494	3.835
54	Hf	-2.989	9.199	3.836
55	Hf	8.032	2.499	3.848
56	Hf	4.483	9.209	3.847
57	Hf	4.111	4.751	6.544
58	Hf	0.578	11.486	6.610
59	Hf	11.611	4.755	6.644
60	Hf	8.065	11.468	6.652
61	Hf	3.761	0.287	9.434
62	Hf	0.251	7.096	9.483

63	Hf	11.232	0.344	9.484
64	Hf	7.700	7.066	9.497
65	Hf	3.362	5.361	12.385
66	Hf	3.737	9.379	12.505
67	H	-0.003	2.374	10.759
68	H	-3.605	9.255	10.660
69	H	7.234	3.837	11.232
70	H	3.160	2.333	10.969
71	H	-0.779	9.728	12.091
72	H	9.907	2.971	12.055
73	H	6.388	9.070	11.821
74	H	-1.737	12.569	11.506
75	H	9.314	5.884	11.531
76	H	5.817	12.545	11.546
77	H	5.101	2.826	12.453
78	H	1.071	8.399	11.880
79	H	12.042	1.720	11.916
80	H	8.559	8.494	11.939
81	H	1.388	3.219	12.411
82	H	-2.271	9.198	11.959
83	H	8.190	1.838	11.469
84	H	2.328	0.518	11.698
85	H	-1.292	7.362	11.551
86	H	9.992	0.662	11.813
87	H	6.420	6.673	11.872
88	H	5.066	1.826	19.748
89	H	1.532	8.541	19.745

90	H	12.532	1.827	19.744
91	H	8.994	8.536	19.743
92	H	1.652	0.378	19.974
93	H	-1.883	7.105	19.979
94	H	9.119	0.381	19.972
95	H	5.586	7.102	19.951
96	H	0.430	4.706	20.580
97	H	-3.104	11.413	20.593
98	H	7.913	4.708	20.589
99	H	4.381	11.414	20.593
100	H	3.693	4.517	20.221
101	H	0.171	11.203	20.239
102	H	11.135	4.517	20.225
103	H	7.620	11.202	20.242
104	H	1.507	2.701	19.900
105	H	-2.019	9.437	19.895
106	H	8.971	2.714	19.907
107	H	5.445	9.439	19.902
108	H	3.417	2.005	20.027
109	H	-0.120	8.723	20.028
110	H	10.884	2.001	20.032
111	H	7.344	8.720	20.037
112	H	-3.057	6.667	18.935
113	H	-6.592	13.354	18.936
114	H	4.406	6.704	18.904
115	H	0.875	13.360	18.936
116	H	-1.485	4.360	19.908

117	H	-5.002	11.067	19.900
118	H	6.011	4.370	19.913
119	H	2.493	11.078	19.899
120	H	-1.832	5.544	11.301
121	H	-5.333	12.237	11.219
122	H	1.942	12.185	11.436
123	H	1.412	6.574	13.089
124	H	6.585	1.597	11.553
125	H	-4.215	8.065	11.668
126	H	14.232	1.255	11.704
127	H	1.719	6.277	15.966
128	H	1.210	7.641	14.917
129	H	2.937	7.083	14.928
130	H	0.041	4.654	13.050
131	H	-0.492	6.108	13.908
132	H	0.112	4.691	14.842
133	H	6.343	5.679	14.506
134	H	6.325	5.031	12.856
135	H	6.523	3.934	14.228
136	H	3.040	4.201	15.353
137	H	4.465	5.021	16.026
138	H	4.561	3.312	15.578
139	H	3.398	11.797	15.436
140	H	3.042	12.942	14.119
141	H	4.518	11.943	14.048
142	H	0.759	10.102	13.625
143	H	0.812	11.877	13.783

144	H	1.255	10.853	15.170
145	H	6.722	9.903	15.226
146	H	6.988	9.564	13.518
147	H	6.854	8.215	14.679
148	H	3.302	9.140	15.469
149	H	4.768	9.780	16.247
150	H	4.625	8.030	15.967
151	N	4.549	4.671	13.938
152	N	1.577	5.876	13.845
153	N	5.002	9.209	14.219
154	N	2.714	10.893	13.622
155	C	1.881	6.760	14.998
156	C	0.234	5.277	13.932
157	C	5.992	4.839	13.885
158	C	4.131	4.282	15.273
159	C	3.454	11.932	14.331
160	C	1.331	10.933	14.062
161	C	6.441	9.213	14.402
162	C	4.398	9.029	15.520
163	O	0.481	3.273	1.818
164	O	-3.061	9.987	1.827
165	O	7.952	3.293	1.834
166	O	4.410	10.003	1.839
167	O	4.003	5.644	4.650
168	O	0.474	12.374	4.692
169	O	11.496	5.633	4.700
170	O	7.954	12.334	4.704

171	O	3.672	1.216	7.499
172	O	0.154	7.825	7.443
173	O	11.122	1.140	7.444
174	O	7.572	7.853	7.440
175	O	-0.192	3.339	10.340
176	O	-3.717	10.132	10.168
177	O	7.151	3.946	10.259
178	O	3.626	10.182	10.458
179	O	4.073	4.689	0.134
180	O	0.552	11.390	0.149
181	O	11.538	4.695	0.127
182	O	8.017	11.390	0.145
183	O	3.857	0.096	3.017
184	O	0.318	6.805	3.008
185	O	11.321	0.100	3.020
186	O	7.781	6.810	3.017
187	O	-0.040	2.348	5.855
188	O	-3.588	9.051	5.851
189	O	7.453	2.352	5.866
190	O	3.893	9.061	5.864
191	O	3.561	4.594	8.605
192	O	0.022	11.440	8.684
193	O	11.027	4.694	8.711
194	O	7.441	11.370	8.690
195	O	-2.034	5.001	2.276
196	O	-5.563	11.714	2.292
197	O	5.443	5.007	2.284

198	O	1.905	11.719	2.300
199	O	5.152	0.603	5.153
200	O	1.633	7.326	5.121
201	O	12.639	0.595	5.140
202	O	9.094	7.288	5.148
203	O	1.283	2.888	7.924
204	O	-2.212	9.581	7.877
205	O	8.642	2.834	8.004
206	O	5.097	9.511	7.985
207	O	-2.557	5.147	10.762
208	O	-6.113	11.845	10.746
209	O	4.599	5.088	10.829
210	O	1.265	11.896	10.780
211	O	6.288	1.188	0.787
212	O	2.752	7.901	0.784
213	O	13.763	1.178	0.784
214	O	10.224	7.894	0.784
215	O	2.436	3.446	3.468
216	O	-1.103	10.157	3.475
217	O	9.920	3.441	3.470
218	O	6.370	10.145	3.485
219	O	-1.444	5.691	6.247
220	O	-4.979	12.415	6.253
221	O	6.011	5.710	6.247
222	O	2.475	12.432	6.267
223	O	5.664	1.330	9.108
224	O	2.196	8.000	9.065

225	O	13.157	1.212	9.055
226	O	9.626	7.942	9.033
227	O	2.381	0.208	0.522
228	O	-1.156	6.919	0.513
229	O	9.857	0.199	0.516
230	O	6.319	6.911	0.511
231	O	6.018	2.457	3.328
232	O	2.476	9.176	3.325
233	O	13.494	2.457	3.320
234	O	9.949	9.164	3.329
235	O	2.077	4.710	6.079
236	O	-1.439	11.418	6.084
237	O	9.605	4.625	6.089
238	O	6.039	11.377	6.124
239	O	1.755	0.258	8.892
240	O	-1.768	7.020	8.928
241	O	9.203	0.295	8.949
242	O	5.638	6.933	8.985
243	O	2.558	5.697	2.112
244	O	-0.968	12.407	2.121
245	O	10.038	5.697	2.132
246	O	6.504	12.405	2.142
247	O	2.218	1.275	4.916
248	O	-1.318	7.977	4.904
249	O	9.690	1.278	4.920
250	O	6.139	7.984	4.921
251	O	-1.704	3.535	7.775

252	O	-5.239	10.262	7.745
253	O	5.812	3.573	7.757
254	O	2.218	10.283	7.750
255	O	2.010	5.824	10.498
256	O	-1.588	12.514	10.543
257	O	9.497	5.820	10.576
258	O	5.907	12.453	10.581
259	O	1.184	5.211	0.041
260	O	-2.350	11.922	0.052
261	O	8.665	5.215	0.052
262	O	5.133	11.923	0.056
263	O	0.889	0.739	2.868
264	O	-2.650	7.451	2.859
265	O	8.370	0.754	2.861
266	O	4.834	7.466	2.855
267	O	4.506	3.020	5.619
268	O	0.939	9.749	5.634
269	O	11.983	3.030	5.639
270	O	8.420	9.731	5.647
271	O	0.527	5.292	8.482
272	O	-2.868	12.005	8.426
273	O	8.200	5.366	8.385
274	O	4.526	11.975	8.502
275	O	3.997	2.422	1.682
276	O	0.455	9.131	1.686
277	O	11.472	2.421	1.684
278	O	7.931	9.131	1.693

279	O	0.097	4.620	4.468
280	O	-3.434	11.330	4.481
281	O	7.587	4.635	4.497
282	O	4.039	11.340	4.506
283	O	7.213	0.209	7.332
284	O	3.665	6.857	7.292
285	O	14.717	0.184	7.304
286	O	11.199	6.889	7.311
287	O	3.256	2.439	9.994
288	O	-0.169	9.174	9.818
289	O	10.840	2.430	9.822
290	O	7.280	9.128	9.782
291	O	2.135	3.618	11.904
292	O	-1.695	10.011	11.879
293	O	9.052	3.154	11.627
294	O	5.647	9.692	11.649
295	O	5.382	2.441	11.598
296	O	1.648	9.186	11.761
297	O	12.783	2.320	11.697
298	O	9.312	9.036	11.626
299	O	3.095	0.019	11.351
300	O	-0.425	6.909	11.434
301	O	10.715	0.127	11.450
302	O	7.269	6.967	11.499
303	O	4.251	1.331	19.966
304	O	0.714	8.046	19.959
305	O	11.718	1.331	19.969

306	O	8.180	8.045	19.974
307	O	2.357	2.895	20.337
308	O	-1.171	9.610	20.342
309	O	9.820	2.890	20.352
310	O	6.290	9.606	20.357
311	O	-0.912	3.704	20.337
312	O	-4.434	10.422	20.351
313	O	6.572	3.709	20.349
314	O	3.046	10.421	20.350
315	O	0.682	0.486	19.708
316	O	-2.852	7.218	19.707
317	O	8.148	0.488	19.711
318	O	4.613	7.208	19.707
319	O	3.605	7.321	12.252
320	O	7.485	1.106	11.313
321	O	-3.333	7.802	11.249
322	O	0.134	1.032	11.224

SI Fig. 3c

Simulation box:

a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

322 atoms

Atomic id	element	x	y	z
1	Hf	2.365	3.812	1.278
2	Hf	-1.173	10.525	1.279
3	Hf	9.838	3.816	1.269
4	Hf	6.304	10.524	1.280

5	Hf	-1.554	6.015	4.002
6	Hf	-5.090	12.740	4.030
7	Hf	5.934	6.033	3.993
8	Hf	2.391	12.742	4.015
9	Hf	5.589	1.633	6.887
10	Hf	2.007	8.372	6.837
11	Hf	13.057	1.611	6.875
12	Hf	9.499	8.323	6.882
13	Hf	1.621	3.982	9.719
14	Hf	-1.775	10.567	9.568
15	Hf	9.250	3.873	9.614
16	Hf	5.647	10.501	9.670
17	Hf	-1.500	3.217	1.338
18	Hf	-5.063	9.950	1.309
19	Hf	5.957	3.225	1.314
20	Hf	2.413	9.951	1.308
21	Hf	1.977	5.598	4.134
22	Hf	-1.545	12.313	4.150
23	Hf	9.482	5.579	4.154
24	Hf	5.944	12.292	4.160
25	Hf	1.651	1.174	6.974
26	Hf	-1.886	7.834	6.919
27	Hf	9.115	1.158	6.928
28	Hf	5.590	7.858	6.930
29	Hf	5.168	3.491	9.768
30	Hf	1.630	10.113	9.797
31	Hf	12.618	3.330	9.832

32	Hf	9.068	10.051	9.828
33	Hf	-6.614	13.306	1.098
34	Hf	-3.086	6.609	1.074
35	Hf	0.857	13.303	1.087
36	Hf	4.386	6.605	1.080
37	Hf	4.086	2.043	3.880
38	Hf	0.540	8.765	3.870
39	Hf	11.563	2.046	3.883
40	Hf	8.026	8.760	3.885
41	Hf	0.157	4.322	6.736
42	Hf	-3.394	11.020	6.678
43	Hf	7.640	4.347	6.709
44	Hf	4.095	11.036	6.726
45	Hf	3.676	6.563	9.308
46	Hf	7.324	0.005	9.529
47	Hf	11.265	6.637	9.489
48	Hf	7.722	13.311	9.505
49	Hf	4.353	0.297	0.963
50	Hf	0.815	7.010	0.956
51	Hf	11.826	0.298	0.962
52	Hf	8.292	7.010	0.962
53	Hf	0.574	2.500	3.861
54	Hf	-2.981	9.208	3.823
55	Hf	8.042	2.505	3.830
56	Hf	4.489	9.221	3.829
57	Hf	4.115	4.767	6.543
58	Hf	0.567	11.525	6.624

59	Hf	11.603	4.762	6.616
60	Hf	8.066	11.489	6.635
61	Hf	3.753	0.312	9.441
62	Hf	0.210	7.140	9.489
63	Hf	11.212	0.376	9.431
64	Hf	7.678	7.066	9.473
65	Hf	3.066	5.396	12.227
66	Hf	3.578	9.327	12.242
67	H	-0.056	2.512	10.804
68	H	-3.628	9.312	10.695
69	H	7.209	3.945	11.193
70	H	3.123	2.454	10.955
71	H	-0.670	9.566	11.887
72	H	9.912	3.129	12.072
73	H	6.423	9.751	12.205
74	H	-1.755	12.617	11.500
75	H	9.307	5.816	11.496
76	H	5.860	12.529	11.519
77	H	4.919	3.569	12.901
78	H	3.123	10.110	14.865
79	H	11.947	1.789	11.896
80	H	8.504	8.415	11.827
81	H	1.989	4.564	14.703
82	H	-2.203	9.208	11.958
83	H	8.141	1.916	11.425
84	H	2.354	0.581	11.706
85	H	-1.404	7.298	11.524

86	H	9.788	0.697	11.582
87	H	6.270	7.099	11.661
88	H	5.071	1.854	19.769
89	H	1.543	8.561	19.769
90	H	12.534	1.869	19.771
91	H	9.010	8.549	19.754
92	H	1.662	0.394	20.023
93	H	-1.879	7.135	20.006
94	H	9.124	0.382	20.016
95	H	5.610	7.120	20.063
96	H	0.390	4.709	20.582
97	H	-3.119	11.418	20.574
98	H	7.875	4.714	20.568
99	H	4.369	11.424	20.570
100	H	3.569	4.538	20.199
101	H	0.102	11.205	20.219
102	H	11.026	4.605	20.178
103	H	7.587	11.235	20.217
104	H	1.505	2.664	19.907
105	H	-2.011	9.418	19.878
106	H	8.956	2.663	19.912
107	H	5.450	9.412	19.892
108	H	3.417	2.018	20.023
109	H	-0.116	8.734	20.015
110	H	10.880	2.012	20.025
111	H	7.356	8.726	20.015
112	H	-3.020	6.670	18.936

113	H	-6.544	13.348	18.944
114	H	4.530	6.509	19.005
115	H	0.887	13.323	18.971
116	H	-1.580	4.392	20.001
117	H	-5.041	11.096	19.928
118	H	5.915	4.392	19.973
119	H	2.428	11.120	19.960
120	H	-1.837	5.571	11.196
121	H	-5.362	12.277	11.217
122	H	2.140	12.409	11.139
123	H	6.085	1.961	11.663
124	H	-4.228	8.059	11.657
125	H	14.162	1.289	11.657
126	H	0.992	6.404	15.953
127	H	1.345	7.426	14.527
128	H	2.685	6.677	15.442
129	H	0.196	4.071	13.284
130	H	-0.210	5.798	13.193
131	H	-0.399	4.919	14.759
132	H	5.650	5.785	14.752
133	H	6.269	5.516	13.088
134	H	6.634	4.346	14.385
135	H	3.322	2.861	14.521
136	H	3.873	4.169	15.633
137	H	4.973	2.846	15.192
138	H	3.569	12.448	15.169
139	H	3.708	12.581	13.382

140	H	4.873	11.574	14.294
141	H	0.886	10.220	14.089
142	H	1.265	11.721	13.233
143	H	1.308	11.698	15.029
144	H	6.713	10.273	15.164
145	H	7.182	9.143	13.869
146	H	7.245	8.619	15.565
147	H	3.638	8.369	16.036
148	H	4.678	9.727	16.541
149	H	5.235	8.063	16.773
150	H	5.230	7.864	14.307
151	N	4.628	4.281	13.645
152	N	1.613	5.364	14.182
153	N	5.267	8.794	14.739
154	N	2.946	10.723	14.061
155	C	1.658	6.532	15.083
156	C	0.206	5.014	13.841
157	C	5.861	5.024	13.982
158	C	4.170	3.499	14.808
159	C	3.829	11.907	14.244
160	C	1.514	11.117	14.114
161	C	6.670	9.223	14.837
162	C	4.677	8.725	16.081
163	O	0.495	3.265	1.822
164	O	-3.058	9.982	1.802
165	O	7.952	3.285	1.810
166	O	4.414	10.000	1.807

167	O	4.000	5.639	4.642
168	O	0.461	12.391	4.681
169	O	11.486	5.646	4.681
170	O	7.950	12.344	4.685
171	O	3.654	1.229	7.488
172	O	0.118	7.864	7.421
173	O	11.121	1.169	7.409
174	O	7.553	7.912	7.450
175	O	-0.251	3.406	10.320
176	O	-3.750	10.199	10.223
177	O	7.136	4.002	10.217
178	O	3.712	9.960	10.293
179	O	4.015	4.736	0.075
180	O	0.521	11.413	0.107
181	O	11.464	4.757	0.066
182	O	7.997	11.419	0.114
183	O	3.848	0.112	3.007
184	O	0.301	6.816	2.993
185	O	11.313	0.112	2.996
186	O	7.763	6.829	2.996
187	O	-0.032	2.379	5.873
188	O	-3.592	9.065	5.836
189	O	7.437	2.368	5.838
190	O	3.886	9.084	5.842
191	O	3.508	4.648	8.592
192	O	-0.016	11.444	8.682
193	O	10.999	4.693	8.678

194	O	7.448	11.377	8.686
195	O	-2.055	5.007	2.250
196	O	-5.572	11.720	2.278
197	O	5.428	5.013	2.250
198	O	1.888	11.719	2.275
199	O	5.132	0.610	5.152
200	O	1.619	7.336	5.104
201	O	12.636	0.606	5.124
202	O	9.072	7.299	5.140
203	O	1.258	2.903	7.977
204	O	-2.270	9.587	7.894
205	O	8.608	2.849	7.991
206	O	5.147	9.561	7.939
207	O	-2.623	5.162	10.736
208	O	-6.145	11.862	10.760
209	O	4.521	5.193	10.833
210	O	1.363	11.948	10.709
211	O	6.283	1.188	0.770
212	O	2.747	7.905	0.760
213	O	13.764	1.182	0.775
214	O	10.215	7.903	0.763
215	O	2.445	3.457	3.466
216	O	-1.103	10.168	3.454
217	O	9.920	3.454	3.445
218	O	6.375	10.159	3.459
219	O	-1.456	5.710	6.237
220	O	-4.983	12.429	6.239

221	O	6.007	5.729	6.222
222	O	2.470	12.448	6.228
223	O	5.640	1.353	9.079
224	O	2.157	8.030	9.010
225	O	13.140	1.237	9.019
226	O	9.601	7.984	9.033
227	O	2.376	0.216	0.505
228	O	-1.164	6.933	0.493
229	O	9.853	0.188	0.486
230	O	6.307	6.933	0.485
231	O	6.018	2.456	3.318
232	O	2.475	9.182	3.307
233	O	13.505	2.459	3.331
234	O	9.953	9.164	3.310
235	O	2.077	4.715	6.080
236	O	-1.449	11.414	6.075
237	O	9.593	4.623	6.061
238	O	6.034	11.405	6.103
239	O	1.746	0.256	8.885
240	O	-1.799	7.026	8.891
241	O	9.217	0.281	8.852
242	O	5.624	6.976	8.965
243	O	2.544	5.710	2.103
244	O	-0.984	12.417	2.108
245	O	10.009	5.714	2.111
246	O	6.495	12.412	2.118
247	O	2.204	1.295	4.916

248	O	-1.331	7.988	4.883
249	O	9.684	1.297	4.886
250	O	6.129	8.003	4.898
251	O	-1.720	3.564	7.755
252	O	-5.253	10.282	7.743
253	O	5.784	3.609	7.734
254	O	2.210	10.319	7.721
255	O	1.984	5.996	10.518
256	O	-1.594	12.542	10.541
257	O	9.440	5.873	10.532
258	O	5.861	12.510	10.545
259	O	1.151	5.210	0.038
260	O	-2.364	11.926	0.033
261	O	8.629	5.217	0.029
262	O	5.123	11.929	0.028
263	O	0.884	0.751	2.863
264	O	-2.662	7.455	2.845
265	O	8.365	0.759	2.837
266	O	4.818	7.470	2.838
267	O	4.499	3.037	5.613
268	O	0.923	9.778	5.612
269	O	11.981	3.043	5.614
270	O	8.423	9.753	5.623
271	O	0.545	5.335	8.499
272	O	-2.888	12.025	8.416
273	O	8.200	5.404	8.340
274	O	4.523	11.988	8.490

275	O	3.992	2.432	1.666
276	O	0.453	9.137	1.665
277	O	11.478	2.435	1.662
278	O	7.931	9.141	1.666
279	O	0.095	4.629	4.463
280	O	-3.441	11.338	4.463
281	O	7.576	4.641	4.465
282	O	4.040	11.349	4.474
283	O	7.198	0.228	7.309
284	O	3.664	6.886	7.240
285	O	14.713	0.194	7.288
286	O	11.163	6.902	7.293
287	O	3.246	2.433	9.965
288	O	-0.198	9.185	9.811
289	O	10.790	2.435	9.816
290	O	7.220	9.147	9.872
291	O	2.154	3.740	11.744
292	O	-1.571	9.972	11.864
293	O	9.066	3.360	11.651
294	O	5.578	10.092	11.862
295	O	5.336	2.611	11.615
296	O	1.712	9.393	11.737
297	O	12.725	2.330	11.665
298	O	9.239	9.042	11.647
299	O	3.075	0.020	11.356
300	O	-0.574	6.802	11.361
301	O	10.530	0.084	11.393

302	O	7.198	6.875	11.466
303	O	4.254	1.344	19.956
304	O	0.722	8.054	19.944
305	O	11.725	1.349	19.958
306	O	8.190	8.048	19.948
307	O	2.354	2.909	20.317
308	O	-1.163	9.626	20.313
309	O	9.804	2.886	20.336
310	O	6.301	9.622	20.317
311	O	-0.969	3.723	20.355
312	O	-4.465	10.428	20.336
313	O	6.510	3.711	20.332
314	O	3.003	10.425	20.323
315	O	0.703	0.517	19.696
316	O	-2.838	7.264	19.683
317	O	8.160	0.512	19.701
318	O	4.665	7.220	19.654
319	O	3.710	7.387	12.432
320	O	7.616	1.100	11.190
321	O	-3.354	7.824	11.217
322	O	0.066	1.023	11.206

SI Fig. 4a is a duplicate of Fig. 2.

SI Fig. 4b					
Simulation box:					
a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

319 atoms

Atomic id	element	x	y	z
1	Hf	2.359	3.826	1.274
2	Hf	-1.177	10.539	1.304
3	Hf	9.834	3.843	1.304
4	Hf	6.302	10.540	1.323
5	Hf	-1.557	6.067	4.042
6	Hf	-5.080	12.753	4.019
7	Hf	5.931	6.062	4.036
8	Hf	2.400	12.774	4.031
9	Hf	5.599	1.643	6.842
10	Hf	2.016	8.359	6.853
11	Hf	13.037	1.686	6.852
12	Hf	9.498	8.366	6.962
13	Hf	1.560	3.676	9.750
14	Hf	-1.851	10.662	9.669
15	Hf	9.016	3.891	9.764
16	Hf	5.679	10.654	9.612
17	Hf	-1.536	3.259	1.318
18	Hf	-5.061	9.964	1.331
19	Hf	5.947	3.257	1.309
20	Hf	2.412	9.963	1.331
21	Hf	2.002	5.601	4.144
22	Hf	-1.549	12.318	4.153
23	Hf	9.459	5.635	4.178
24	Hf	5.943	12.329	4.168

25	Hf	1.672	1.196	6.896
26	Hf	-1.936	7.898	6.967
27	Hf	9.119	1.204	6.944
28	Hf	5.575	7.868	6.975
29	Hf	5.209	3.407	9.703
30	Hf	1.576	10.185	9.686
31	Hf	12.545	3.530	9.675
32	Hf	9.043	10.183	9.875
33	Hf	-6.615	13.321	1.092
34	Hf	-3.067	6.611	1.116
35	Hf	0.866	13.324	1.102
36	Hf	4.413	6.616	1.113
37	Hf	4.081	2.064	3.860
38	Hf	0.517	8.782	3.890
39	Hf	11.540	2.081	3.887
40	Hf	8.019	8.785	3.930
41	Hf	0.166	4.359	6.651
42	Hf	-3.390	11.071	6.750
43	Hf	7.653	4.367	6.749
44	Hf	4.105	11.089	6.723
45	Hf	3.674	6.557	9.387
46	Hf	7.349	0.013	9.528
47	Hf	11.291	6.627	9.647
48	Hf	14.835	0.083	9.439
49	Hf	4.362	0.301	0.962
50	Hf	0.833	7.018	0.984
51	Hf	11.829	0.314	0.981

52	Hf	8.316	7.035	0.996
53	Hf	0.549	2.526	3.812
54	Hf	-2.998	9.248	3.870
55	Hf	8.025	2.544	3.839
56	Hf	4.480	9.242	3.865
57	Hf	4.135	4.765	6.573
58	Hf	0.567	11.540	6.607
59	Hf	11.572	4.841	6.631
60	Hf	8.071	11.535	6.645
61	Hf	3.720	0.469	9.470
62	Hf	0.240	6.962	9.345
63	Hf	11.229	0.486	9.483
64	Hf	7.671	7.133	9.489
65	Hf	3.655	9.219	11.965
66	Hf	-0.153	8.691	12.210
67	Hf	2.792	5.482	12.374
68	Hf	-0.814	4.855	11.982
69	H	-3.650	9.370	10.762
70	H	9.966	2.990	11.947
71	H	6.443	9.847	12.122
72	H	-1.600	12.674	11.529
73	H	9.279	5.813	11.572
74	H	5.817	12.685	11.508
75	H	4.644	1.754	11.922
76	H	12.617	2.511	12.326
77	H	8.443	8.614	11.932
78	H	-2.323	10.330	12.434

79	H	8.148	1.913	11.460
80	H	2.443	0.827	11.646
81	H	9.994	0.620	11.786
82	H	5.068	1.829	19.741
83	H	1.540	8.586	19.804
84	H	12.535	1.854	19.761
85	H	9.010	8.591	19.782
86	H	1.654	0.395	20.005
87	H	-1.870	7.084	20.014
88	H	9.126	0.401	19.997
89	H	5.614	7.105	20.043
90	H	0.440	4.732	20.575
91	H	-3.091	11.423	20.581
92	H	7.926	4.747	20.587
93	H	4.384	11.429	20.596
94	H	3.716	4.520	20.231
95	H	0.141	11.240	20.238
96	H	11.164	4.510	20.250
97	H	7.600	11.229	20.244
98	H	1.520	2.737	19.878
99	H	-2.030	9.410	19.924
100	H	8.981	2.749	19.909
101	H	5.441	9.400	19.947
102	H	3.415	2.018	20.019
103	H	-0.123	8.734	20.059
104	H	10.879	2.032	20.040
105	H	7.352	8.748	20.063

106	H	-3.049	6.624	18.977
107	H	-6.571	13.350	18.946
108	H	4.486	6.584	18.980
109	H	0.897	13.362	18.938
110	H	-1.466	4.396	19.919
111	H	-5.012	11.118	19.955
112	H	6.034	4.392	19.899
113	H	2.457	11.147	19.990
114	H	-5.374	12.452	11.238
115	H	2.162	12.393	11.134
116	H	6.261	1.805	11.636
117	H	-4.344	8.179	11.684
118	H	-0.150	2.039	11.191
119	H	5.631	9.853	14.853
120	H	5.572	8.142	14.328
121	H	4.964	8.587	15.934
122	H	1.833	10.002	14.638
123	H	3.208	11.111	14.940
124	H	2.820	9.816	16.112
125	H	0.294	8.186	15.990
126	H	-0.451	7.065	14.801
127	H	-1.473	8.092	15.816
128	H	-0.715	11.215	14.104
129	H	-0.166	10.622	15.690
130	H	-1.862	10.413	15.219
131	H	5.310	5.869	15.308
132	H	5.910	5.493	13.667

133	H	5.740	4.202	14.880
134	H	2.142	3.964	14.791
135	H	2.976	5.010	15.980
136	H	3.647	3.414	15.560
137	H	-0.577	4.153	15.842
138	H	-0.022	3.249	14.402
139	H	13.292	2.967	15.067
140	H	-2.988	6.184	13.847
141	H	-2.432	5.843	15.507
142	H	11.522	4.646	14.644
143	H	5.423	5.431	11.372
144	H	6.155	7.357	11.539
145	H	3.197	8.224	14.292
146	H	1.435	6.592	14.240
147	N	3.707	9.132	14.294
148	N	-0.494	9.106	14.225
149	N	3.899	4.893	14.047
150	N	-1.403	4.785	13.979
151	C	5.042	8.926	14.890
152	C	2.851	10.077	15.046
153	C	-0.524	8.069	15.247
154	C	-0.825	10.392	14.825
155	C	5.270	5.124	14.478
156	C	3.134	4.301	15.137
157	C	-0.894	3.748	14.859
158	C	-2.613	5.390	14.510
159	O	0.466	3.324	1.807

160	O	-3.070	10.049	1.854
161	O	7.944	3.334	1.825
162	O	4.406	10.039	1.855
163	O	3.997	5.726	4.676
164	O	0.460	12.411	4.695
165	O	11.461	5.751	4.710
166	O	7.948	12.415	4.710
167	O	3.648	1.332	7.456
168	O	0.080	8.060	7.531
169	O	11.119	1.298	7.455
170	O	7.541	7.985	7.495
171	O	-0.398	4.188	10.051
172	O	-3.802	10.280	10.316
173	O	7.055	3.845	10.132
174	O	3.632	10.206	10.234
175	O	4.091	4.705	0.143
176	O	0.530	11.420	0.144
177	O	11.557	4.701	0.149
178	O	8.004	11.414	0.143
179	O	3.851	0.108	3.003
180	O	0.307	6.842	3.024
181	O	11.321	0.120	3.016
182	O	7.790	6.844	3.041
183	O	-0.028	2.369	5.824
184	O	-3.581	9.112	5.908
185	O	7.463	2.369	5.850
186	O	3.874	9.112	5.879

187	O	3.702	4.645	8.618
188	O	-0.003	11.390	8.705
189	O	11.009	4.701	8.705
190	O	7.470	11.477	8.711
191	O	-2.063	5.023	2.321
192	O	-5.586	11.731	2.301
193	O	5.431	5.029	2.307
194	O	1.895	11.736	2.308
195	O	5.132	0.623	5.134
196	O	1.555	7.309	5.180
197	O	12.600	0.636	5.150
198	O	9.055	7.343	5.208
199	O	1.167	2.892	7.951
200	O	-2.313	9.618	8.019
201	O	8.677	2.902	7.991
202	O	5.153	9.627	7.966
203	O	-2.637	5.210	10.886
204	O	-6.181	12.065	10.791
205	O	4.574	5.044	11.034
206	O	1.355	11.949	10.714
207	O	6.289	1.210	0.774
208	O	2.767	7.925	0.789
209	O	13.758	1.209	0.778
210	O	10.239	7.928	0.797
211	O	2.438	3.477	3.432
212	O	-1.102	10.197	3.480
213	O	9.909	3.501	3.469

214	O	6.377	10.193	3.492
215	O	-1.458	5.794	6.239
216	O	-4.980	12.477	6.244
217	O	6.009	5.774	6.261
218	O	2.480	12.482	6.246
219	O	5.645	1.364	9.045
220	O	2.115	8.049	9.105
221	O	13.159	1.409	9.052
222	O	9.583	8.053	9.110
223	O	2.381	0.199	0.504
224	O	-1.141	6.900	0.521
225	O	9.855	0.201	0.506
226	O	6.333	6.927	0.522
227	O	6.024	2.466	3.303
228	O	2.471	9.158	3.340
229	O	13.493	2.461	3.307
230	O	9.953	9.171	3.345
231	O	2.136	4.589	6.002
232	O	-1.450	11.426	6.110
233	O	9.588	4.675	6.075
234	O	6.046	11.430	6.106
235	O	1.794	0.225	8.783
236	O	-1.773	6.978	8.927
237	O	9.236	0.327	8.884
238	O	5.626	6.990	8.966
239	O	2.545	5.728	2.110
240	O	-0.976	12.438	2.122

241	O	10.026	5.747	2.133
242	O	6.504	12.437	2.134
243	O	2.229	1.316	4.878
244	O	-1.350	8.055	4.932
245	O	9.698	1.327	4.901
246	O	6.130	8.040	4.937
247	O	-1.734	3.662	7.671
248	O	-5.255	10.345	7.791
249	O	5.808	3.582	7.656
250	O	2.219	10.345	7.727
251	O	2.047	5.687	10.366
252	O	-1.580	12.648	10.555
253	O	9.372	5.876	10.600
254	O	5.953	12.683	10.544
255	O	1.202	5.237	0.025
256	O	-2.339	11.934	0.034
257	O	8.680	5.255	0.046
258	O	5.132	11.941	0.058
259	O	0.901	0.777	2.840
260	O	-2.622	7.513	2.855
261	O	8.378	0.789	2.852
262	O	4.854	7.507	2.854
263	O	4.543	3.077	5.556
264	O	0.965	9.798	5.613
265	O	11.985	3.119	5.582
266	O	8.445	9.808	5.652
267	O	0.808	5.503	8.155

268	O	-2.873	12.094	8.476
269	O	8.181	5.463	8.380
270	O	4.587	12.112	8.447
271	O	3.992	2.434	1.666
272	O	0.452	9.153	1.697
273	O	11.453	2.439	1.687
274	O	7.932	9.155	1.710
275	O	0.088	4.660	4.472
276	O	-3.442	11.357	4.502
277	O	7.564	4.663	4.506
278	O	4.042	11.372	4.496
279	O	7.217	0.227	7.329
280	O	3.632	6.927	7.286
281	O	14.691	0.262	7.311
282	O	11.149	6.946	7.365
283	O	3.261	2.499	10.040
284	O	-0.201	9.169	10.092
285	O	10.842	2.464	10.026
286	O	7.208	9.250	9.912
287	O	1.215	4.271	12.261
288	O	-1.575	10.198	11.827
289	O	9.060	3.294	11.758
290	O	5.557	10.152	11.840
291	O	5.387	2.355	11.709
292	O	1.684	9.443	11.872
293	O	13.277	2.839	11.697
294	O	9.170	9.238	11.734

295	O	3.111	0.143	11.426
296	O	-0.335	6.833	11.468
297	O	3.504	13.355	11.398
298	O	6.980	6.852	11.422
299	O	4.248	1.338	19.954
300	O	0.726	8.073	19.988
301	O	11.719	1.356	19.972
302	O	8.201	8.082	19.995
303	O	2.365	2.905	20.333
304	O	-1.188	9.600	20.372
305	O	9.827	2.914	20.361
306	O	6.288	9.619	20.371
307	O	-0.909	3.726	20.348
308	O	-4.456	10.431	20.360
309	O	6.591	3.734	20.349
310	O	3.008	10.433	20.354
311	O	0.686	0.505	19.707
312	O	-2.838	7.211	19.723
313	O	8.161	0.515	19.707
314	O	4.658	7.218	19.705
315	O	3.833	7.379	11.466
316	O	7.571	1.128	11.194
317	O	-3.494	7.873	11.259
318	O	0.596	1.721	10.620
319	O	1.793	6.968	13.402

SI Fig. 4c

Simulation box:					
a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78
328 atoms					
Atomic id	element	x	y	z	
1	Hf	2.434	3.782	1.251	
2	Hf	-1.080	10.486	1.287	
3	Hf	9.914	3.789	1.299	
4	Hf	6.387	10.502	1.309	
5	Hf	-1.464	6.008	4.026	
6	Hf	-5.011	12.680	3.998	
7	Hf	6.015	6.001	4.030	
8	Hf	2.469	12.676	4.049	
9	Hf	5.691	1.534	6.830	
10	Hf	2.099	8.227	6.922	
11	Hf	13.135	1.623	6.868	
12	Hf	9.551	8.304	6.929	
13	Hf	1.685	3.565	9.693	
14	Hf	-1.732	10.518	9.676	
15	Hf	9.127	3.742	9.756	
16	Hf	5.681	10.568	9.699	
17	Hf	-1.467	3.225	1.296	
18	Hf	-4.951	9.897	1.346	
19	Hf	6.033	3.213	1.301	
20	Hf	2.525	9.907	1.356	
21	Hf	2.091	5.549	4.131	
22	Hf	-1.438	12.230	4.153	

23	Hf	9.544	5.575	4.166
24	Hf	6.006	12.270	4.176
25	Hf	1.766	1.084	6.871
26	Hf	-1.872	7.809	6.951
27	Hf	9.216	1.107	6.960
28	Hf	5.584	7.796	6.981
29	Hf	5.311	3.256	9.668
30	Hf	1.757	9.912	9.890
31	Hf	12.675	3.547	9.713
32	Hf	9.061	10.148	9.839
33	Hf	-6.564	13.295	1.077
34	Hf	-2.984	6.569	1.106
35	Hf	0.925	13.293	1.106
36	Hf	4.491	6.573	1.105
37	Hf	4.156	1.997	3.845
38	Hf	0.628	8.723	3.916
39	Hf	11.625	2.010	3.889
40	Hf	8.092	8.733	3.921
41	Hf	0.283	4.285	6.650
42	Hf	-3.301	10.992	6.743
43	Hf	7.741	4.284	6.730
44	Hf	4.173	10.981	6.781
45	Hf	3.759	6.365	9.511
46	Hf	0.362	13.278	9.536
47	Hf	11.243	6.559	9.583
48	Hf	14.911	0.025	9.443
49	Hf	4.410	0.274	0.945

50	Hf	0.910	6.987	0.967
51	Hf	11.887	0.275	0.979
52	Hf	8.373	6.995	0.975
53	Hf	0.620	2.471	3.796
54	Hf	-2.896	9.183	3.869
55	Hf	8.105	2.462	3.838
56	Hf	4.584	9.177	3.883
57	Hf	4.220	4.689	6.569
58	Hf	0.656	11.411	6.672
59	Hf	11.662	4.767	6.615
60	Hf	8.125	11.461	6.653
61	Hf	3.815	0.330	9.444
62	Hf	0.226	6.831	9.326
63	Hf	11.334	0.430	9.503
64	Hf	7.707	7.076	9.420
65	Hf	3.935	8.991	12.251
66	Hf	-0.151	8.633	12.415
67	Hf	2.119	6.103	12.587
68	Hf	-0.931	5.154	12.082
69	H	-3.665	9.432	10.852
70	H	10.107	2.763	11.863
71	H	6.369	10.040	12.338
72	H	-1.537	12.568	11.533
73	H	9.350	5.773	11.517
74	H	5.920	12.551	11.496
75	H	4.662	1.549	11.820
76	H	12.717	2.510	12.304

77	H	8.453	8.915	12.133
78	H	-2.291	10.365	12.411
79	H	8.147	1.678	11.485
80	H	2.532	0.769	11.595
81	H	10.010	0.555	11.779
82	H	5.158	1.784	19.728
83	H	1.632	8.577	19.802
84	H	12.623	1.775	19.751
85	H	9.086	8.583	19.793
86	H	1.719	0.418	20.008
87	H	-1.797	7.071	20.009
88	H	9.205	0.413	20.009
89	H	5.689	7.082	20.030
90	H	0.500	4.695	20.567
91	H	-3.061	11.383	20.593
92	H	7.986	4.694	20.590
93	H	4.412	11.388	20.604
94	H	3.757	4.488	20.212
95	H	0.123	11.294	20.200
96	H	11.241	4.441	20.252
97	H	7.540	11.287	20.200
98	H	1.610	2.694	19.846
99	H	-1.949	9.362	19.907
100	H	9.093	2.717	19.879
101	H	5.502	9.342	19.948
102	H	3.503	1.995	19.987
103	H	-0.026	8.709	20.034

104	H	10.971	1.996	20.021
105	H	7.429	8.720	20.049
106	H	-2.974	6.626	18.961
107	H	-6.439	13.321	18.919
108	H	4.574	6.559	18.964
109	H	1.022	13.360	18.923
110	H	-1.410	4.359	19.911
111	H	-5.042	11.086	20.014
112	H	6.080	4.364	19.923
113	H	2.438	11.088	20.028
114	H	-5.307	12.373	11.252
115	H	2.318	12.278	11.102
116	H	6.300	1.631	11.643
117	H	10.437	8.162	11.626
118	H	-0.087	2.151	11.163
119	H	4.643	10.705	16.214
120	H	5.311	9.294	15.320
121	H	3.634	9.272	15.952
122	H	2.492	11.820	13.486
123	H	2.876	12.012	15.225
124	H	1.866	10.633	14.653
125	H	-0.242	9.425	16.378
126	H	-0.817	7.990	15.480
127	H	-1.914	9.359	15.787
128	H	-0.271	11.628	13.438
129	H	-0.163	11.565	15.209
130	H	-1.745	11.391	14.436

131	H	5.266	5.356	14.677
132	H	5.608	4.309	13.260
133	H	5.355	3.583	14.857
134	H	1.804	4.050	15.063
135	H	3.057	5.059	15.850
136	H	3.272	3.294	15.787
137	H	-1.797	3.579	16.007
138	H	-0.445	3.400	14.825
139	H	12.920	2.649	14.508
140	H	11.291	5.922	13.850
141	H	11.174	4.900	15.323
142	H	11.020	4.168	13.700
143	H	4.505	4.877	11.590
144	H	6.540	7.357	12.061
145	H	1.177	7.915	14.480
146	H	6.319	5.916	11.330
147	H	-1.501	5.552	14.652
148	H	-2.548	7.357	12.216
149	H	3.393	3.479	13.392
150	H	5.490	7.513	13.659
151	H	3.149	7.554	14.761
152	H	4.665	11.043	13.828
153	N	3.923	10.443	14.212
154	N	-0.461	9.680	14.259
155	N	3.572	4.334	13.932
156	N	-1.949	4.739	14.209
157	C	4.413	9.900	15.495

158	C	2.721	11.280	14.412
159	C	-0.869	9.087	15.522
160	C	-0.669	11.115	14.327
161	C	5.033	4.400	14.187
162	C	2.880	4.165	15.233
163	C	-1.528	3.527	14.938
164	C	11.537	4.944	14.281
165	O	0.546	3.247	1.776
166	O	-2.967	9.960	1.847
167	O	8.036	3.231	1.801
168	O	4.509	9.963	1.862
169	O	4.090	5.639	4.655
170	O	0.562	12.273	4.720
171	O	11.560	5.663	4.692
172	O	8.023	12.318	4.706
173	O	3.743	1.172	7.420
174	O	0.138	7.875	7.502
175	O	11.237	1.129	7.460
176	O	7.593	7.892	7.481
177	O	-0.287	4.423	10.229
178	O	-3.772	10.222	10.255
179	O	7.223	3.479	10.075
180	O	3.790	9.847	10.355
181	O	4.156	4.680	0.113
182	O	0.548	11.441	0.095
183	O	11.649	4.658	0.144
184	O	7.996	11.447	0.078

185	O	3.907	0.057	2.973
186	O	0.394	6.803	3.009
187	O	11.394	0.062	3.020
188	O	7.866	6.798	3.021
189	O	0.039	2.326	5.801
190	O	-3.516	9.039	5.894
191	O	7.543	2.283	5.841
192	O	3.957	9.019	5.907
193	O	3.762	4.498	8.599
194	O	0.043	11.286	8.734
195	O	11.103	4.634	8.666
196	O	7.543	11.415	8.733
197	O	-1.954	4.989	2.290
198	O	-5.509	11.683	2.254
199	O	5.530	4.986	2.276
200	O	1.989	11.683	2.284
201	O	5.241	0.544	5.097
202	O	1.653	7.240	5.178
203	O	12.724	0.594	5.134
204	O	9.130	7.285	5.181
205	O	1.275	2.794	7.885
206	O	-2.225	9.514	7.996
207	O	8.860	2.854	7.911
208	O	5.254	9.552	7.987
209	O	-2.712	5.200	10.874
210	O	-6.131	12.026	10.809
211	O	5.103	5.019	10.837

212	O	1.539	11.807	10.666
213	O	6.350	1.153	0.767
214	O	2.853	7.873	0.785
215	O	13.817	1.166	0.765
216	O	10.314	7.867	0.792
217	O	2.509	3.409	3.414
218	O	-1.006	10.116	3.478
219	O	9.982	3.416	3.473
220	O	6.461	10.137	3.500
221	O	-1.367	5.712	6.249
222	O	-4.909	12.386	6.232
223	O	6.086	5.686	6.249
224	O	2.555	12.350	6.307
225	O	5.738	1.204	9.021
226	O	2.145	7.790	9.135
227	O	13.269	1.358	9.064
228	O	9.604	7.983	9.084
229	O	2.428	0.215	0.488
230	O	-1.064	6.888	0.505
231	O	9.910	0.210	0.522
232	O	6.405	6.900	0.498
233	O	6.098	2.427	3.294
234	O	2.568	9.113	3.363
235	O	13.558	2.444	3.298
236	O	10.036	9.131	3.361
237	O	2.218	4.544	5.984
238	O	-1.364	11.342	6.116

239	O	9.666	4.663	6.068
240	O	6.096	11.400	6.145
241	O	1.867	0.157	8.796
242	O	-1.771	6.916	8.963
243	O	9.303	0.359	8.963
244	O	5.667	6.922	8.965
245	O	2.633	5.674	2.097
246	O	-0.883	12.368	2.135
247	O	10.121	5.674	2.132
248	O	6.572	12.391	2.142
249	O	2.308	1.233	4.860
250	O	-1.271	7.983	4.932
251	O	9.793	1.216	4.919
252	O	6.198	7.970	4.939
253	O	-1.591	3.600	7.709
254	O	-5.207	10.274	7.778
255	O	5.902	3.472	7.645
256	O	2.302	10.162	7.837
257	O	2.463	5.111	10.772
258	O	-1.519	12.511	10.561
259	O	9.376	5.753	10.542
260	O	6.032	12.672	10.534
261	O	1.260	5.200	0.022
262	O	-2.308	11.886	0.056
263	O	8.738	5.202	0.056
264	O	5.161	11.893	0.070
265	O	0.938	0.704	2.853

266	O	-2.550	7.448	2.854
267	O	8.416	0.696	2.892
268	O	4.930	7.447	2.855
269	O	4.596	2.979	5.564
270	O	1.039	9.687	5.673
271	O	12.037	3.027	5.626
272	O	8.484	9.728	5.660
273	O	1.013	5.312	8.278
274	O	-2.806	11.973	8.466
275	O	8.179	5.364	8.396
276	O	4.570	11.981	8.553
277	O	4.074	2.399	1.642
278	O	0.557	9.121	1.681
279	O	11.532	2.394	1.680
280	O	8.021	9.125	1.693
281	O	0.174	4.610	4.456
282	O	-3.347	11.297	4.484
283	O	7.652	4.596	4.484
284	O	4.119	11.294	4.514
285	O	7.331	0.121	7.330
286	O	3.708	6.813	7.308
287	O	14.772	0.188	7.308
288	O	11.198	6.883	7.340
289	O	3.367	2.362	9.975
290	O	-0.129	9.031	10.166
291	O	11.007	2.430	10.019
292	O	7.248	9.164	9.972

293	O	0.776	4.681	13.019
294	O	-1.623	10.045	11.781
295	O	9.195	3.088	11.745
296	O	5.589	10.420	11.890
297	O	5.401	2.191	11.700
298	O	1.830	9.272	11.986
299	O	13.373	2.980	11.761
300	O	9.267	9.261	11.731
301	O	3.200	0.074	11.426
302	O	0.484	6.761	11.400
303	O	3.595	13.342	11.426
304	O	7.018	6.650	11.455
305	O	4.328	1.303	19.926
306	O	0.822	8.050	19.968
307	O	11.793	1.297	19.953
308	O	8.278	8.060	19.981
309	O	2.458	2.899	20.282
310	O	-1.105	9.576	20.344
311	O	9.941	2.907	20.320
312	O	6.350	9.586	20.359
313	O	-0.835	3.693	20.324
314	O	-4.441	10.405	20.364
315	O	6.655	3.698	20.336
316	O	3.038	10.400	20.366
317	O	0.767	0.524	19.654
318	O	-2.765	7.196	19.720
319	O	8.251	0.529	19.680

320	O	4.734	7.196	19.681
321	O	3.648	7.205	11.403
322	O	7.543	0.896	11.308
323	O	-3.667	7.708	11.293
324	O	0.652	1.803	10.591
325	O	0.795	7.292	13.838
326	O	-1.645	7.103	12.663
327	O	5.778	8.215	13.046
328	O	3.395	7.361	13.841

SI Fig. 4c

Simulation box:

a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

328 atoms

Atomic id	element	x	y	z
1	Hf	2.429	3.788	1.242
2	Hf	-1.081	10.493	1.284
3	Hf	9.912	3.793	1.291
4	Hf	6.384	10.508	1.302
5	Hf	-1.468	6.016	4.016
6	Hf	-5.011	12.689	3.983
7	Hf	6.013	6.008	4.023
8	Hf	2.464	12.684	4.040
9	Hf	5.685	1.553	6.820
10	Hf	2.085	8.245	6.910
11	Hf	13.127	1.626	6.860
12	Hf	9.541	8.320	6.915

13	Hf	1.668	3.569	9.676
14	Hf	-1.751	10.550	9.667
15	Hf	9.126	3.756	9.747
16	Hf	5.683	10.578	9.689
17	Hf	-1.471	3.229	1.284
18	Hf	-4.953	9.900	1.339
19	Hf	6.028	3.221	1.295
20	Hf	2.523	9.915	1.347
21	Hf	2.085	5.559	4.123
22	Hf	-1.445	12.245	4.146
23	Hf	9.541	5.583	4.156
24	Hf	6.003	12.276	4.167
25	Hf	1.761	1.091	6.859
26	Hf	-1.895	7.826	6.939
27	Hf	9.207	1.116	6.953
28	Hf	5.576	7.805	6.971
29	Hf	5.308	3.276	9.660
30	Hf	1.725	9.931	9.871
31	Hf	12.665	3.564	9.701
32	Hf	9.053	10.158	9.828
33	Hf	-6.568	13.298	1.060
34	Hf	-2.978	6.570	1.096
35	Hf	0.921	13.301	1.097
36	Hf	4.496	6.575	1.096
37	Hf	4.152	2.009	3.833
38	Hf	0.624	8.735	3.908
39	Hf	11.624	2.012	3.881

40	Hf	8.088	8.741	3.907
41	Hf	0.268	4.285	6.625
42	Hf	-3.307	11.006	6.736
43	Hf	7.737	4.296	6.720
44	Hf	4.167	10.992	6.770
45	Hf	3.748	6.375	9.486
46	Hf	0.355	13.298	9.535
47	Hf	11.230	6.580	9.566
48	Hf	14.901	0.033	9.432
49	Hf	4.409	0.276	0.940
50	Hf	0.914	6.990	0.961
51	Hf	11.884	0.277	0.969
52	Hf	8.376	6.995	0.970
53	Hf	0.616	2.475	3.781
54	Hf	-2.897	9.191	3.861
55	Hf	8.103	2.472	3.829
56	Hf	4.581	9.184	3.875
57	Hf	4.214	4.698	6.558
58	Hf	0.647	11.430	6.665
59	Hf	11.656	4.774	6.603
60	Hf	8.122	11.472	6.639
61	Hf	3.803	0.356	9.440
62	Hf	0.213	6.819	9.280
63	Hf	11.326	0.437	9.498
64	Hf	7.697	7.084	9.411
65	Hf	3.926	9.015	12.216
66	Hf	-0.228	8.688	12.413

67	Hf	2.006	6.257	12.447
68	Hf	-0.959	5.159	12.080
69	H	-3.674	9.433	10.822
70	H	10.099	2.765	11.847
71	H	6.374	10.023	12.327
72	H	-1.561	12.589	11.526
73	H	9.343	5.784	11.509
74	H	5.918	12.566	11.491
75	H	4.655	1.615	11.833
76	H	12.695	2.532	12.298
77	H	8.446	8.906	12.115
78	H	-2.367	10.413	12.400
79	H	8.145	1.707	11.479
80	H	2.531	0.779	11.611
81	H	9.997	0.553	11.773
82	H	5.151	1.781	19.712
83	H	1.628	8.577	19.791
84	H	12.617	1.779	19.740
85	H	9.081	8.585	19.782
86	H	1.721	0.420	19.993
87	H	-1.796	7.071	19.993
88	H	9.201	0.411	19.998
89	H	5.686	7.075	20.002
90	H	0.500	4.703	20.555
91	H	-3.060	11.389	20.587
92	H	7.986	4.697	20.583
93	H	4.411	11.391	20.595

94	H	3.774	4.486	20.207
95	H	0.126	11.295	20.195
96	H	11.241	4.441	20.245
97	H	7.538	11.291	20.189
98	H	1.609	2.707	19.833
99	H	-1.952	9.370	19.904
100	H	9.087	2.720	19.872
101	H	5.494	9.342	19.941
102	H	3.499	1.995	19.982
103	H	-0.029	8.710	20.032
104	H	10.964	1.998	20.013
105	H	7.425	8.718	20.046
106	H	-2.982	6.627	18.955
107	H	-6.446	13.328	18.911
108	H	4.552	6.576	18.945
109	H	1.006	13.373	18.914
110	H	-1.407	4.362	19.893
111	H	-5.040	11.088	20.005
112	H	6.089	4.346	19.888
113	H	2.443	11.093	20.018
114	H	-5.315	12.388	11.237
115	H	2.306	12.278	11.106
116	H	6.292	1.657	11.637
117	H	10.431	8.172	11.612
118	H	-0.097	2.157	11.155
119	H	4.606	10.634	16.216
120	H	5.278	9.237	15.302

121	H	3.598	9.201	15.919
122	H	2.478	11.803	13.489
123	H	2.885	11.996	15.223
124	H	1.848	10.631	14.668
125	H	-0.221	9.462	16.362
126	H	-0.835	8.037	15.470
127	H	-1.912	9.410	15.827
128	H	-0.348	11.689	13.438
129	H	-0.178	11.614	15.204
130	H	-1.787	11.449	14.486
131	H	6.374	4.036	15.807
132	H	6.618	3.075	14.326
133	H	6.491	2.262	15.923
134	H	2.866	2.775	16.170
135	H	4.065	3.823	16.959
136	H	4.294	2.057	16.983
137	H	-1.740	3.569	16.006
138	H	-0.372	3.440	14.836
139	H	13.017	2.638	14.501
140	H	11.301	5.888	13.872
141	H	11.209	4.857	15.339
142	H	11.057	4.130	13.714
143	H	4.614	4.818	11.680
144	H	6.506	7.348	12.046
145	H	1.182	7.985	14.436
146	H	6.306	5.912	11.313
147	H	-1.482	5.555	14.656

148	H	-2.569	7.364	12.228
149	H	4.425	2.287	14.469
150	H	5.395	7.469	13.613
151	H	3.133	7.222	14.750
152	H	4.652	11.008	13.840
153	N	3.899	10.409	14.207
154	N	-0.514	9.737	14.252
155	N	4.661	3.056	15.101
156	N	-1.917	4.732	14.216
157	C	4.379	9.840	15.484
158	C	2.710	11.263	14.415
159	C	-0.879	9.133	15.525
160	C	-0.716	11.172	14.337
161	C	6.105	3.096	15.298
162	C	3.942	2.906	16.358
163	C	-1.461	3.529	14.940
164	C	11.565	4.911	14.296
165	O	0.540	3.254	1.767
166	O	-2.969	9.968	1.841
167	O	8.033	3.240	1.796
168	O	4.504	9.977	1.859
169	O	4.082	5.657	4.648
170	O	0.556	12.293	4.715
171	O	11.555	5.674	4.683
172	O	8.019	12.331	4.695
173	O	3.734	1.198	7.413
174	O	0.122	7.892	7.488

175	O	11.228	1.144	7.456
176	O	7.584	7.913	7.474
177	O	-0.299	4.431	10.222
178	O	-3.788	10.231	10.234
179	O	7.219	3.506	10.061
180	O	3.769	9.899	10.358
181	O	4.160	4.676	0.113
182	O	0.549	11.444	0.091
183	O	11.649	4.658	0.137
184	O	7.992	11.448	0.068
185	O	3.905	0.063	2.968
186	O	0.388	6.811	3.006
187	O	11.393	0.067	3.013
188	O	7.863	6.804	3.014
189	O	0.034	2.324	5.788
190	O	-3.523	9.051	5.887
191	O	7.540	2.294	5.833
192	O	3.948	9.029	5.900
193	O	3.764	4.502	8.585
194	O	0.040	11.309	8.727
195	O	11.100	4.648	8.658
196	O	7.532	11.419	8.721
197	O	-1.962	4.993	2.283
198	O	-5.511	11.686	2.246
199	O	5.524	4.991	2.276
200	O	1.981	11.688	2.280
201	O	5.234	0.558	5.093

202	O	1.641	7.248	5.174
203	O	12.716	0.599	5.129
204	O	9.124	7.292	5.175
205	O	1.260	2.799	7.877
206	O	-2.235	9.533	7.988
207	O	8.855	2.863	7.906
208	O	5.233	9.555	7.987
209	O	-2.713	5.222	10.865
210	O	-6.139	12.034	10.796
211	O	5.066	5.023	10.844
212	O	1.520	11.813	10.678
213	O	6.347	1.161	0.761
214	O	2.854	7.879	0.781
215	O	13.815	1.172	0.753
216	O	10.315	7.871	0.784
217	O	2.505	3.418	3.404
218	O	-1.007	10.128	3.474
219	O	9.984	3.425	3.464
220	O	6.457	10.146	3.491
221	O	-1.375	5.721	6.234
222	O	-4.914	12.399	6.220
223	O	6.081	5.697	6.238
224	O	2.549	12.361	6.301
225	O	5.732	1.225	9.015
226	O	2.117	7.808	9.119
227	O	13.261	1.366	9.058
228	O	9.596	7.997	9.073

229	O	2.428	0.214	0.484
230	O	-1.063	6.886	0.499
231	O	9.909	0.209	0.515
232	O	6.407	6.895	0.493
233	O	6.097	2.431	3.287
234	O	2.563	9.116	3.356
235	O	13.556	2.446	3.288
236	O	10.034	9.134	3.352
237	O	2.212	4.547	5.972
238	O	-1.370	11.356	6.109
239	O	9.664	4.664	6.058
240	O	6.091	11.404	6.136
241	O	1.858	0.167	8.786
242	O	-1.785	6.923	8.937
243	O	9.299	0.361	8.958
244	O	5.669	6.912	8.947
245	O	2.623	5.680	2.089
246	O	-0.887	12.379	2.127
247	O	10.115	5.682	2.122
248	O	6.569	12.399	2.131
249	O	2.303	1.242	4.847
250	O	-1.280	7.995	4.923
251	O	9.787	1.225	4.913
252	O	6.192	7.982	4.934
253	O	-1.599	3.607	7.699
254	O	-5.217	10.288	7.765
255	O	5.901	3.487	7.633

256	O	2.287	10.178	7.831
257	O	2.388	5.194	10.686
258	O	-1.529	12.540	10.554
259	O	9.371	5.770	10.534
260	O	6.025	12.680	10.527
261	O	1.260	5.204	0.012
262	O	-2.305	11.890	0.048
263	O	8.741	5.205	0.046
264	O	5.160	11.898	0.059
265	O	0.939	0.711	2.838
266	O	-2.550	7.456	2.843
267	O	8.420	0.706	2.880
268	O	4.932	7.457	2.842
269	O	4.595	2.993	5.550
270	O	1.034	9.703	5.665
271	O	12.037	3.035	5.614
272	O	8.481	9.739	5.644
273	O	0.990	5.309	8.243
274	O	-2.815	12.001	8.454
275	O	8.185	5.381	8.380
276	O	4.575	11.996	8.539
277	O	4.070	2.403	1.638
278	O	0.553	9.125	1.677
279	O	11.529	2.396	1.671
280	O	8.017	9.130	1.685
281	O	0.167	4.613	4.443
282	O	-3.351	11.305	4.476

283	O	7.648	4.604	4.478
284	O	4.113	11.303	4.507
285	O	7.323	0.136	7.326
286	O	3.694	6.826	7.302
287	O	14.763	0.193	7.299
288	O	11.183	6.895	7.328
289	O	3.356	2.382	9.977
290	O	-0.166	9.094	10.173
291	O	11.004	2.440	10.016
292	O	7.239	9.169	9.963
293	O	0.816	4.759	12.965
294	O	-1.683	10.099	11.784
295	O	9.191	3.103	11.735
296	O	5.599	10.414	11.880
297	O	5.410	2.231	11.693
298	O	1.809	9.222	11.977
299	O	13.359	3.000	11.762
300	O	9.258	9.263	11.721
301	O	3.183	0.075	11.416
302	O	0.363	6.822	11.358
303	O	3.589	13.348	11.421
304	O	6.996	6.654	11.440
305	O	4.324	1.302	19.925
306	O	0.819	8.051	19.967
307	O	11.787	1.300	19.943
308	O	8.275	8.061	19.976
309	O	2.453	2.896	20.281

310	O	-1.108	9.579	20.344
311	O	9.936	2.905	20.315
312	O	6.342	9.583	20.357
313	O	-0.836	3.698	20.314
314	O	-4.440	10.409	20.359
315	O	6.662	3.700	20.332
316	O	3.041	10.404	20.358
317	O	0.766	0.523	19.651
318	O	-2.766	7.195	19.714
319	O	8.245	0.532	19.677
320	O	4.727	7.192	19.678
321	O	3.649	7.250	11.348
322	O	7.550	0.918	11.300
323	O	-3.669	7.728	11.272
324	O	0.637	1.809	10.579
325	O	0.752	7.372	13.816
326	O	-1.681	7.117	12.701
327	O	5.714	8.196	13.041
328	O	3.386	7.141	13.815

SI Fig. 5a

Simulation box:

a=14.949	b=15.168	c=25.974	α=90.00	β90.00	γ=117.78

308 atoms

Atomic id	element	x	y	z
1	Hf	2.291	3.818	1.298
2	Hf	-1.245	10.525	1.307

3	Hf	9.766	3.817	1.297
4	Hf	6.226	10.526	1.307
5	Hf	-1.607	6.037	4.035
6	Hf	-5.153	12.743	4.050
7	Hf	5.855	6.038	4.025
8	Hf	2.320	12.736	4.041
9	Hf	5.513	1.594	6.902
10	Hf	1.956	8.296	6.923
11	Hf	12.978	1.648	6.891
12	Hf	9.431	8.324	6.882
13	Hf	1.704	3.812	9.656
14	Hf	-1.855	10.497	9.675
15	Hf	9.051	3.851	9.539
16	Hf	5.568	10.544	9.666
17	Hf	-1.599	3.251	1.318
18	Hf	-5.134	9.964	1.320
19	Hf	5.870	3.248	1.311
20	Hf	2.337	9.958	1.317
21	Hf	1.935	5.601	4.160
22	Hf	-1.610	12.303	4.175
23	Hf	9.409	5.602	4.158
24	Hf	5.860	12.308	4.179
25	Hf	1.560	1.143	6.951
26	Hf	-1.971	7.836	6.956
27	Hf	9.044	1.110	6.943
28	Hf	5.499	7.841	6.951
29	Hf	5.108	3.330	9.806

30	Hf	1.572	10.038	9.816
31	Hf	12.493	3.406	9.777
32	Hf	8.961	10.070	9.803
33	Hf	-6.668	13.309	1.123
34	Hf	-3.133	6.603	1.109
35	Hf	0.804	13.307	1.109
36	Hf	4.347	6.607	1.097
37	Hf	4.009	2.059	3.904
38	Hf	0.471	8.769	3.909
39	Hf	11.482	2.059	3.903
40	Hf	7.940	8.765	3.889
41	Hf	0.100	4.345	6.731
42	Hf	-3.454	11.026	6.750
43	Hf	7.535	4.323	6.665
44	Hf	4.015	11.014	6.740
45	Hf	3.720	6.569	9.518
46	Hf	0.195	13.272	9.552
47	Hf	11.146	6.615	9.534
48	Hf	7.642	13.328	9.473
49	Hf	4.284	0.305	0.994
50	Hf	0.753	7.020	0.991
51	Hf	11.761	0.309	0.993
52	Hf	8.226	7.024	0.983
53	Hf	0.482	2.523	3.852
54	Hf	-3.063	9.224	3.857
55	Hf	7.945	2.510	3.834
56	Hf	4.412	9.223	3.855

57	Hf	4.037	4.765	6.626
58	Hf	0.495	11.466	6.638
59	Hf	11.512	4.796	6.620
60	Hf	7.978	11.474	6.627
61	Hf	3.660	0.345	9.456
62	Hf	0.115	7.029	9.480
63	Hf	11.135	0.369	9.496
64	Hf	7.581	7.084	9.465
65	Hf	1.776	9.597	14.099
66	Hf	9.713	3.306	14.462
67	Hf	5.277	2.481	14.174
68	Hf	0.721	3.931	15.058
69	H	-0.350	3.750	11.159
70	H	-3.815	9.258	10.638
71	H	7.278	2.426	10.912
72	H	3.799	9.123	10.835
73	H	2.239	2.965	12.134
74	H	-1.288	9.750	12.486
75	H	10.085	2.508	11.624
76	H	6.800	9.904	12.169
77	H	1.850	5.754	11.569
78	H	-1.765	12.518	11.586
79	H	9.320	5.775	11.551
80	H	5.857	12.533	11.508
81	H	4.577	1.656	11.888
82	H	0.894	8.471	11.937
83	H	12.442	2.438	12.465

84	H	8.379	8.422	11.867
85	H	0.648	1.768	11.439
86	H	-2.573	9.055	11.876
87	H	8.713	1.868	12.127
88	H	5.261	9.917	12.586
89	H	2.610	0.549	12.007
90	H	-0.901	7.239	12.070
91	H	10.605	0.167	12.269
92	H	6.144	7.371	11.568
93	H	4.984	1.817	24.744
94	H	1.453	8.535	24.746
95	H	12.467	1.824	24.749
96	H	8.930	8.549	24.744
97	H	1.572	0.391	24.955
98	H	-1.958	7.107	24.950
99	H	9.049	0.394	24.943
100	H	5.513	7.109	24.918
101	H	0.376	4.724	25.591
102	H	-3.152	11.432	25.594
103	H	7.848	4.724	25.594
104	H	4.316	11.433	25.599
105	H	3.657	4.515	25.241
106	H	0.126	11.213	25.253
107	H	11.141	4.509	25.246
108	H	7.607	11.219	25.257
109	H	1.434	2.747	24.905
110	H	-2.096	9.467	24.904

111	H	8.916	2.754	24.899
112	H	5.378	9.475	24.902
113	H	3.331	2.013	25.046
114	H	-0.200	8.729	25.047
115	H	10.815	2.017	25.043
116	H	7.275	8.735	25.043
117	H	-3.169	6.723	23.929
118	H	0.362	0.009	23.932
119	H	4.294	6.731	23.907
120	H	7.836	0.012	23.924
121	H	-1.502	4.344	24.872
122	H	-5.030	11.068	24.877
123	H	5.970	4.342	24.861
124	H	2.441	11.059	24.871
125	H	-2.082	5.569	11.348
126	H	-5.437	12.291	11.225
127	H	5.614	5.526	11.286
128	H	2.127	12.341	11.184
129	H	3.895	7.583	12.092
130	H	7.022	0.667	12.096
131	H	10.491	8.072	11.657
132	H	13.979	1.579	11.507
133	O	0.400	3.309	1.843
134	O	-3.137	10.025	1.849
135	O	7.874	3.299	1.831
136	O	4.335	10.020	1.847
137	O	3.935	5.666	4.706

138	O	0.403	12.361	4.721
139	O	11.413	5.666	4.700
140	O	7.868	12.377	4.717
141	O	3.583	1.173	7.459
142	O	0.029	7.892	7.486
143	O	11.040	1.219	7.501
144	O	7.501	7.882	7.427
145	O	-0.425	3.856	10.187
146	O	-3.893	10.137	10.144
147	O	7.226	3.305	10.375
148	O	3.654	10.045	10.370
149	O	4.023	4.686	0.159
150	O	0.494	11.389	0.169
151	O	11.503	4.683	0.164
152	O	7.970	11.391	0.176
153	O	3.778	0.115	3.041
154	O	0.244	6.830	3.037
155	O	11.254	0.112	3.039
156	O	7.714	6.820	3.022
157	O	-0.118	2.373	5.871
158	O	-3.656	9.076	5.880
159	O	7.337	2.358	5.852
160	O	3.805	9.070	5.879
161	O	3.505	4.631	8.706
162	O	-0.073	11.366	8.710
163	O	10.928	4.649	8.688
164	O	7.385	11.398	8.687

165	O	-2.101	5.023	2.308
166	O	-5.641	11.730	2.321
167	O	5.367	5.024	2.296
168	O	1.835	11.727	2.312
169	O	5.095	0.616	5.155
170	O	1.539	7.310	5.173
171	O	12.549	0.621	5.167
172	O	9.026	7.330	5.132
173	O	1.113	2.846	7.987
174	O	-2.325	9.572	7.946
175	O	8.659	2.884	7.875
176	O	5.090	9.581	7.956
177	O	12.135	5.163	10.829
178	O	-6.205	11.901	10.730
179	O	4.885	5.124	10.744
180	O	1.363	11.852	10.723
181	O	6.217	1.198	0.805
182	O	2.683	7.915	0.801
183	O	13.692	1.201	0.814
184	O	10.157	7.916	0.807
185	O	2.370	3.463	3.480
186	O	-1.173	10.170	3.497
187	O	9.833	3.459	3.487
188	O	6.295	10.174	3.494
189	O	-1.528	5.724	6.263
190	O	-5.074	12.436	6.282
191	O	5.933	5.706	6.249

192	O	2.402	12.422	6.295
193	O	5.614	1.243	9.153
194	O	2.063	7.966	9.144
195	O	13.031	1.319	9.078
196	O	9.503	7.951	9.050
197	O	2.312	0.207	0.546
198	O	-1.220	6.924	0.540
199	O	9.786	0.217	0.545
200	O	6.254	6.934	0.529
201	O	5.936	2.484	3.329
202	O	2.401	9.181	3.342
203	O	13.415	2.483	3.343
204	O	9.879	9.189	3.335
205	O	2.044	4.641	6.083
206	O	-1.516	11.409	6.118
207	O	9.484	4.726	6.106
208	O	5.945	11.418	6.130
209	O	1.662	0.305	8.917
210	O	-1.892	6.963	8.940
211	O	9.133	0.338	8.940
212	O	5.603	6.951	8.863
213	O	2.487	5.713	2.134
214	O	-1.043	12.416	2.146
215	O	9.974	5.708	2.133
216	O	6.431	12.417	2.149
217	O	2.141	1.300	4.931
218	O	-1.402	8.004	4.932

219	O	9.612	1.283	4.928
220	O	6.064	7.999	4.917
221	O	-1.786	3.602	7.764
222	O	-5.345	10.275	7.744
223	O	5.717	3.543	7.793
224	O	2.151	10.260	7.804
225	O	1.978	5.743	10.593
226	O	-1.554	12.417	10.630
227	O	9.308	5.751	10.563
228	O	5.875	12.549	10.533
229	O	1.128	5.231	0.054
230	O	-2.400	11.939	0.057
231	O	8.601	5.232	0.055
232	O	5.070	11.941	0.060
233	O	0.819	0.768	2.883
234	O	-2.714	7.481	2.871
235	O	8.286	0.756	2.877
236	O	4.754	7.479	2.863
237	O	4.444	3.044	5.651
238	O	0.890	9.747	5.663
239	O	11.880	3.058	5.647
240	O	8.338	9.760	5.629
241	O	0.683	5.371	8.389
242	O	-2.953	12.006	8.490
243	O	7.972	5.288	8.457
244	O	4.437	12.014	8.521
245	O	3.918	2.430	1.696

246	O	0.382	9.142	1.704
247	O	11.393	2.432	1.701
248	O	7.855	9.144	1.700
249	O	0.036	4.650	4.503
250	O	-3.510	11.354	4.518
251	O	7.502	4.642	4.484
252	O	3.959	11.348	4.515
253	O	7.145	0.190	7.350
254	O	3.587	6.888	7.331
255	O	14.607	0.212	7.330
256	O	11.081	6.899	7.326
257	O	3.328	2.421	9.902
258	O	-0.244	9.137	9.939
259	O	10.589	2.513	10.101
260	O	7.107	9.161	9.834
261	O	1.434	3.122	11.606
262	O	-2.025	9.900	11.841
263	O	9.398	2.586	12.386
264	O	5.930	10.308	11.963
265	O	5.065	2.498	12.040
266	O	1.553	9.198	12.033
267	O	12.865	2.393	11.587
268	O	9.060	9.090	11.642
269	O	3.126	0.006	11.388
270	O	-0.378	6.734	11.424
271	O	3.418	13.283	11.356
272	O	6.962	6.856	11.389

273	O	4.168	1.335	24.988
274	O	0.638	8.051	24.987
275	O	11.651	1.339	24.987
276	O	8.115	8.060	24.981
277	O	2.281	2.896	25.363
278	O	-1.250	9.610	25.368
279	O	9.763	2.903	25.357
280	O	6.224	9.615	25.365
281	O	-0.956	3.704	25.357
282	O	-4.486	10.422	25.359
283	O	6.520	3.710	25.353
284	O	2.989	10.423	25.360
285	O	0.594	0.491	24.744
286	O	-2.937	7.207	24.739
287	O	8.070	0.490	24.738
288	O	4.534	7.204	24.722
289	O	4.165	7.717	11.163
290	O	7.569	0.980	11.343
291	O	-3.586	7.798	11.233
292	O	-0.060	1.051	11.252
293	Cl	1.852	9.183	16.427
294	Cl	4.089	8.858	14.004
295	Cl	-0.518	8.810	14.205
296	Cl	1.852	11.911	14.103
297	Cl	9.794	3.933	16.707
298	Cl	9.999	5.491	13.628
299	Cl	11.530	1.847	14.511

300	Cl	7.819	1.876	14.810
301	Cl	5.070	2.440	16.545
302	Cl	6.060	4.706	13.998
303	Cl	5.429	0.059	13.833
304	Cl	2.811	2.397	14.255
305	Cl	1.178	4.114	17.306
306	Cl	1.980	5.646	13.936
307	Cl	-0.180	1.781	14.754
308	Cl	-1.319	5.030	14.829

SI Fig. 5b

Simulation box:

a=14.949	b=15.168	c=25.974	α=90.00	β90.00	γ=117.78

311 atoms

Atomic id	element	x	y	z
1	Hf	2.288	3.804	1.310
2	Hf	-1.246	10.511	1.318
3	Hf	9.766	3.801	1.317
4	Hf	6.226	10.518	1.314
5	Hf	-1.617	6.024	4.045
6	Hf	-5.162	12.734	4.052
7	Hf	5.862	6.020	4.038
8	Hf	2.310	12.731	4.057
9	Hf	5.499	1.574	6.896
10	Hf	1.963	8.289	6.927
11	Hf	12.992	1.636	6.898
12	Hf	9.428	8.315	6.889

13	Hf	1.706	3.790	9.698
14	Hf	-1.848	10.503	9.667
15	Hf	8.973	3.867	9.737
16	Hf	5.596	10.506	9.656
17	Hf	-1.602	3.242	1.327
18	Hf	-5.139	9.954	1.324
19	Hf	5.877	3.235	1.329
20	Hf	2.334	9.954	1.321
21	Hf	1.932	5.583	4.170
22	Hf	-1.611	12.286	4.178
23	Hf	9.406	5.581	4.174
24	Hf	5.860	12.296	4.180
25	Hf	1.567	1.133	6.959
26	Hf	-1.962	7.817	6.957
27	Hf	9.056	1.125	6.976
28	Hf	5.506	7.814	6.950
29	Hf	5.070	3.345	9.745
30	Hf	1.583	10.033	9.841
31	Hf	12.553	3.421	9.777
32	Hf	8.985	10.084	9.823
33	Hf	-6.672	13.304	1.124
34	Hf	-3.141	6.591	1.120
35	Hf	0.805	13.296	1.125
36	Hf	4.333	6.590	1.114
37	Hf	4.008	2.039	3.902
38	Hf	0.473	8.751	3.918
39	Hf	11.489	2.043	3.916

40	Hf	7.942	8.746	3.893
41	Hf	0.111	4.336	6.750
42	Hf	-3.453	11.006	6.749
43	Hf	7.565	4.295	6.739
44	Hf	4.018	10.990	6.721
45	Hf	3.719	6.563	9.520
46	Hf	0.194	13.274	9.499
47	Hf	11.151	6.592	9.514
48	Hf	7.648	13.319	9.479
49	Hf	4.286	0.295	0.994
50	Hf	0.750	7.009	0.994
51	Hf	11.761	0.297	0.996
52	Hf	8.225	7.005	0.989
53	Hf	0.478	2.513	3.863
54	Hf	-3.072	9.216	3.862
55	Hf	7.950	2.506	3.862
56	Hf	4.407	9.211	3.852
57	Hf	4.046	4.749	6.621
58	Hf	0.501	11.458	6.640
59	Hf	11.511	4.774	6.649
60	Hf	7.980	11.462	6.632
61	Hf	3.675	0.320	9.488
62	Hf	0.117	7.028	9.482
63	Hf	11.176	0.270	9.458
64	Hf	7.586	7.090	9.474
65	Hf	1.864	9.342	14.110
66	Hf	9.194	3.755	14.042

67	Hf	5.447	2.229	14.230
68	Hf	1.021	4.488	15.171
69	H	-0.310	3.700	11.199
70	H	-3.788	9.226	10.600
71	H	7.171	2.385	10.853
72	H	3.814	9.136	10.845
73	H	2.225	2.942	12.196
74	H	-1.289	9.837	12.515
75	H	10.546	2.219	11.029
76	H	6.910	10.046	12.185
77	H	1.877	5.804	11.575
78	H	-1.560	12.568	11.566
79	H	9.398	5.874	11.576
80	H	5.905	12.471	11.497
81	H	4.339	1.719	11.997
82	H	0.897	8.444	11.904
83	H	12.425	2.628	12.474
84	H	8.377	8.427	11.872
85	H	0.634	1.688	11.522
86	H	-2.549	9.112	11.888
87	H	8.715	2.319	11.931
88	H	5.378	9.924	12.618
89	H	3.463	-0.445	12.136
90	H	-0.917	7.227	12.068
91	H	10.841	-0.076	12.217
92	H	6.128	7.371	11.557
93	H	4.988	1.821	24.757

94	H	1.449	8.522	24.750
95	H	12.464	1.819	24.759
96	H	8.929	8.528	24.753
97	H	1.573	0.380	24.961
98	H	-1.961	7.094	24.961
99	H	9.051	0.381	24.964
100	H	5.514	7.093	24.962
101	H	0.379	4.710	25.599
102	H	-3.150	11.419	25.601
103	H	7.857	4.706	25.601
104	H	4.319	11.422	25.601
105	H	3.647	4.502	25.252
106	H	0.129	11.204	25.263
107	H	11.133	4.500	25.258
108	H	7.606	11.208	25.261
109	H	1.432	2.723	24.921
110	H	-2.096	9.446	24.917
111	H	8.912	2.727	24.921
112	H	5.382	9.446	24.914
113	H	3.333	2.008	25.056
114	H	-0.207	8.721	25.056
115	H	10.809	2.008	25.058
116	H	7.273	8.721	25.054
117	H	-3.167	6.714	23.931
118	H	0.359	0.003	23.938
119	H	4.307	6.714	23.931
120	H	7.845	-0.007	23.939

121	H	-1.501	4.340	24.882
122	H	-5.028	11.051	24.878
123	H	5.971	4.346	24.897
124	H	2.442	11.047	24.873
125	H	-2.006	5.611	11.284
126	H	-5.465	12.377	11.208
127	H	5.597	5.502	11.269
128	H	2.060	12.357	11.210
129	H	3.952	7.591	12.086
130	H	7.204	0.682	12.040
131	H	10.534	8.052	11.650
132	H	13.955	1.559	11.535
133	H	5.577	3.010	16.841
134	H	6.766	3.912	16.210
135	O	0.397	3.300	1.852
136	O	-3.139	10.010	1.853
137	O	7.877	3.292	1.855
138	O	4.333	10.008	1.847
139	O	3.939	5.649	4.713
140	O	0.399	12.349	4.722
141	O	11.410	5.636	4.721
142	O	7.868	12.362	4.718
143	O	3.576	1.163	7.463
144	O	0.037	7.881	7.488
145	O	11.061	1.208	7.515
146	O	7.508	7.840	7.425
147	O	-0.405	3.827	10.229

148	O	-3.883	10.133	10.140
149	O	7.080	3.299	10.337
150	O	3.671	10.059	10.381
151	O	4.018	4.673	0.167
152	O	0.497	11.376	0.179
153	O	11.499	4.671	0.176
154	O	7.969	11.381	0.179
155	O	3.779	0.096	3.041
156	O	0.246	6.814	3.041
157	O	11.259	0.101	3.049
158	O	7.713	6.801	3.030
159	O	-0.108	2.364	5.886
160	O	-3.655	9.055	5.886
161	O	7.369	2.356	5.900
162	O	3.807	9.051	5.875
163	O	3.494	4.607	8.709
164	O	-0.064	11.345	8.697
165	O	10.922	4.591	8.734
166	O	7.383	11.393	8.686
167	O	-2.106	5.010	2.317
168	O	-5.643	11.721	2.321
169	O	5.368	5.004	2.311
170	O	1.835	11.717	2.323
171	O	5.094	0.597	5.156
172	O	1.543	7.297	5.179
173	O	12.558	0.607	5.179
174	O	9.035	7.315	5.137

175	O	1.117	2.832	8.014
176	O	-2.323	9.555	7.949
177	O	8.659	2.856	8.009
178	O	5.098	9.548	7.952
179	O	12.185	5.170	10.817
180	O	-6.235	11.906	10.746
181	O	4.843	5.108	10.759
182	O	1.320	11.852	10.743
183	O	6.221	1.186	0.816
184	O	2.679	7.903	0.810
185	O	13.692	1.194	0.817
186	O	10.154	7.902	0.814
187	O	2.368	3.448	3.487
188	O	-1.176	10.154	3.503
189	O	9.840	3.444	3.505
190	O	6.295	10.161	3.493
191	O	-1.527	5.707	6.273
192	O	-5.073	12.425	6.284
193	O	5.948	5.685	6.260
194	O	2.409	12.408	6.287
195	O	5.596	1.241	9.110
196	O	2.070	7.959	9.143
197	O	13.049	1.301	9.086
198	O	9.514	7.945	9.040
199	O	2.313	0.199	0.548
200	O	-1.226	6.914	0.550
201	O	9.788	0.201	0.553

202	O	6.251	6.907	0.540
203	O	5.944	2.464	3.348
204	O	2.401	9.168	3.343
205	O	13.415	2.471	3.354
206	O	9.874	9.183	3.340
207	O	2.046	4.630	6.094
208	O	-1.513	11.392	6.118
209	O	9.487	4.703	6.145
210	O	5.949	11.396	6.124
211	O	1.669	0.294	8.938
212	O	-1.882	6.941	8.923
213	O	9.173	0.237	8.902
214	O	5.608	6.925	8.865
215	O	2.492	5.699	2.145
216	O	-1.038	12.402	2.152
217	O	9.969	5.694	2.150
218	O	6.432	12.410	2.151
219	O	2.139	1.286	4.934
220	O	-1.398	7.988	4.935
221	O	9.614	1.276	4.949
222	O	6.070	7.982	4.920
223	O	-1.759	3.592	7.777
224	O	-5.346	10.270	7.746
225	O	5.691	3.542	7.770
226	O	2.167	10.249	7.815
227	O	1.976	5.743	10.598
228	O	-1.561	12.454	10.577

229	O	9.328	5.802	10.588
230	O	5.839	12.533	10.525
231	O	1.130	5.218	0.062
232	O	-2.399	11.927	0.063
233	O	8.608	5.214	0.064
234	O	5.072	11.930	0.062
235	O	0.816	0.759	2.885
236	O	-2.727	7.464	2.886
237	O	8.291	0.753	2.890
238	O	4.753	7.461	2.873
239	O	4.437	3.024	5.647
240	O	0.898	9.737	5.667
241	O	11.889	3.042	5.666
242	O	8.333	9.741	5.636
243	O	0.674	5.354	8.417
244	O	-2.945	12.002	8.477
245	O	7.962	5.250	8.547
246	O	4.486	11.966	8.489
247	O	3.922	2.417	1.706
248	O	0.381	9.130	1.712
249	O	11.394	2.419	1.713
250	O	7.854	9.128	1.704
251	O	0.035	4.637	4.512
252	O	-3.513	11.338	4.523
253	O	7.513	4.621	4.512
254	O	3.961	11.333	4.512
255	O	7.152	0.181	7.337

256	O	3.590	6.870	7.334
257	O	14.615	0.197	7.332
258	O	11.084	6.869	7.330
259	O	3.325	2.388	9.957
260	O	-0.236	9.129	9.951
261	O	10.621	2.422	10.064
262	O	7.131	9.152	9.820
263	O	1.436	3.119	11.650
264	O	-2.011	9.957	11.840
265	O	9.169	3.207	12.011
266	O	6.004	10.363	11.974
267	O	5.030	2.387	12.204
268	O	1.600	9.125	12.003
269	O	12.773	2.387	11.591
270	O	9.053	9.101	11.650
271	O	2.973	-0.109	11.361
272	O	-0.450	6.689	11.405
273	O	3.362	13.408	11.340
274	O	6.950	6.859	11.385
275	O	4.174	1.332	24.994
276	O	0.633	8.041	24.994
277	O	11.649	1.331	24.996
278	O	8.113	8.042	24.989
279	O	2.279	2.882	25.375
280	O	-1.250	9.598	25.375
281	O	9.759	2.883	25.378
282	O	6.227	9.599	25.373

283	O	-0.957	3.697	25.366
284	O	-4.485	10.409	25.365
285	O	6.519	3.696	25.368
286	O	2.990	10.414	25.365
287	O	0.595	0.486	24.749
288	O	-2.939	7.195	24.745
289	O	8.074	0.482	24.748
290	O	4.537	7.199	24.742
291	O	4.188	7.724	11.146
292	O	7.575	1.035	11.205
293	O	-3.558	7.817	11.188
294	O	-0.109	1.030	11.294
295	O	5.863	3.518	16.053
296	Cl	1.953	8.855	16.430
297	Cl	4.275	8.857	14.001
298	Cl	-0.546	8.994	14.237
299	Cl	2.033	11.658	14.138
300	Cl	8.805	4.331	16.374
301	Cl	10.047	5.911	13.585
302	Cl	11.169	2.505	14.463
303	Cl	7.879	1.558	14.531
304	Cl	4.413	1.140	16.145
305	Cl	6.754	4.413	13.541
306	Cl	5.404	-0.213	13.539
307	Cl	3.320	3.671	14.251
308	Cl	1.656	4.647	17.378
309	Cl	1.844	6.396	13.813

310	Cl	0.263	2.307	14.826
311	Cl	-1.112	5.418	15.209

SI Fig. 5c is a duplicate of Fig. 3.

SI Fig. 5d

Simulation box:

a=14.949	b=15.168	c=25.974	α=90.00	β90.00	γ=117.78

323 atoms

Atomic id	element	x	y	z
1	Hf	2.302	3.785	1.231
2	Hf	-1.229	10.496	1.258
3	Hf	9.782	3.789	1.254
4	Hf	6.245	10.499	1.258
5	Hf	-1.592	6.008	3.980
6	Hf	-5.154	12.711	3.960
7	Hf	5.871	5.986	3.957
8	Hf	2.322	12.702	3.958
9	Hf	5.506	1.562	6.809
10	Hf	1.971	8.260	6.851
11	Hf	12.963	1.624	6.806
12	Hf	9.434	8.321	6.813
13	Hf	1.699	3.776	9.609
14	Hf	-1.833	10.460	9.638
15	Hf	9.113	3.850	9.572
16	Hf	5.569	10.539	9.577
17	Hf	-1.601	3.227	1.252

18	Hf	-5.117	9.920	1.272
19	Hf	5.887	3.200	1.234
20	Hf	2.357	9.906	1.259
21	Hf	1.941	5.558	4.083
22	Hf	-1.621	12.276	4.093
23	Hf	9.405	5.578	4.099
24	Hf	5.850	12.285	4.105
25	Hf	1.538	1.133	6.846
26	Hf	-1.947	7.825	6.901
27	Hf	9.030	1.117	6.869
28	Hf	5.503	7.815	6.872
29	Hf	5.117	3.261	9.698
30	Hf	1.642	9.941	9.794
31	Hf	12.497	3.413	9.700
32	Hf	8.951	10.067	9.729
33	Hf	-6.656	13.279	1.022
34	Hf	-3.106	6.575	1.053
35	Hf	0.821	13.271	1.022
36	Hf	4.363	6.560	1.019
37	Hf	4.010	2.029	3.823
38	Hf	0.483	8.724	3.842
39	Hf	11.479	2.026	3.830
40	Hf	7.947	8.733	3.831
41	Hf	0.111	4.321	6.677
42	Hf	-3.439	11.018	6.694
43	Hf	7.569	4.291	6.643
44	Hf	4.019	10.994	6.654

45	Hf	3.750	6.518	9.473
46	Hf	0.166	13.192	9.390
47	Hf	11.153	6.647	9.472
48	Hf	7.607	13.338	9.400
49	Hf	4.293	0.263	0.913
50	Hf	0.774	6.976	0.916
51	Hf	11.779	0.265	0.920
52	Hf	8.250	6.978	0.916
53	Hf	0.473	2.484	3.770
54	Hf	-3.053	9.198	3.804
55	Hf	7.950	2.472	3.767
56	Hf	4.426	9.167	3.779
57	Hf	4.040	4.745	6.557
58	Hf	0.503	11.433	6.546
59	Hf	11.522	4.786	6.559
60	Hf	7.978	11.471	6.557
61	Hf	3.603	0.331	9.347
62	Hf	0.141	7.008	9.421
63	Hf	11.125	0.392	9.399
64	Hf	7.589	7.076	9.390
65	Hf	1.897	9.807	14.108
66	Hf	9.529	3.883	13.935
67	Hf	5.108	2.162	13.939
68	Hf	0.500	4.169	16.785
69	H	-0.355	3.790	11.116
70	H	-3.858	9.388	10.729
71	H	7.330	2.588	11.005

72	H	3.882	9.052	10.832
73	H	2.100	2.857	12.156
74	H	-1.310	9.760	12.484
75	H	10.123	2.840	11.687
76	H	6.969	10.068	12.070
77	H	1.681	5.827	11.452
78	H	-1.620	12.451	11.558
79	H	9.265	5.901	11.426
80	H	5.886	12.507	11.433
81	H	4.630	1.403	11.633
82	H	1.001	8.477	11.980
83	H	12.370	2.472	12.400
84	H	8.330	8.419	11.747
85	H	0.608	1.763	11.382
86	H	-2.506	8.901	11.798
87	H	8.820	0.638	11.437
88	H	5.440	10.041	12.556
89	H	2.862	0.376	12.088
90	H	-0.781	7.027	12.023
91	H	10.677	0.007	12.170
92	H	6.150	7.352	11.523
93	H	4.974	1.790	24.664
94	H	1.441	8.526	24.685
95	H	12.468	1.794	24.687
96	H	8.933	8.547	24.706
97	H	1.570	0.355	24.813
98	H	-1.957	7.045	24.845

99	H	9.061	0.356	24.853
100	H	5.527	7.053	24.835
101	H	0.388	4.687	25.523
102	H	-3.152	11.386	25.533
103	H	7.872	4.687	25.530
104	H	4.318	11.390	25.537
105	H	3.654	4.474	25.165
106	H	0.077	11.194	25.176
107	H	11.175	4.459	25.204
108	H	7.564	11.196	25.179
109	H	1.423	2.727	24.841
110	H	-2.115	9.403	24.877
111	H	8.931	2.729	24.849
112	H	5.371	9.404	24.873
113	H	3.320	1.975	24.981
114	H	-0.216	8.693	25.004
115	H	10.811	1.986	24.995
116	H	7.272	8.700	25.005
117	H	-3.214	6.708	23.864
118	H	0.313	0.018	23.836
119	H	4.274	6.713	23.847
120	H	7.836	-0.023	23.850
121	H	-1.473	4.300	24.780
122	H	-5.051	11.048	24.854
123	H	5.988	4.335	24.814
124	H	2.420	11.046	24.847
125	H	-2.846	5.306	11.739

126	H	-5.526	12.271	11.213
127	H	5.676	5.467	11.177
128	H	2.131	12.232	11.083
129	H	3.863	7.526	12.065
130	H	7.346	0.507	12.134
131	H	10.494	8.052	11.625
132	H	13.941	1.562	11.447
133	H	10.091	2.566	17.014
134	H	6.180	4.591	16.980
135	H	1.091	7.205	14.991
136	H	2.658	7.335	15.279
137	H	3.144	5.081	16.568
138	H	3.237	3.487	16.884
139	H	4.822	6.202	16.407
140	H	4.139	5.790	15.095
141	H	6.972	5.471	15.995
142	H	8.351	6.217	14.318
143	O	0.401	3.294	1.777
144	O	-3.127	10.003	1.801
145	O	7.884	3.270	1.769
146	O	4.349	9.980	1.786
147	O	3.941	5.643	4.636
148	O	0.397	12.332	4.633
149	O	11.419	5.654	4.641
150	O	7.869	12.358	4.641
151	O	3.568	1.158	7.361
152	O	0.047	7.870	7.425

153	O	11.040	1.150	7.393
154	O	7.511	7.845	7.348
155	O	-0.433	3.907	10.143
156	O	-3.903	10.174	10.121
157	O	7.216	3.275	10.304
158	O	3.722	9.970	10.344
159	O	4.028	4.643	0.080
160	O	0.470	11.364	0.082
161	O	11.530	4.638	0.124
162	O	7.946	11.367	0.090
163	O	3.777	0.080	2.963
164	O	0.257	6.788	2.969
165	O	11.252	0.074	2.967
166	O	7.728	6.780	2.960
167	O	-0.109	2.345	5.797
168	O	-3.645	9.072	5.825
169	O	7.364	2.328	5.800
170	O	3.820	9.033	5.803
171	O	3.508	4.601	8.633
172	O	-0.113	11.339	8.577
173	O	10.940	4.686	8.621
174	O	7.375	11.407	8.627
175	O	-2.098	4.989	2.262
176	O	-5.651	11.694	2.241
177	O	5.370	4.970	2.232
178	O	1.833	11.683	2.234
179	O	5.089	0.587	5.076

180	O	1.542	7.269	5.109
181	O	12.550	0.599	5.084
182	O	9.034	7.308	5.074
183	O	1.093	2.819	7.929
184	O	-2.340	9.546	7.902
185	O	8.672	2.868	7.866
186	O	5.105	9.564	7.871
187	O	11.973	5.112	10.788
188	O	-6.266	11.897	10.680
189	O	4.957	5.062	10.631
190	O	1.410	11.788	10.557
191	O	6.227	1.162	0.715
192	O	2.703	7.874	0.723
193	O	13.701	1.174	0.735
194	O	10.179	7.882	0.749
195	O	2.373	3.434	3.407
196	O	-1.161	10.143	3.435
197	O	9.839	3.434	3.427
198	O	6.304	10.145	3.432
199	O	-1.515	5.712	6.212
200	O	-5.072	12.426	6.212
201	O	5.943	5.671	6.193
202	O	2.396	12.389	6.213
203	O	5.607	1.172	9.076
204	O	2.092	7.901	9.102
205	O	13.039	1.315	8.988
206	O	9.514	7.977	8.972

207	O	2.323	0.158	0.458
208	O	-1.199	6.868	0.471
209	O	9.801	0.165	0.462
210	O	6.278	6.864	0.455
211	O	5.948	2.428	3.256
212	O	2.417	9.122	3.275
213	O	13.417	2.441	3.269
214	O	9.891	9.152	3.282
215	O	2.051	4.604	6.012
216	O	-1.518	11.382	6.040
217	O	9.495	4.708	6.051
218	O	5.946	11.408	6.058
219	O	1.626	0.288	8.835
220	O	-1.864	6.947	8.927
221	O	9.114	0.311	8.855
222	O	5.608	6.952	8.806
223	O	2.497	5.684	2.059
224	O	-1.046	12.396	2.072
225	O	9.981	5.685	2.075
226	O	6.426	12.398	2.076
227	O	2.138	1.273	4.842
228	O	-1.392	7.985	4.878
229	O	9.610	1.253	4.851
230	O	6.076	7.958	4.843
231	O	-1.791	3.586	7.684
232	O	-5.353	10.280	7.681
233	O	5.722	3.492	7.718

234	O	2.170	10.206	7.752
235	O	2.074	5.650	10.570
236	O	-1.390	12.307	10.611
237	O	9.265	5.856	10.453
238	O	5.754	12.591	10.468
239	O	1.149	5.194	-0.027
240	O	-2.398	11.895	-0.012
241	O	8.631	5.193	-0.013
242	O	5.075	11.896	-0.006
243	O	0.830	0.738	2.787
244	O	-2.683	7.461	2.807
245	O	8.302	0.725	2.790
246	O	4.781	7.433	2.781
247	O	4.457	3.022	5.567
248	O	0.911	9.712	5.588
249	O	11.876	3.039	5.574
250	O	8.339	9.746	5.563
251	O	0.698	5.353	8.327
252	O	-2.941	11.985	8.446
253	O	7.975	5.253	8.426
254	O	4.428	11.990	8.445
255	O	3.927	2.393	1.626
256	O	0.396	9.105	1.645
257	O	11.397	2.394	1.643
258	O	7.869	9.108	1.646
259	O	0.036	4.617	4.442
260	O	-3.514	11.330	4.447

261	O	7.512	4.601	4.428
262	O	3.960	11.312	4.439
263	O	7.139	0.161	7.246
264	O	3.599	6.858	7.266
265	O	14.593	0.194	7.241
266	O	11.106	6.904	7.265
267	O	3.321	2.392	9.807
268	O	-0.204	9.120	9.841
269	O	10.646	2.460	9.855
270	O	7.113	9.151	9.736
271	O	1.389	3.011	11.506
272	O	-1.989	9.770	11.757
273	O	9.468	3.541	11.949
274	O	6.070	10.415	11.874
275	O	5.131	2.230	11.848
276	O	1.604	9.265	12.029
277	O	12.815	2.428	11.532
278	O	9.023	9.096	11.584
279	O	3.230	-0.042	11.285
280	O	-0.021	6.847	11.447
281	O	10.268	0.149	11.298
282	O	6.988	6.867	11.341
283	O	4.164	1.303	24.917
284	O	0.637	8.028	24.933
285	O	11.654	1.307	24.927
286	O	8.128	8.038	24.934
287	O	2.271	2.845	25.308

288	O	-1.266	9.554	25.331
289	O	9.776	2.863	25.315
290	O	6.219	9.559	25.327
291	O	-0.936	3.676	25.294
292	O	-4.500	10.387	25.305
293	O	6.540	3.690	25.286
294	O	2.979	10.394	25.302
295	O	0.587	0.456	24.660
296	O	-2.939	7.159	24.681
297	O	8.082	0.461	24.657
298	O	4.546	7.168	24.662
299	O	4.190	7.652	11.156
300	O	7.796	0.826	11.315
301	O	-3.590	7.756	11.215
302	O	-0.119	1.030	11.196
303	O	6.397	5.529	16.798
304	O	1.908	7.675	14.720
305	O	2.620	4.264	16.969
306	O	3.912	6.208	15.967
307	O	8.223	5.266	14.471
308	Cl	2.101	10.230	16.460
309	Cl	4.303	9.203	13.985
310	Cl	-0.506	9.531	14.357
311	Cl	2.187	12.128	13.726
312	Cl	9.536	3.734	17.012
313	Cl	11.230	5.571	13.876
314	Cl	11.122	2.123	14.457

315	Cl	7.697	2.195	14.362
316	Cl	5.021	2.354	16.426
317	Cl	5.117	4.563	13.712
318	Cl	-1.386	13.214	13.716
319	Cl	2.779	1.642	14.013
320	Cl	0.517	3.893	19.161
321	Cl	0.943	4.701	14.455
322	Cl	-0.542	2.145	16.321
323	Cl	-0.874	6.072	16.892

SI Fig. 6a

Simulation box:

a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

290 atoms

Atomic id	element	x	y	z
1	Hf	2.315	3.813	1.360
2	Hf	-1.218	10.521	1.362
3	Hf	9.791	3.819	1.363
4	Hf	6.255	10.529	1.363
5	Hf	-1.597	6.051	4.102
6	Hf	-5.133	12.742	4.098
7	Hf	5.879	6.029	4.063
8	Hf	2.332	12.742	4.081
9	Hf	5.525	1.612	6.963
10	Hf	1.983	8.338	6.956
11	Hf	13.016	1.639	6.962
12	Hf	9.461	8.352	6.961

13	Hf	1.686	3.776	9.752
14	Hf	-1.866	10.692	9.690
15	Hf	9.174	3.853	9.655
16	Hf	5.564	10.651	9.590
17	Hf	-1.577	3.257	1.383
18	Hf	-5.106	9.964	1.384
19	Hf	5.904	3.236	1.361
20	Hf	2.364	9.955	1.365
21	Hf	1.945	5.604	4.226
22	Hf	-1.585	12.306	4.228
23	Hf	9.428	5.612	4.235
24	Hf	5.891	12.318	4.235
25	Hf	1.605	1.127	7.012
26	Hf	-1.958	7.871	7.014
27	Hf	9.075	1.141	6.988
28	Hf	5.526	7.836	6.965
29	Hf	5.080	3.267	9.896
30	Hf	1.662	10.062	9.782
31	Hf	12.576	3.393	9.908
32	Hf	9.009	10.082	9.895
33	Hf	-6.652	13.313	1.171
34	Hf	-3.110	6.599	1.175
35	Hf	0.829	13.301	1.159
36	Hf	4.365	6.598	1.151
37	Hf	4.033	2.043	3.949
38	Hf	0.500	8.781	3.970
39	Hf	11.510	2.069	3.972

40	Hf	7.969	8.781	3.967
41	Hf	0.105	4.327	6.785
42	Hf	-3.419	11.046	6.824
43	Hf	7.573	4.314	6.755
44	Hf	4.016	11.044	6.748
45	Hf	3.706	6.501	9.436
46	Hf	0.127	13.383	9.618
47	Hf	11.222	6.659	9.626
48	Hf	7.693	13.355	9.623
49	Hf	4.320	0.292	1.046
50	Hf	0.785	7.001	1.061
51	Hf	11.793	0.309	1.065
52	Hf	8.258	7.021	1.059
53	Hf	0.495	2.523	3.909
54	Hf	-3.039	9.237	3.915
55	Hf	7.970	2.518	3.895
56	Hf	4.433	9.228	3.893
57	Hf	4.071	4.753	6.655
58	Hf	0.518	11.514	6.719
59	Hf	11.545	4.805	6.706
60	Hf	8.009	11.510	6.700
61	Hf	3.726	0.340	9.597
62	Hf	0.151	7.020	9.513
63	Hf	11.178	0.434	9.498
64	Hf	7.629	7.039	9.476
65	Hf	3.679	9.377	12.572
66	Hf	0.101	10.143	12.647

67	Hf	6.156	8.109	12.174
68	H	-0.183	2.568	10.802
69	H	-3.709	9.434	10.933
70	H	7.320	2.597	10.803
71	H	4.389	6.916	11.786
72	H	10.233	3.041	12.125
73	H	1.859	5.820	11.608
74	H	9.221	5.837	11.594
75	H	5.497	12.664	11.557
76	H	4.552	1.694	11.973
77	H	11.980	1.700	11.881
78	H	8.473	8.445	12.016
79	H	1.216	2.470	12.081
80	H	-1.827	9.445	12.236
81	H	8.761	2.462	12.009
82	H	2.238	0.582	11.735
83	H	-0.646	7.314	12.102
84	H	9.902	0.498	11.864
85	H	4.997	1.829	19.800
86	H	1.463	8.525	19.801
87	H	12.498	1.840	19.826
88	H	8.956	8.558	19.821
89	H	1.597	0.378	20.022
90	H	-1.935	7.086	20.012
91	H	9.083	0.388	20.011
92	H	5.538	7.104	19.947
93	H	0.406	4.720	20.645

94	H	-3.124	11.426	20.642
95	H	7.882	4.733	20.649
96	H	4.346	11.442	20.653
97	H	3.662	4.537	20.286
98	H	0.140	11.220	20.294
99	H	11.153	4.501	20.311
100	H	7.599	11.226	20.303
101	H	1.426	2.726	19.989
102	H	-2.103	9.440	19.986
103	H	8.928	2.749	19.976
104	H	5.378	9.464	19.984
105	H	3.349	1.993	20.108
106	H	-0.183	8.697	20.112
107	H	10.849	2.006	20.106
108	H	7.307	8.715	20.106
109	H	-3.160	6.702	19.008
110	H	-6.693	13.408	19.011
111	H	4.280	6.809	18.950
112	H	0.810	13.417	18.983
113	H	-1.485	4.353	19.945
114	H	-5.024	11.077	19.963
115	H	5.989	4.358	19.929
116	H	2.472	11.037	19.899
117	H	-1.883	5.653	11.323
118	H	-5.400	12.253	11.341
119	H	5.595	5.507	11.294
120	H	1.679	12.143	11.709

121	H	6.768	1.323	11.794
122	H	10.580	8.088	11.740
123	H	14.192	1.325	11.800
124	H	1.971	9.759	12.949
125	O	0.418	3.324	1.907
126	O	-3.113	10.036	1.915
127	O	7.899	3.303	1.890
128	O	4.359	10.023	1.899
129	O	3.960	5.654	4.748
130	O	0.424	12.366	4.778
131	O	11.430	5.694	4.779
132	O	7.893	12.380	4.777
133	O	3.603	1.165	7.519
134	O	0.082	7.887	7.535
135	O	11.075	1.188	7.489
136	O	7.499	7.971	7.554
137	O	-0.300	3.452	10.294
138	O	-3.867	10.187	10.309
139	O	7.201	3.467	10.291
140	O	3.742	10.195	10.571
141	O	4.028	4.687	0.207
142	O	0.508	11.382	0.211
143	O	11.523	4.682	0.225
144	O	7.974	11.398	0.216
145	O	3.799	0.104	3.087
146	O	0.268	6.837	3.108
147	O	11.278	0.114	3.101

148	O	7.743	6.828	3.098
149	O	-0.104	2.380	5.929
150	O	-3.638	9.090	5.948
151	O	7.377	2.365	5.914
152	O	3.833	9.072	5.924
153	O	3.486	4.648	8.728
154	O	-0.016	11.396	8.804
155	O	10.950	4.737	8.772
156	O	7.415	11.386	8.785
157	O	-2.090	5.027	2.381
158	O	-5.630	11.727	2.373
159	O	5.389	5.019	2.346
160	O	1.850	11.728	2.357
161	O	5.113	0.615	5.205
162	O	1.580	7.346	5.228
163	O	12.590	0.629	5.217
164	O	9.020	7.339	5.240
165	O	1.198	2.869	7.984
166	O	-2.324	9.586	8.043
167	O	8.680	2.888	7.972
168	O	5.070	9.565	8.017
169	O	-2.637	5.218	10.847
170	O	-6.200	11.862	10.856
171	O	4.818	5.172	10.826
172	O	1.240	11.829	10.904
173	O	6.247	1.196	0.844
174	O	2.709	7.914	0.852

175	O	13.719	1.208	0.868
176	O	10.187	7.919	0.864
177	O	2.389	3.463	3.541
178	O	-1.142	10.177	3.552
179	O	9.858	3.471	3.547
180	O	6.320	10.178	3.548
181	O	-1.507	5.737	6.330
182	O	-5.044	12.428	6.332
183	O	5.963	5.731	6.302
184	O	2.424	12.430	6.330
185	O	5.639	1.283	9.108
186	O	2.122	7.985	9.201
187	O	13.102	1.266	9.123
188	O	9.493	7.991	9.146
189	O	2.343	0.175	0.594
190	O	-1.188	6.889	0.603
191	O	9.818	0.201	0.597
192	O	6.283	6.914	0.597
193	O	5.964	2.480	3.384
194	O	2.426	9.198	3.394
195	O	13.438	2.484	3.397
196	O	9.904	9.182	3.402
197	O	2.046	4.702	6.162
198	O	-1.483	11.417	6.191
199	O	9.520	4.716	6.169
200	O	5.972	11.399	6.182
201	O	1.671	0.285	8.991

202	O	-1.828	6.992	8.977
203	O	9.184	0.293	8.984
204	O	5.624	6.920	8.918
205	O	2.498	5.722	2.192
206	O	-1.025	12.423	2.192
207	O	9.988	5.720	2.200
208	O	6.452	12.427	2.202
209	O	2.156	1.290	4.982
210	O	-1.381	8.023	4.999
211	O	9.630	1.291	4.973
212	O	6.091	8.005	4.976
213	O	-1.766	3.594	7.831
214	O	-5.323	10.292	7.852
215	O	5.720	3.574	7.806
216	O	2.200	10.283	7.898
217	O	2.009	5.772	10.648
218	O	-1.614	12.579	10.596
219	O	9.363	5.815	10.633
220	O	5.868	12.505	10.665
221	O	1.161	5.225	0.103
222	O	-2.368	11.929	0.098
223	O	8.634	5.236	0.116
224	O	5.099	11.943	0.116
225	O	0.842	0.774	2.930
226	O	-2.686	7.494	2.931
227	O	8.307	0.763	2.925
228	O	4.773	7.480	2.921

229	O	4.432	3.043	5.695
230	O	0.920	9.779	5.736
231	O	11.911	3.082	5.708
232	O	8.381	9.784	5.704
233	O	0.603	5.331	8.547
234	O	-2.969	12.003	8.538
235	O	8.048	5.343	8.511
236	O	4.507	12.049	8.493
237	O	3.947	2.422	1.748
238	O	0.411	9.137	1.761
239	O	11.417	2.432	1.765
240	O	7.884	9.144	1.763
241	O	0.048	4.653	4.565
242	O	-3.479	11.354	4.572
243	O	7.525	4.642	4.551
244	O	3.981	11.353	4.564
245	O	7.186	0.200	7.386
246	O	3.613	6.891	7.378
247	O	14.649	0.195	7.389
248	O	11.103	6.949	7.402
249	O	3.243	2.436	9.940
250	O	-0.205	9.149	9.976
251	O	10.723	2.482	9.864
252	O	7.039	9.173	10.131
253	O	1.759	3.289	11.970
254	O	-1.671	10.351	11.837
255	O	9.303	3.306	11.946

256	O	5.648	10.247	11.997
257	O	5.262	2.340	11.704
258	O	1.663	9.143	11.677
259	O	12.648	2.396	11.720
260	O	9.147	9.077	11.764
261	O	3.028	0.062	11.486
262	O	-0.428	6.637	11.451
263	O	10.759	0.223	11.501
264	O	7.015	6.754	11.415
265	O	4.190	1.329	20.038
266	O	0.657	8.032	20.047
267	O	11.686	1.340	20.048
268	O	8.146	8.054	20.044
269	O	2.274	2.861	20.450
270	O	-1.256	9.570	20.450
271	O	9.776	2.893	20.434
272	O	6.229	9.596	20.438
273	O	-0.939	3.701	20.414
274	O	-4.478	10.414	20.415
275	O	6.539	3.713	20.403
276	O	3.017	10.417	20.408
277	O	0.618	0.498	19.801
278	O	-2.915	7.202	19.803
279	O	8.104	0.488	19.790
280	O	4.552	7.204	19.793
281	O	4.292	7.697	11.223
282	O	7.652	1.105	11.337

283	O	-3.518	7.782	11.332
284	O	0.087	1.096	11.330
285	Cl	3.630	7.599	14.173
286	Cl	3.536	11.287	13.888
287	Cl	0.211	8.372	14.192
288	Cl	0.134	12.026	13.890
289	Cl	6.204	6.508	13.904
290	Cl	6.157	10.223	13.689

SI Fig. 6b

Simulation box:

a=14.949	b=15.168	c=20.974	α=90.00	β90.00	γ=117.78

290 atoms

Atomic id	element	x	y	z
1	Hf	2.309	3.814	1.362
2	Hf	-1.219	10.525	1.349
3	Hf	9.792	3.809	1.363
4	Hf	6.255	10.527	1.348
5	Hf	-1.598	6.029	4.106
6	Hf	-5.151	12.746	4.078
7	Hf	5.873	6.029	4.078
8	Hf	2.332	12.727	4.069
9	Hf	5.506	1.630	6.934
10	Hf	1.959	8.327	6.913
11	Hf	12.986	1.605	6.965
12	Hf	9.440	8.317	6.907
13	Hf	1.673	3.829	9.778

14	Hf	-1.949	10.678	9.685
15	Hf	9.155	3.810	9.653
16	Hf	5.513	10.531	9.773
17	Hf	-1.581	3.246	1.379
18	Hf	-5.107	9.940	1.353
19	Hf	5.900	3.240	1.362
20	Hf	2.370	9.939	1.355
21	Hf	1.937	5.589	4.223
22	Hf	-1.617	12.326	4.188
23	Hf	9.428	5.582	4.224
24	Hf	5.858	12.308	4.197
25	Hf	1.592	1.133	7.027
26	Hf	-1.962	7.882	7.013
27	Hf	9.050	1.090	7.000
28	Hf	5.498	7.870	6.981
29	Hf	5.092	3.363	9.890
30	Hf	1.593	10.096	9.728
31	Hf	12.550	3.332	9.912
32	Hf	8.966	10.093	9.723
33	Hf	-6.645	13.298	1.153
34	Hf	-3.116	6.585	1.164
35	Hf	0.832	13.304	1.139
36	Hf	4.358	6.591	1.149
37	Hf	4.012	2.056	3.941
38	Hf	0.478	8.766	3.928
39	Hf	11.499	2.040	3.968
40	Hf	7.955	8.765	3.925

41	Hf	0.109	4.303	6.812
42	Hf	-3.457	11.039	6.727
43	Hf	7.568	4.307	6.751
44	Hf	4.041	11.037	6.777
45	Hf	3.710	6.594	9.521
46	Hf	0.057	13.319	9.562
47	Hf	11.184	6.620	9.583
48	Hf	7.662	13.298	9.569
49	Hf	4.325	0.294	1.029
50	Hf	0.779	6.996	1.038
51	Hf	11.806	0.299	1.035
52	Hf	8.235	7.006	1.026
53	Hf	0.483	2.515	3.915
54	Hf	-3.047	9.218	3.885
55	Hf	7.960	2.499	3.891
56	Hf	4.432	9.219	3.886
57	Hf	4.064	4.775	6.685
58	Hf	0.490	11.505	6.639
59	Hf	11.551	4.777	6.700
60	Hf	7.968	11.502	6.651
61	Hf	3.717	0.342	9.578
62	Hf	0.129	7.052	9.570
63	Hf	11.106	0.349	9.516
64	Hf	7.605	7.030	9.483
65	Hf	3.654	9.349	12.355
66	Hf	-0.097	10.161	12.443
67	Hf	7.200	8.677	12.322

68	H	-0.167	2.504	10.812
69	H	-3.861	9.519	10.938
70	H	7.304	2.539	10.785
71	H	4.206	6.813	12.090
72	H	10.238	3.027	12.143
73	H	1.863	5.700	11.559
74	H	9.192	5.791	11.568
75	H	5.867	12.497	11.634
76	H	4.427	2.141	12.148
77	H	11.911	1.658	11.929
78	H	9.902	8.462	11.812
79	H	1.522	2.846	12.302
80	H	-2.456	9.260	11.952
81	H	8.758	2.491	12.069
82	H	2.171	0.599	11.678
83	H	-0.459	6.963	12.301
84	H	9.605	0.517	11.631
85	H	4.983	1.831	19.780
86	H	1.454	8.513	19.782
87	H	12.501	1.842	19.812
88	H	8.924	8.517	19.766
89	H	1.596	0.363	19.977
90	H	-1.942	7.073	19.974
91	H	9.083	0.380	19.988
92	H	5.523	7.093	19.897
93	H	0.408	4.704	20.640
94	H	-3.133	11.422	20.629

95	H	7.884	4.707	20.645
96	H	4.342	11.429	20.630
97	H	3.682	4.536	20.285
98	H	0.119	11.219	20.277
99	H	11.173	4.481	20.310
100	H	7.612	11.216	20.282
101	H	1.422	2.717	19.986
102	H	-2.096	9.441	19.967
103	H	8.942	2.742	19.961
104	H	5.381	9.459	19.954
105	H	3.330	2.000	20.109
106	H	-0.195	8.700	20.101
107	H	10.846	2.010	20.101
108	H	7.274	8.714	20.091
109	H	-3.185	6.733	18.976
110	H	-6.703	13.408	18.979
111	H	4.265	6.831	18.900
112	H	7.856	0.010	18.975
113	H	-1.471	4.357	19.945
114	H	-5.011	11.031	19.898
115	H	6.005	4.364	19.923
116	H	2.444	11.059	19.934
117	H	-1.844	5.629	11.237
118	H	-5.427	12.241	11.261
119	H	5.704	5.666	11.219
120	H	1.729	12.189	11.493
121	H	6.853	1.131	11.839

122	H	-3.259	7.205	12.147
123	H	14.140	1.254	11.771
124	H	2.765	11.080	14.845
125	O	0.411	3.327	1.913
126	O	-3.115	10.011	1.881
127	O	7.893	3.311	1.892
128	O	4.358	10.013	1.884
129	O	3.945	5.674	4.766
130	O	0.400	12.384	4.720
131	O	11.432	5.669	4.775
132	O	7.864	12.378	4.731
133	O	3.599	1.153	7.510
134	O	0.060	7.965	7.603
135	O	11.039	1.125	7.490
136	O	7.496	7.970	7.527
137	O	-0.328	3.362	10.285
138	O	-3.933	10.117	10.164
139	O	7.204	3.427	10.296
140	O	3.548	10.222	10.444
141	O	4.032	4.672	0.213
142	O	0.497	11.389	0.190
143	O	11.534	4.660	0.228
144	O	7.977	11.383	0.200
145	O	3.792	0.106	3.070
146	O	0.258	6.815	3.086
147	O	11.273	0.094	3.078
148	O	7.729	6.810	3.068

149	O	-0.123	2.366	5.933
150	O	-3.657	9.069	5.907
151	O	7.354	2.358	5.902
152	O	3.850	9.071	5.919
153	O	3.488	4.696	8.772
154	O	0.016	11.321	8.708
155	O	10.930	4.716	8.752
156	O	7.374	11.328	8.734
157	O	-2.091	5.009	2.380
158	O	-5.639	11.713	2.350
159	O	5.374	5.007	2.358
160	O	1.840	11.713	2.337
161	O	5.083	0.626	5.185
162	O	1.540	7.324	5.208
163	O	12.561	0.602	5.210
164	O	9.011	7.313	5.198
165	O	1.194	2.875	8.005
166	O	-2.286	9.639	7.948
167	O	8.664	2.849	7.959
168	O	5.065	9.563	8.058
169	O	-2.662	5.184	10.817
170	O	-6.213	11.818	10.796
171	O	4.908	5.235	10.798
172	O	0.983	11.741	11.024
173	O	6.246	1.202	0.833
174	O	2.706	7.902	0.836
175	O	13.725	1.204	0.852

176	O	10.175	7.896	0.846
177	O	2.377	3.471	3.546
178	O	-1.156	10.172	3.523
179	O	9.851	3.454	3.547
180	O	6.316	10.174	3.521
181	O	-1.507	5.730	6.349
182	O	-5.071	12.425	6.275
183	O	5.950	5.746	6.317
184	O	2.406	12.408	6.290
185	O	5.631	1.326	9.093
186	O	2.054	8.049	9.217
187	O	13.053	1.217	9.108
188	O	9.504	7.968	9.116
189	O	2.344	0.174	0.584
190	O	-1.194	6.879	0.592
191	O	9.825	0.185	0.573
192	O	6.268	6.898	0.580
193	O	5.955	2.465	3.376
194	O	2.422	9.169	3.380
195	O	13.430	2.460	3.395
196	O	9.900	9.160	3.369
197	O	2.032	4.723	6.187
198	O	-1.520	11.447	6.129
199	O	9.515	4.710	6.168
200	O	5.962	11.390	6.149
201	O	1.665	0.261	8.959
202	O	-1.871	7.086	9.016

203	O	9.114	0.161	8.956
204	O	5.595	7.018	8.945
205	O	2.498	5.715	2.189
206	O	-1.034	12.429	2.164
207	O	10.003	5.698	2.197
208	O	6.438	12.426	2.171
209	O	2.140	1.297	4.974
210	O	-1.382	8.009	4.986
211	O	9.610	1.270	4.969
212	O	6.087	8.008	4.959
213	O	-1.802	3.559	7.833
214	O	-5.338	10.279	7.756
215	O	5.694	3.593	7.793
216	O	2.211	10.271	7.769
217	O	1.933	5.845	10.593
218	O	-1.650	12.538	10.433
219	O	9.369	5.760	10.609
220	O	5.825	12.475	10.660
221	O	1.162	5.215	0.094
222	O	-2.376	11.927	0.087
223	O	8.638	5.217	0.105
224	O	5.098	11.931	0.090
225	O	0.841	0.773	2.907
226	O	-2.684	7.469	2.920
227	O	8.323	0.763	2.894
228	O	4.775	7.468	2.910
229	O	4.411	3.061	5.682

230	O	0.886	9.758	5.679
231	O	11.889	3.045	5.705
232	O	8.364	9.766	5.654
233	O	0.515	5.333	8.574
234	O	-3.118	12.004	8.479
235	O	8.023	5.293	8.502
236	O	4.496	11.993	8.549
237	O	3.935	2.424	1.748
238	O	0.405	9.129	1.739
239	O	11.413	2.416	1.761
240	O	7.875	9.133	1.736
241	O	0.043	4.636	4.573
242	O	-3.503	11.344	4.517
243	O	7.514	4.637	4.553
244	O	3.972	11.337	4.540
245	O	7.118	0.177	7.356
246	O	3.578	6.925	7.392
247	O	14.628	0.175	7.361
248	O	11.108	6.934	7.394
249	O	3.259	2.418	9.868
250	O	-0.232	9.316	10.316
251	O	10.688	2.429	9.870
252	O	7.146	9.173	10.110
253	O	1.898	3.595	11.809
254	O	-2.048	10.157	11.855
255	O	9.312	3.310	11.972
256	O	5.575	9.875	11.948

257	O	5.245	2.376	11.675
258	O	1.696	9.436	12.009
259	O	12.588	2.339	11.742
260	O	9.099	9.058	11.698
261	O	2.918	0.019	11.423
262	O	-0.560	6.561	11.415
263	O	10.451	0.055	11.445
264	O	7.026	6.908	11.410
265	O	4.178	1.335	20.035
266	O	0.645	8.026	20.036
267	O	11.689	1.342	20.035
268	O	8.114	8.037	20.029
269	O	2.268	2.855	20.448
270	O	-1.248	9.574	20.429
271	O	9.786	2.884	20.426
272	O	6.226	9.583	20.423
273	O	-0.933	3.698	20.413
274	O	-4.463	10.406	20.399
275	O	6.546	3.718	20.407
276	O	3.003	10.414	20.398
277	O	0.617	0.475	19.783
278	O	-2.923	7.180	19.799
279	O	8.105	0.497	19.780
280	O	4.539	7.173	19.769
281	O	3.921	7.533	11.491
282	O	7.655	1.059	11.263
283	O	-3.615	7.737	11.413

284	O	0.020	1.005	11.283
285	Cl	3.423	8.350	14.543
286	Cl	3.577	11.672	14.024
287	Cl	-0.581	8.418	14.025
288	Cl	0.026	11.907	14.065
289	Cl	6.819	7.205	14.272
290	Cl	7.710	10.177	14.294