

0 Structures, Relative Stabilities and Binding Energies of Neutral Water Clusters, (H₂O)₂-30
1
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9 Cartesian coordinates of neutral water clusters.

12 Cartesian coordinates of the water dimer

14 Cartesian coordinates of : L2

16	H	-0.544272	-0.000062	0.047845
17	O	-1.498434	0.000031	-0.121161
18	H	-1.924602	-0.000332	0.740065
19	O	1.368843	-0.000053	0.104166
20	H	1.753272	-0.770836	-0.326307
21	H	1.752330	0.771408	-0.325646

24 Cartesian coordinates of the water trimer

26 Cartesian coordinates of : CY3

28	H	-0.287455	-1.226281	-0.050901
29	O	-1.235827	-1.002689	-0.077795
30	H	-1.687940	-1.588389	0.535688
31	O	1.494614	-0.561686	-0.087505
32	H	1.189512	0.362574	-0.029973
33	H	2.223390	-0.661644	0.531274
34	O	-0.259308	1.568191	0.102850
35	H	-0.911964	0.845649	0.048968
36	H	-0.521377	2.237556	-0.535453

39 Cartesian coordinates of the water tetramer

42 Cartesian coordinates of : CY4_1

44	H	-0.838159	-2.329628	0.852888
45	O	-0.739369	-1.765150	0.080913
46	H	-1.542934	-0.215994	-0.009441
47	H	0.215264	-1.541234	0.008030
48	O	-1.765979	0.739004	-0.080794
49	H	-2.332639	0.839241	-0.850791
50	H	-0.214897	1.542573	0.007142
51	O	0.739862	1.765784	0.080665
52	H	0.839023	2.327890	0.854186
53	H	1.543376	0.215933	-0.010043
54	O	1.765657	-0.739302	-0.080756
55	H	2.329590	-0.841473	-0.852198

57 Cartesian coordinates of : CY4_2

59	H	0.405149	2.556911	-0.572700
60	O	0.396544	1.868866	0.098691
61	H	1.484816	0.501107	-0.036982
62	H	-0.506387	1.483541	0.103491
63	O	1.898047	-0.387760	-0.102080
64	H	2.613763	-0.414198	0.539268
65	H	0.504582	-1.484976	-0.099534
66	O	-0.397363	-1.871854	-0.079482
67	H	-0.405271	-2.526138	0.624555
68	H	-1.482892	-0.500735	0.029836
69	O	-1.899822	0.387396	0.082276
70	H	-2.593006	0.411299	-0.583171

72 Cartesian coordinates of : P4
73
74 H -1.179886 -0.898340 -0.085493
75 O -1.628067 -0.257858 0.496149
76 H 0.297006 -0.006483 1.699672
77 H -2.532667 -0.558027 0.623316
78 O 1.170418 0.101057 1.297228
79 H 1.073215 0.904083 0.754621
80 H 0.985483 -1.002501 -0.126047
81 O 0.491914 -1.297563 -0.923003
82 H 0.914515 -2.090853 -1.264475
83 H 0.305363 0.907522 -1.438154
84 O 0.080143 1.627151 -0.832265
85 H -0.778300 1.362309 -0.468305

86
87
88 Cartesian coordinates of the water pentamer
89

90 Cartesian coordinates of : CY5
91
92 H -0.419153 -1.877743 -0.070940
93 H 2.760042 -0.392233 1.017445
94 O 0.502300 -2.220429 -0.142168
95 O -1.976599 -1.174063 0.010860
96 H -1.954492 -0.189983 0.011213
97 H -2.569128 -1.442540 0.718331
98 O -1.707661 1.525867 0.007760
99 H -2.106865 2.136237 0.633756
100 H -0.754505 1.768987 -0.059607
101 O 0.924032 2.084684 -0.138335
102 H 1.460741 1.271578 0.013700
103 H 1.263590 2.492324 -0.940472
104 O 2.271990 -0.221928 0.206790
105 H 1.663695 -0.986760 0.072261
106 H 0.543579 -2.732914 -0.954939

107
108
109 Cartesian coordinates of the water hexamer
110

111 Cartesian coordinates of : Prism
112
113 H -0.008612 -0.688794 1.738084
114 O 0.869814 -0.308378 1.899670
115 H 1.460453 -0.714180 1.245674
116 H -0.639320 1.585287 -0.394370
117 O -1.538103 1.248020 -0.689795
118 H -2.064517 2.006738 -0.957852
119 H 0.855950 1.309476 0.991971
120 O 0.847644 1.825352 0.158655
121 H 1.484921 1.336578 -0.387661
122 H -2.532079 -1.205578 1.442529
123 O -1.760550 -0.950397 0.928560
124 H -1.944978 -0.083888 0.512023
125 H -0.844826 -1.599945 -0.793796
126 O -0.385224 -1.194789 -1.544733
127 H -0.833734 -0.337689 -1.640882
128 H 1.257252 -0.898923 -1.115408
129 O 2.089047 -0.584294 -0.688915
130 H 2.828470 -0.993202 -1.147856

131
132 Cartesian coordinates of : Cage
133

134 H 0.012888 1.306374 -0.681344
135 O 0.555138 1.765134 0.026494
136 H 0.441222 2.714170 -0.080285
137 H 2.111003 0.892091 0.104111
138 H -1.670053 0.118025 -1.225438
139 O 2.735792 0.138275 0.153918
140 H 1.708880 -1.198914 -0.276736
141 H 3.124983 0.156553 1.033594
142 O 0.891481 -1.727664 -0.426295
143 H 1.154411 -2.618614 -0.675040
144 H -0.306296 -0.588822 -1.460170
145 H -0.113520 -1.004689 1.101415
146 O -0.784255 0.243298 -1.616470

147	O	-0.582714	-0.339955	1.632208
148	H	-2.207879	-0.206545	0.874841
149	H	-0.179903	0.508074	1.382962
150	O	-2.864123	-0.030115	0.168055
151	H	-3.686286	-0.469485	0.398818
152				
153	Cartesian coordinates of : Book			
154				
155	O	0.150582	1.525049	0.875919
156	H	1.004130	1.486264	0.366834
157	H	0.297982	2.086304	1.643359
158	O	-0.038727	-1.352947	0.845896
159	H	-0.082960	-0.412468	1.083390
160	H	-0.891603	-1.552138	0.413062
161	O	-2.266779	1.376806	-0.459407
162	H	-1.413254	1.546020	-0.013086
163	H	-2.250465	1.861014	-1.289920
164	O	-2.531641	-1.358867	-0.377372
165	H	-2.586784	-0.387058	-0.477653
166	H	-3.336215	-1.642989	0.065359
167	O	2.405819	1.162849	-0.447075
168	H	2.488429	0.174813	-0.482720
169	H	2.545287	1.490111	-1.340434
170	O	2.273755	-1.479982	-0.437682
171	H	1.392306	-1.574528	0.008158
172	H	2.889074	-2.058613	0.021416
173				
174	Cartesian coordinates of : Cyclic			
175				
176	H	-2.161842	0.890001	0.025346
177	O	-2.678338	0.062599	0.170413
178	H	-3.193878	0.197131	0.970757
179	H	-1.855727	-1.413313	-0.025462
180	O	-1.277740	2.330493	-0.170146
181	H	-1.423417	2.862775	-0.957488
182	H	-0.302207	2.297062	-0.029184
183	O	1.387058	2.270465	0.165032
184	H	1.855344	1.413670	0.024991
185	H	1.758265	2.658987	0.962640
186	O	2.679109	-0.062806	-0.162124
187	H	3.202984	-0.198070	-0.957007
188	H	2.161591	-0.890347	-0.021290
189	O	1.276958	-2.331550	0.166992
190	H	0.301697	-2.297205	0.024410
191	H	1.420785	-2.865972	0.953243
192	O	-1.387583	-2.269340	-0.170329
193	H	-1.759307	-2.653607	-0.969654
194				
195				
196	Cartesian coordinates of the water heptamer			
197				
198	Cartesian coordinates of : W 7_1			
199				
200	O	1.107206	-1.164052	1.491072
201	H	0.284374	-0.600226	1.647315
202	H	1.280019	-1.662599	2.295015
203	O	2.375150	0.714382	-0.159439
204	H	2.215486	0.147711	0.616732
205	H	2.308023	0.096497	-0.902836
206	O	0.172798	2.210155	-0.183600
207	H	1.073157	1.797286	-0.190276
208	H	0.280451	3.163326	-0.253393
209	O	-0.923597	0.407201	1.713223
210	H	-0.685886	1.199728	1.200764
211	H	-1.724818	0.037449	1.286180
212	O	-1.040588	0.155278	-1.748664
213	H	-0.299379	-0.472330	-1.686659
214	H	-0.704930	0.995745	-1.394131
215	O	-2.837535	-0.661540	0.080931
216	H	-3.757149	-0.440128	-0.088139
217	H	-2.313666	-0.407726	-0.713772
218	O	1.126559	-1.615406	-1.192935
219	H	1.151744	-2.487081	-1.598756
220	H	1.052631	-1.735810	-0.222749
221				

222 Cartesian coordinates of : W 7_ 2

223
224 O -1.274524 0.237979 -1.614222
225 H -2.043529 0.128330 -1.019917
226 H -0.744218 -0.571095 -1.516672
227 O 1.352522 1.132537 1.293383
228 H 1.560940 1.725715 2.021286
229 H 0.913734 1.666469 0.569969
230 O 2.762340 -0.686063 -0.175195
231 H 2.419157 -0.006429 0.442387
232 H 3.343494 -0.232828 -0.793042
233 O -2.959893 -0.078480 0.532678
234 H -3.749098 -0.557154 0.798521
235 H -2.210125 -0.399809 1.081011
236 O 0.117206 2.244198 -0.696290
237 H -0.442752 1.517426 -1.098761
238 H 0.468596 2.779046 -1.412695
239 O 0.472113 -1.905103 -0.881578
240 H 1.378374 -1.546180 -0.736400
241 H 0.562404 -2.811160 -1.191320
242 O -0.618500 -0.945561 1.583772
243 H -0.280881 -1.475959 0.842920
244 H 0.013786 -0.212421 1.672337

245

246 Cartesian coordinates of : W 7_ 3

247
248 O -2.929753 1.317109 -0.569458
249 H -2.933529 0.352379 -0.735162
250 H -3.798374 1.548460 -0.229122
251 O 3.019794 0.132593 -0.847769
252 H 2.575523 0.949573 -0.498525
253 H 3.137030 0.266372 -1.792905
254 O 1.830770 -2.067487 0.003412
255 H 2.288342 -1.255330 -0.341620
256 H 2.508559 -2.618933 0.404334
257 O -0.498803 -1.479555 1.094116
258 H -0.629473 -1.937598 1.930029
259 H 0.391937 -1.746492 0.740663
260 O -2.561982 -1.395771 -0.754971
261 H -2.303649 -1.809942 -1.583617
262 H -1.828271 -1.542290 -0.125327
263 O -0.610985 1.383310 0.961357
264 H -0.576343 0.425001 1.120534
265 H -1.421712 1.533600 0.436872
266 O 1.712462 2.240685 0.058839
267 H 2.087926 2.817137 0.730307
268 H 0.810014 1.971001 0.379339

269

270 Cartesian coordinates of : W 7_ 4

271
272 O 2.108069 0.815053 1.679460
273 H 1.262241 0.535883 1.263653
274 H 2.106819 0.474765 2.578784
275 O -3.865618 0.087223 -0.236844
276 H -4.332910 -0.159589 -1.040259
277 H -3.250333 0.814451 -0.474094
278 O 0.001151 -0.070066 0.186313
279 H -0.664923 -0.711225 0.520174
280 H 0.523548 -0.513422 -0.517991
281 O -1.799223 1.807561 -0.676352
282 H -1.047747 1.233637 -0.410490
283 H -1.514680 2.313292 -1.442494
284 O -2.113962 -1.606460 0.956143
285 H -2.361509 -1.768013 1.871426
286 H -2.846737 -1.091285 0.550285
287 O 1.788125 -1.017005 -1.643873
288 H 2.624408 -0.679724 -1.253710
289 H 1.935823 -1.939850 -1.869722
290 O 3.860140 0.029957 -0.235731
291 H 3.350859 0.349980 0.542119
292 H 4.385691 0.770997 -0.550602

293

294 Cartesian coordinates of : W 7_ 5

295
296 O 2.956177 -0.919040 0.467302

297	H	2.255700	-1.560062	0.191717
298	H	3.238827	-1.184442	1.347196
299	O	-1.927723	1.163213	-0.784547
300	H	-2.268547	1.589540	-1.576735
301	H	-1.183907	1.733906	-0.455476
302	O	-3.224260	-0.418406	1.113076
303	H	-2.994708	0.333724	0.539367
304	H	-4.162362	-0.359042	1.311811
305	O	0.062434	2.690532	0.045703
306	H	0.971335	2.301753	0.008511
307	H	-0.010816	3.129971	0.897996
308	O	-1.383160	-1.631688	-0.611861
309	H	-1.400738	-0.700498	-0.891243
310	H	-2.036014	-1.654415	0.106572
311	O	2.525206	1.676925	0.023185
312	H	2.667880	0.714286	0.198391
313	H	3.150804	1.930457	-0.661269
314	O	1.047043	-2.651986	-0.219943
315	H	0.135309	-2.285082	-0.335233
316	H	1.191504	-3.266495	-0.944928

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318

319 Cartesian coordinates of the water octamer

320

321 Cartesian coordinates of : W 8_1

322

323	O	1.852228	0.234856	1.291998
324	O	-0.261865	2.069991	1.320087
325	O	-1.852039	-0.234172	1.292484
326	O	0.262046	-2.069213	1.321135
327	O	2.069706	0.261646	-1.320754
328	O	-0.234750	1.851538	-1.292680
329	O	-2.069809	-0.262314	-1.320418
330	O	0.234445	-1.852357	-1.291913
331	H	1.220555	0.941619	1.517566
332	H	1.416529	-0.607065	1.517920
333	H	-1.220175	-0.940781	1.518005
334	H	-1.416238	0.607890	1.517689
335	H	0.607297	1.415772	-1.517993
336	H	-0.941386	1.219638	-1.518019
337	H	-0.607550	-1.416595	-1.517426
338	H	0.941142	-1.220570	-1.517392
339	H	-0.374738	2.960828	1.664545
340	H	0.374962	-2.959920	1.665921
341	H	2.960451	0.374449	-1.665453
342	H	-2.960609	-0.375290	-1.664935
343	H	-0.268044	2.117459	0.322156
344	H	0.268071	-2.117083	0.323224
345	H	-2.117397	-0.268147	-0.322495
346	H	2.117442	0.268001	-0.322825

347

348 Cartesian coordinates of : W 8_2

349

350	O	1.299951	-1.822449	-0.239397
351	O	1.482866	-0.114817	1.982252
352	O	1.305859	1.818066	0.242482
353	O	1.487333	0.109947	-1.979831
354	O	-1.488417	-1.979495	-0.113827
355	O	-1.305346	-0.238559	1.818904
356	O	-1.481681	1.983983	0.110720
357	O	-1.300425	0.243210	-1.821432
358	H	1.476922	-1.430836	0.635477
359	H	-1.480632	0.636504	1.426998
360	H	1.483393	1.425854	-0.631999
361	H	-1.479713	-0.631265	-1.430039
362	H	0.369870	-2.114530	-0.222850
363	H	-0.376000	-0.222712	2.113382
364	H	0.376797	2.113242	0.223942
365	H	-0.370593	0.224023	-2.114168
366	H	2.120515	-0.018304	-2.692317
367	H	-2.122714	-2.691287	0.012872
368	H	2.113792	0.011259	2.697113
369	H	-2.112872	2.698322	-0.016894
370	H	1.515779	-0.690065	-1.378866
371	H	-1.518682	-1.378161	0.685815

372	H	1.515451	0.685623	1.381962
373	H	-1.512427	1.383238	-0.689398
374				
375	Cartesian coordinates of : W 8_ 3			
376				
377	O	-0.642597	-2.300541	0.674363
378	O	0.642597	2.300541	-0.674363
379	O	1.019881	-0.751536	1.864351
380	O	-1.019881	0.751536	-1.864351
381	O	0.374431	-1.712621	-1.778017
382	O	-0.374431	1.712621	1.778017
383	O	2.272971	-0.018075	-0.440777
384	O	-2.272971	0.018075	0.440777
385	H	0.018349	-1.767374	1.225404
386	H	-0.018349	1.767374	-1.225404
387	H	-0.781548	-3.148142	1.107720
388	H	0.781548	3.148142	-1.107720
389	H	1.635693	-0.511720	1.134228
390	H	-1.635693	0.511720	-1.134228
391	H	0.577493	0.083504	2.094490
392	H	-0.577493	-0.083504	-2.094490
393	H	-0.021108	-2.091349	-0.960169
394	H	0.021108	2.091349	0.960169
395	H	0.486073	-2.430351	-2.408651
396	H	-0.486073	2.430351	2.408651
397	H	1.811120	-0.591674	-1.073980
398	H	-1.811120	0.591674	1.073980
399	H	1.935894	0.880278	-0.597440
400	H	-1.935894	-0.880278	0.597440
401				
402	Cartesian coordinates of : W 8_ 4			
403				
404	O	-0.236424	-1.407148	-1.863753
405	O	0.236080	-1.405553	1.864730
406	O	2.121829	-1.318919	-0.282766
407	O	-2.122155	-1.318259	0.283725
408	O	-0.276177	1.319174	-1.782231
409	O	0.276517	1.320683	1.781298
410	O	2.010279	1.395025	-0.112260
411	O	-2.009967	1.395512	0.111211
412	H	-0.940044	-1.609824	-1.225925
413	H	0.939664	-1.608777	1.227034
414	H	0.604083	-1.600147	-1.416435
415	H	-0.604447	-1.598602	1.417461
416	H	2.258972	-0.344562	-0.263644
417	H	-2.259091	-0.343885	0.263845
418	H	2.980150	-1.735228	-0.406742
419	H	-2.980443	-1.734246	0.408976
420	H	1.377688	1.453614	0.676237
421	H	-1.377271	1.453221	-0.677274
422	H	2.723336	2.025547	0.027696
423	H	-2.722918	2.025980	-0.029523
424	H	0.250068	0.360509	1.996298
425	H	-0.249990	0.358847	-1.996568
426	H	-0.601065	1.527460	1.416160
427	H	0.601454	1.525977	-1.417223
428				
429	Cartesian coordinates of : W 8_ 5			
430				
431	O	-0.715395	-0.011736	2.153740
432	O	2.606833	0.007388	-0.162832
433	O	0.785179	0.011271	-2.083356
434	O	-2.352439	-0.006822	0.259624
435	O	0.924984	-1.920320	1.086685
436	O	0.913055	1.915402	1.101786
437	O	-0.988646	-1.940446	-1.078683
438	O	-1.000324	1.944850	-1.063436
439	H	-0.133618	-0.784106	1.973302
440	H	-0.138097	0.765483	1.980009
441	H	0.212127	-0.762758	-1.944782
442	H	0.208083	0.781095	-1.938283
443	H	2.042743	0.009227	-0.979079
444	H	3.529211	0.011015	-0.435265
445	H	-1.738077	-0.009160	1.098122
446	H	-3.266519	-0.010901	0.561179

447	H	1.679287	-1.399276	0.761738
448	H	1.670226	1.401473	0.772212
449	H	0.402391	-2.149487	0.302023
450	H	0.389142	2.148839	0.319284
451	H	-1.643619	-1.350150	-0.642322
452	H	-1.651942	1.347565	-0.631584
453	H	-1.465744	-2.682102	-1.462688
454	H	-1.481576	2.686546	-1.442094

455

456 Cartesian coordinates of : W 8_ 6

457

458	O	1.014877	2.073752	-0.847699
459	H	1.480394	2.862630	-1.141683
460	H	1.681655	1.427658	-0.533276
461	O	-2.581184	0.006191	-0.234221
462	H	-3.500805	0.014926	-0.515257
463	H	-2.007679	0.102312	-1.038387
464	O	0.802483	-1.899488	-1.072324
465	H	0.124094	-1.998268	-0.310855
466	H	1.003453	-2.775720	-1.414997
467	O	-0.932980	1.800431	1.260875
468	H	-1.677973	1.318002	0.865424
469	H	-0.383622	2.098256	0.519138
470	O	-0.723202	0.225591	-2.110224
471	H	-0.165084	-0.564361	-1.995146
472	H	-0.157150	0.980744	-1.876429
473	O	2.444465	-0.093179	0.024990
474	H	1.974225	-0.842586	-0.417611
475	H	3.386688	-0.287057	0.008818
476	O	0.644351	-0.202410	2.340900
477	H	0.112114	0.598681	2.155359
478	H	1.436988	-0.110786	1.791861
479	O	-0.835694	-1.916140	0.856394
480	H	-0.354387	-1.393086	1.541810
481	H	-1.617843	-1.389322	0.611696

482

483 Cartesian coordinates of : W 8_ 7

484

485	O	0.003126	0.708831	2.304641
486	O	0.951159	2.220269	0.167819
487	O	2.431848	-0.037147	-0.730266
488	O	1.408250	-1.368211	1.249483
489	O	-0.887623	-2.189114	-0.271682
490	O	0.111536	-0.635261	-2.082664
491	O	-1.474420	1.543626	-1.243793
492	O	-2.321663	-0.152006	0.759513
493	H	-0.896702	0.537766	1.989903
494	H	-1.171975	-3.048584	-0.597326
495	H	3.369110	-0.179552	-0.891232
496	H	-2.108860	2.118129	-1.682777
497	H	0.356730	1.395607	1.703530
498	H	-0.504881	-1.671029	-1.045711
499	H	2.155595	-0.592936	0.060326
500	H	-1.944674	1.059892	-0.533959
501	H	1.618033	1.619899	-0.206790
502	H	0.192574	2.192220	-0.434408
503	H	1.025805	-0.417204	-1.810789
504	H	-0.399588	0.190455	-2.028602
505	H	0.959005	-0.677572	1.791205
506	H	0.689276	-1.906211	0.881542
507	H	-3.191278	-0.345198	1.123138
508	H	-1.925861	-1.003573	0.457545

509

510 Cartesian coordinates of : W 8_ 8

511

512	O	-1.459613	1.902232	-0.400252
513	O	0.049850	0.644623	-2.076442
514	O	2.405149	0.519800	-0.653109
515	O	0.816522	1.761727	1.366618
516	O	0.086533	-0.754536	2.281559
517	O	1.560220	-1.767123	0.237850
518	O	-0.918123	-1.883647	-1.231695
519	O	-2.316634	-0.427389	0.647852
520	H	-1.938178	2.652457	-0.765597
521	H	-0.824845	-0.771510	1.954536

522	H	3.341729	0.574414	-0.864025
523	H	-1.377522	-2.589736	-1.696519
524	H	-0.899014	1.496970	-1.131487
525	H	0.367358	0.176625	2.164846
526	H	2.208264	-0.403035	-0.309832
527	H	-1.534445	-1.515611	-0.564873
528	H	0.973172	0.684018	-1.755364
529	H	-0.218589	-0.288346	-2.011779
530	H	1.101861	-1.529015	1.078560
531	H	0.847161	-2.067568	-0.346592
532	H	0.044701	2.060211	0.861311
533	H	1.494191	1.532622	0.707938
534	H	-2.153685	0.493515	0.333324
535	H	-3.223407	-0.471506	0.966500

536
537 Cartesian coordinates of : W 8_9

538				
539	O	3.215777	1.422562	0.167569
540	H	3.534168	1.852305	0.966656
541	H	2.254659	1.608001	0.108364
542	O	-1.938443	-0.927481	-1.545434
543	H	-2.182519	-1.381475	-0.720505
544	H	-0.990398	-1.123631	-1.623287
545	O	-2.117687	1.672988	-0.995014
546	H	-2.140420	0.736930	-1.320442
547	H	-2.650828	2.205950	-1.592056
548	O	0.491326	1.357018	0.073270
549	H	-0.186762	1.769187	-0.487603
550	H	0.476715	0.397610	-0.152578
551	O	-1.780890	0.845777	1.694606
552	H	-2.253592	1.253982	0.949551
553	H	-0.861711	1.119994	1.533444
554	O	-1.709638	-1.764557	1.147969
555	H	-2.108842	-2.350508	1.797594
556	H	-1.794181	-0.835562	1.483697
557	O	0.571772	-1.326530	-0.402370
558	H	1.530632	-1.518916	-0.317041
559	H	0.082409	-1.763874	0.314095
560	O	3.270605	-1.290717	-0.150015
561	H	3.388015	-0.324182	-0.020825
562	H	3.880081	-1.558294	-0.843712

563
564 Cartesian coordinates of : W 8_10

565				
566	O	2.105535	0.969539	-1.058217
567	H	2.430608	0.666338	-0.192732
568	H	1.895064	0.142488	-1.517603
569	O	-2.233806	0.821242	-1.191965
570	H	-1.554511	1.495914	-1.023580
571	H	-2.640845	0.635967	-0.333410
572	O	-2.298246	-0.792851	1.229350
573	H	-2.868527	-1.336102	1.780417
574	H	-1.937966	-1.354805	0.492267
575	O	2.138821	-0.474713	1.357671
576	H	2.660468	-0.599249	2.155728
577	H	1.267044	-0.044540	1.622490
578	O	-1.281574	-1.778065	-0.986510
579	H	-0.313101	-1.858544	-1.017132
580	H	-1.511301	-0.926111	-1.404251
581	O	-0.029547	2.423988	-0.410468
582	H	0.085770	3.367523	-0.557930
583	H	0.777533	1.962783	-0.754286
584	O	-0.092494	0.730986	1.847233
585	H	-0.173258	1.470024	1.218540
586	H	-0.904667	0.191853	1.756129
587	O	1.559573	-1.843373	-0.918801
588	H	1.834981	-1.608159	-0.008043
589	H	2.006611	-2.659411	-1.162950

590
591 Cartesian coordinates of : W 8_11

592				
593	O	-3.215078	0.308335	0.016880
594	H	-2.615466	0.484974	-0.745480
595	H	-4.015390	0.825069	-0.106916
596	O	-0.114583	-1.925670	-1.363048

597	H	-0.559422	-2.608419	-1.874579
598	H	-0.280993	-2.106387	-0.413352
599	O	-1.189479	0.693228	-1.703737
600	H	-0.603573	1.308901	-1.230879
601	H	-0.745368	-0.172588	-1.694196
602	O	-1.076012	0.406043	1.731735
603	H	-1.947631	0.411393	1.285195
604	H	-0.551512	1.104561	1.299488
605	O	0.369805	2.241365	0.114913
606	H	0.293686	3.185660	0.281945
607	H	1.336480	2.026287	0.066525
608	O	0.037069	-1.883518	1.346679
609	H	-0.146425	-2.489935	2.070171
610	H	-0.405403	-1.002247	1.565633
611	O	2.349058	-1.229482	-0.115298
612	H	1.825290	-1.481523	-0.891069
613	H	1.780609	-1.493202	0.630077
614	O	2.875975	1.385062	0.020775
615	H	2.774378	0.402700	-0.037652
616	H	3.566704	1.641841	-0.596111

617

618 Cartesian coordinates of : W 8_12

619

620	O	3.246189	0.445364	-0.625388
621	H	2.693759	1.109114	-0.169555
622	H	4.162846	0.638163	-0.409735
623	O	-0.642921	-1.637684	-1.319397
624	H	-1.290768	-1.643295	-0.584896
625	H	-1.018278	-2.151952	-2.040642
626	O	1.238828	1.852002	0.654536
627	H	0.859497	1.103238	1.212082
628	H	1.209572	2.660669	1.174326
629	O	-0.627515	1.228180	-1.341210
630	H	-0.432632	0.287074	-1.487150
631	H	0.081125	1.577316	-0.769188
632	O	1.801533	-1.818129	0.137166
633	H	2.439346	-1.163933	-0.204352
634	H	1.135114	-1.939827	-0.556445
635	O	0.338537	-0.267643	1.819557
636	H	0.890685	-0.940569	1.356280
637	H	-0.584056	-0.494206	1.615161
638	O	-2.958675	1.253815	-0.126583
639	H	-3.683523	1.500655	-0.707434
640	H	-2.109220	1.363428	-0.635189
641	O	-2.248519	-1.072317	0.831239
642	H	-2.693703	-0.231380	0.541120
643	H	-2.839436	-1.543198	1.426249

644

645 Cartesian coordinates of : W 8_13

646

647	O	2.831410	-1.060561	0.004049
648	H	3.059508	-0.104121	-0.060180
649	H	3.654884	-1.550138	0.088074
650	O	-2.313947	2.193960	0.163261
651	H	-1.345787	2.015061	0.132531
652	H	-2.482863	2.740570	0.935936
653	O	0.471483	-0.890605	-1.596042
654	H	1.343828	-1.162638	-1.266931
655	H	-0.168505	-1.494734	-1.182818
656	O	-3.338757	-0.250464	-0.280458
657	H	-3.046507	0.664435	-0.055126
658	H	-3.693288	-0.205179	-1.173860
659	O	-1.437294	-2.063766	0.143863
660	H	-2.179521	-1.418647	0.011217
661	H	-1.837670	-2.921888	0.313286
662	O	0.550071	-0.789228	1.724039
663	H	-0.139608	-1.365781	1.350785
664	H	1.391606	-1.088154	1.341469
665	O	0.241173	1.304779	0.035206
666	H	0.227349	0.667631	-0.715986
667	H	0.305497	0.693686	0.809064
668	O	2.953890	1.632882	-0.139356
669	H	3.264482	2.154238	-0.885339
670	H	1.982363	1.759674	-0.078618

671

672 Cartesian coordinates of : W 8_14

673
674 O 2.003244 -1.839714 0.396065
675 H 2.377356 -2.689667 0.644630
676 H 1.403239 -1.537580 1.121011
677 O 0.229323 -1.212069 -1.680131
678 H 0.386687 -0.259432 -1.807612
679 H 0.913012 -1.535657 -1.064173
680 O -0.963401 2.340190 0.311842
681 H -0.391325 2.625207 1.032830
682 H -1.518641 1.611202 0.658427
683 O 0.481062 -0.378287 2.014590
684 H -0.467501 -0.301998 1.817178
685 H 0.931503 0.361860 1.565803
686 O 2.245927 1.030485 0.384028
687 H 1.917886 1.313903 -0.484501
688 H 2.648418 0.159558 0.247905
689 O -2.204792 -1.606304 -0.801159
690 H -1.284196 -1.512909 -1.177386
691 H -2.818561 -1.638990 -1.540174
692 O -2.216079 0.064339 1.187671
693 H -2.329401 -0.578678 0.429663
694 H -2.955876 -0.052100 1.791024
695 O 0.528308 1.594445 -1.764739
696 H -0.099521 1.932826 -1.079090
697 H 0.458193 2.157775 -2.540869

698
699 Cartesian coordinates of : W 8_15

700
701 O -0.573433 0.116835 1.410627
702 H -0.554003 -0.785548 1.043216
703 H -0.448683 0.704188 0.637890
704 O -0.205098 1.721918 -0.871907
705 H 0.766249 1.631827 -1.037531
706 H -0.407040 2.659825 -0.795014
707 O 2.159061 -1.401354 -0.430957
708 H 1.258401 -1.761219 -0.525799
709 H 2.278716 -1.207334 0.517800
710 O -3.252053 0.567086 0.905649
711 H -2.428900 0.417280 1.407693
712 H -3.995913 0.466340 1.505326
713 O 2.260831 0.175389 1.868467
714 H 2.498374 0.895366 1.267831
715 H 1.303079 0.260579 2.012635
716 O -2.112908 -0.295088 -1.492373
717 H -2.749795 -0.035382 -0.801022
718 H -1.525161 0.472622 -1.588872
719 O -0.564183 -2.095593 -0.362565
720 H -1.187399 -1.526090 -0.893240
721 H -0.889472 -3.000310 -0.392660
722 O 2.377133 1.126572 -0.997055
723 H 3.029445 1.354564 -1.666124
724 H 2.337296 0.127173 -0.931228

725
726
727 Cartesian coordinates of the water nonamer

728
729 Cartesian coordinates of : W 9_1

730
731 O 0.304876 1.284426 1.795702
732 H -0.462868 1.596837 1.282937
733 H 1.097019 1.533771 1.286193
734 O 0.455282 -1.319329 2.026339
735 H 0.478040 -1.622000 2.938949
736 H 0.347603 -0.325321 2.031824
737 O -1.357148 -2.031934 0.000717
738 H -0.782113 -1.918458 -0.778128
739 H -0.782086 -1.917236 0.779386
740 O 0.304473 1.282945 -1.796470
741 H 1.096676 1.532734 -1.287263
742 H -0.463286 1.595333 -1.283685
743 O 2.451969 1.411490 -0.000681
744 H 2.563779 0.417048 -0.000248
745 H 3.323618 1.817199 -0.000982
746 O -1.749059 2.002393 -0.000489

747	H	-2.222005	2.839752	-0.000860
748	H	-2.421713	1.272760	-0.000118
749	O	-3.203914	-0.175863	0.000003
750	H	-4.102496	-0.512344	0.000192
751	H	-2.567303	-0.942624	0.000014
752	O	0.455231	-1.320890	-2.025509
753	H	0.478413	-1.624290	-2.937867
754	H	0.347522	-0.326889	-2.031778
755	O	2.384804	-1.199843	0.000431
756	H	1.849507	-1.442005	-0.777336
757	H	1.849584	-1.441436	0.778433

758

759 Cartesian coordinates of : W 9_ 2

760

761	O	-0.311095	1.037702	-1.905928
762	H	0.453976	1.392118	-1.415922
763	H	-1.106680	1.351672	-1.439793
764	O	-0.435105	-1.051019	2.146262
765	H	-0.349251	-0.058860	2.047270
766	H	-0.457521	-1.257804	3.085292
767	O	-2.388146	-1.200490	0.143412
768	H	-1.867461	-1.538508	-0.608100
769	H	-1.836493	-1.340616	0.934786
770	O	-0.474217	-1.574560	-1.866531
771	H	-0.483338	-1.975412	-2.740721
772	H	-0.366707	-0.587002	-1.979177
773	O	1.743129	1.948450	-0.199449
774	H	2.222365	2.759674	-0.392897
775	H	2.410933	1.210504	-0.121699
776	O	-2.468934	1.393927	-0.152174
777	H	-3.342637	1.793060	-0.194866
778	H	-2.575826	0.405344	-0.040611
779	O	3.261246	-0.169673	-0.058442
780	H	3.986452	-0.342151	0.548173
781	H	2.599282	-0.909778	0.042676
782	O	-0.326633	1.511394	1.647253
783	H	-1.119474	1.686013	1.108015
784	H	0.440996	1.765153	1.102373
785	O	1.374710	-1.970702	0.206237
786	H	0.798711	-1.992552	-0.579984
787	H	0.793038	-1.761085	0.960063

788

789 Cartesian coordinates of : W 9_ 3

790

791	O	-3.295272	-0.121659	-0.092894
792	H	-2.635936	-0.867379	-0.155036
793	H	-4.001626	-0.302674	-0.718876
794	O	0.342347	-1.546036	1.928848
795	H	0.304509	-1.928591	2.810487
796	H	0.242600	-0.554405	2.015965
797	O	-1.405859	-1.933918	-0.236474
798	H	-0.775662	-1.783524	-0.964410
799	H	-0.870564	-1.956575	0.578140
800	O	0.224805	1.061239	1.901624
801	H	1.048860	1.367543	1.482120
802	H	-0.501815	1.408883	1.351234
803	O	0.669369	-1.262250	-2.021182
804	H	0.955651	-1.755799	-2.795650
805	H	1.385397	-1.333254	-1.324616
806	O	2.335607	-1.264521	-0.016092
807	H	2.585685	-0.333692	0.129777
808	H	1.806821	-1.527649	0.759565
809	O	0.490409	1.506612	-1.634703
810	H	-0.351857	1.712717	-1.189689
811	H	0.433419	0.585016	-1.948502
812	O	-1.717780	1.955434	0.050653
813	H	-2.409711	1.242003	-0.031922
814	H	-2.174156	2.789349	0.197625
815	O	2.377724	1.532006	0.162273
816	H	1.728367	1.619819	-0.594445
817	H	3.059213	2.202946	0.061811

818

819 Cartesian coordinates of : W 9_ 4

820

821	O	-1.454092	0.000487	-1.497031
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822	H	-2.392539	0.000618	-1.733794
823	H	-1.474714	0.000004	-0.514407
824	O	0.576897	-1.891008	-1.279575
825	H	1.364418	-1.346689	-1.461752
826	H	-0.189093	-1.379577	-1.600232
827	O	0.382214	-2.069874	1.316812
828	H	0.360189	-2.965750	1.665894
829	H	0.448676	-2.121700	0.317977
830	O	0.381763	2.068729	1.318393
831	H	0.448250	2.121354	0.319590
832	H	0.359505	2.964361	1.668093
833	O	0.576666	1.892145	-1.278166
834	H	-0.189237	1.380820	-1.599197
835	H	1.364288	1.348119	-1.460770
836	O	-3.892795	0.000205	-0.143441
837	H	-4.795238	-0.001025	0.185533
838	H	-3.299079	-0.000448	0.625344
839	O	2.276101	-0.000378	1.394227
840	H	1.723893	-0.780299	1.584007
841	H	1.723711	0.779270	1.584612
842	O	2.647896	0.000640	-1.203099
843	H	2.645587	0.000264	-0.204677
844	H	3.560622	0.000790	-1.506046
845	O	-1.468820	-0.000759	1.265194
846	H	-0.932875	-0.784940	1.491348
847	H	-0.933000	0.783331	1.491965

848

849 Cartesian coordinates of : W 9_ 5

850

851	O	-0.510061	-0.206772	-1.858959
852	H	-1.391489	-0.570477	-1.677286
853	H	0.118921	-0.949232	-1.805704
854	O	-0.138208	1.582878	0.106992
855	H	0.136015	1.121959	0.924592
856	H	-0.208532	0.890421	-0.600045
857	O	-2.862326	-0.802957	-0.416932
858	H	-3.721348	-1.235169	-0.432688
859	H	-3.002136	0.134431	-0.135492
860	O	2.456350	2.229949	-0.610270
861	H	2.599106	2.590072	-1.490175
862	H	1.494777	2.253686	-0.436578
863	O	0.686277	-0.084303	2.201474
864	H	0.119620	-0.842533	1.883809
865	H	0.587013	-0.004625	3.154626
866	O	-0.685303	-1.952978	0.998311
867	H	-1.487446	-1.609878	0.564188
868	H	-0.072584	-2.224290	0.289838
869	O	2.722742	-0.385944	0.291603
870	H	2.798030	0.502091	-0.110528
871	H	2.252717	-0.255696	1.133788
872	O	1.289800	-2.126747	-0.989291
873	H	1.800114	-2.862865	-1.338837
874	H	1.925292	-1.489401	-0.542933
875	O	-2.820563	1.767194	0.335019
876	H	-3.215247	2.500664	-0.145548
877	H	-1.842487	1.888285	0.301408

878

879 Cartesian coordinates of : W 9_ 6

880

881	O	-0.895923	-0.334876	2.359546
882	H	-1.233558	-0.523535	3.239608
883	H	-1.651402	-0.387773	1.711444
884	O	0.289753	1.902492	1.073468
885	H	-0.505581	2.199354	0.604134
886	H	-0.011462	1.227955	1.704634
887	O	2.416518	1.403230	-0.625021
888	H	1.920194	1.225761	-1.435594
889	H	1.734793	1.661184	0.030922
890	O	-1.245802	-2.262797	-1.266304
891	H	-0.483198	-2.291932	-0.649358
892	H	-1.492440	-3.166356	-1.483943
893	O	-2.629920	-0.406592	0.388886
894	H	-2.603431	0.461059	-0.051072
895	H	-2.328124	-1.063519	-0.264251
896	O	0.683325	-1.462056	0.409277

897	H	1.666616	-1.446312	0.448281
898	H	0.331860	-1.193878	1.277476
899	O	3.314636	-0.983915	0.187599
900	H	4.056441	-0.977083	0.798066
901	H	3.152497	-0.054938	-0.107194
902	O	0.001625	0.248237	-1.700421
903	H	0.272241	-0.159912	-0.848492
904	H	-0.396562	-0.493633	-2.179339
905	O	-1.821912	1.998912	-0.833597
906	H	-2.173952	2.686691	-1.405946
907	H	-1.153325	1.475786	-1.336831

908

909 Cartesian coordinates of : W 9_ 7

910

911	O	-2.835912	0.850038	-0.294370
912	H	-3.019017	-0.084136	-0.028041
913	H	-3.672502	1.324537	-0.281540
914	O	-0.228255	-1.580921	0.132486
915	H	-0.286633	-0.884090	-0.570733
916	H	0.105247	-1.141421	0.939579
917	O	-0.558396	0.205137	-1.843631
918	H	0.091803	0.928765	-1.821042
919	H	-1.415037	0.603149	-1.617440
920	O	0.972166	-0.024842	2.118560
921	H	1.285172	-0.243230	3.001098
922	H	1.767825	0.103922	1.518668
923	O	1.168958	2.220852	-0.962954
924	H	1.420879	3.116218	-1.207224
925	H	0.519361	2.271622	-0.206705
926	O	2.772713	0.279713	0.282841
927	H	2.403481	0.971459	-0.295078
928	H	2.793402	-0.554950	-0.224405
929	O	2.318384	-2.238031	-0.787013
930	H	2.368815	-2.587231	-1.681255
931	H	1.378619	-2.257362	-0.521207
932	O	-2.902433	-1.727943	0.421858
933	H	-1.928316	-1.870400	0.366827
934	H	-3.324689	-2.442975	-0.063021
935	O	-0.571841	1.990603	0.986102
936	H	-0.164131	1.345373	1.592823
937	H	-1.407357	1.603906	0.667675

938

939 Cartesian coordinates of : W 9_ 8

940

941	O	-0.117111	-1.000814	-1.334084
942	H	-1.000947	-1.362285	-1.141326
943	H	0.528938	-1.539088	-0.840726
944	O	-2.685691	-1.455265	-0.307383
945	H	-3.345716	-2.111683	-0.549561
946	H	-3.090402	-0.566103	-0.435592
947	O	2.426243	0.297456	-1.705198
948	H	2.597490	-0.535615	-1.226290
949	H	1.593707	0.131010	-2.169693
950	O	2.003478	2.024829	0.283352
951	H	2.278188	1.487110	-0.502047
952	H	2.611785	2.765000	0.367464
953	O	-0.668914	1.441776	-0.235853
954	H	0.123315	1.970666	-0.041000
955	H	-0.347722	0.629048	-0.688653
956	O	-1.241711	-0.273262	1.931254
957	H	-1.211173	0.458179	1.288736
958	H	-1.719030	-0.977065	1.467043
959	O	1.539014	-0.277164	1.930548
960	H	0.572824	-0.346731	2.079476
961	H	1.710260	0.617741	1.589930
962	O	2.156343	-1.873780	-0.000618
963	H	1.987773	-1.333546	0.830185
964	H	2.614244	-2.683249	0.242332
965	O	-3.359415	1.151254	-0.548657
966	H	-2.459048	1.532022	-0.525310
967	H	-3.862376	1.584352	0.148151

968

969 Cartesian coordinates of : W 9_ 9

970

971	O	-0.056192	-2.159829	-0.186697
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972	H	0.746597	-1.606374	-0.260429
973	H	-0.410440	-1.997753	0.706448
974	O	-1.776590	-1.139621	-1.854940
975	H	-1.138462	-1.648670	-1.273806
976	H	-2.133198	-1.740642	-2.515432
977	O	-0.054175	1.087074	-1.919024
978	H	0.741592	0.668408	-1.535278
979	H	-0.659213	0.357427	-2.143395
980	O	1.845678	-0.142940	-0.309358
981	H	1.521757	0.306236	0.510016
982	H	2.816232	-0.151040	-0.291116
983	O	4.683777	-0.131390	-0.066909
984	H	5.088632	-0.824211	0.464833
985	H	5.107904	0.694854	0.186230
986	O	-2.816608	0.189183	0.385238
987	H	-2.430847	1.080561	0.297562
988	H	-2.683069	-0.245656	-0.477120
989	O	-1.320294	-1.101344	2.095091
990	H	-1.993100	-0.639908	1.516495
991	H	-1.780084	-1.474622	2.852512
992	O	0.562522	0.978500	1.754243
993	H	-0.023647	1.637660	1.341603
994	H	-0.023245	0.284787	2.105261
995	O	-1.155991	2.413122	0.031939
996	H	-1.321275	3.344223	-0.142285
997	H	-0.723161	2.012683	-0.778767

998

999 Cartesian coordinates of : W 9_10

1000

1001	O	-2.829534	0.868971	-0.889981
1002	H	-2.891779	-0.092373	-0.647457
1003	H	-3.685937	1.148749	-1.226301
1004	O	-0.199875	0.546219	-1.836934
1005	H	-1.134150	0.798571	-1.746935
1006	H	0.322820	1.254525	-1.422637
1007	O	3.296840	0.675591	0.475038
1008	H	3.233312	-0.234111	0.089700
1009	H	3.590497	0.566936	1.384315
1010	O	-0.979364	-0.883466	2.008791
1011	H	-0.864496	-1.030295	2.951956
1012	H	-1.015015	0.099821	1.844571
1013	O	-2.630326	-1.660491	-0.106598
1014	H	-1.865678	-2.045619	-0.563143
1015	H	-2.311927	-1.553447	0.807883
1016	O	-1.137083	1.618248	1.245533
1017	H	-0.309566	1.935023	0.839298
1018	H	-1.805969	1.582945	0.538645
1019	O	1.253208	2.239891	-0.119746
1020	H	2.029628	1.672628	0.134683
1021	H	1.599006	3.115671	-0.317276
1022	O	0.260366	-1.701713	-0.410050
1023	H	0.100647	-0.883852	-0.942359
1024	H	0.042025	-1.474034	0.511581
1025	O	2.930554	-1.803964	-0.429901
1026	H	1.947007	-1.901978	-0.480497
1027	H	3.301286	-2.153443	-1.245243

1028

1029 Cartesian coordinates of : W 9_11

1030

1031	O	0.139640	0.026584	2.400109
1032	H	0.846765	0.029826	1.706343
1033	H	0.563407	0.034011	3.263533
1034	O	-3.015179	-0.031517	-0.351129
1035	H	-2.397871	-0.030841	-1.137889
1036	H	-3.920929	-0.047250	-0.674137
1037	O	-1.449632	1.869365	0.976439
1038	H	-1.013490	1.346552	1.671786
1039	H	-2.177789	1.319650	0.632750
1040	O	0.293165	2.064836	-0.963975
1041	H	-0.377443	2.141374	-0.227333
1042	H	0.570234	2.947465	-1.227455
1043	O	0.342688	-2.056252	-0.929287
1044	H	0.651615	-2.933911	-1.173221
1045	H	-0.326676	-2.140229	-0.192458
1046	O	1.731159	0.029904	0.242630

1047	H	1.410350	-0.759743	-0.240436
1048	H	1.394697	0.803333	-0.255159
1049	O	-1.137502	-0.024338	-2.170590
1050	H	-0.570198	-0.795606	-1.992203
1051	H	-0.588871	0.763097	-2.005027
1052	O	4.549696	-0.017411	-0.325230
1053	H	3.619715	0.013627	-0.049006
1054	H	5.072743	0.105200	0.471422
1055	O	-1.407319	-1.875746	1.006216
1056	H	-2.146831	-1.347269	0.653659
1057	H	-0.983152	-1.332690	1.693361

1058
1059 Cartesian coordinates of : W 9_12

1061	O	2.903029	-0.827685	-0.119475
1062	H	2.761668	0.147013	-0.014882
1063	H	3.848534	-0.994621	-0.169507
1064	O	-0.053372	1.689178	-1.719275
1065	H	-0.857951	1.709067	-1.155793
1066	H	-0.241120	2.193497	-2.516781
1067	O	-2.075610	1.543284	0.109812
1068	H	-2.558361	0.643284	0.036641
1069	H	-2.742948	2.220766	0.259035
1070	O	-3.106133	-0.759510	0.016162
1071	H	-3.788964	-1.045359	-0.597209
1072	H	-2.327687	-1.420448	-0.047780
1073	O	2.078246	1.680553	0.148571
1074	H	1.492302	1.685858	0.924596
1075	H	1.485194	1.855000	-0.602070
1076	O	-0.051959	1.254634	1.957644
1077	H	-0.843365	1.375773	1.388835
1078	H	-0.283205	1.555366	2.841938
1079	O	-1.083955	-2.276595	-0.160369
1080	H	-0.516901	-1.966272	-0.899209
1081	H	-0.502412	-2.174879	0.622531
1082	O	0.800351	-1.504319	1.697566
1083	H	1.629994	-1.459967	1.193709
1084	H	0.550118	-0.583280	1.873621
1085	O	0.697955	-1.103031	-1.899929
1086	H	1.551807	-1.153130	-1.437533
1087	H	0.474881	-0.159727	-1.945794

1088
1089 Cartesian coordinates of : W 9_13

1091	O	0.155255	-2.057518	-0.168066
1092	H	-0.650790	-2.154463	-0.702416
1093	H	0.844865	-1.669248	-0.752832
1094	O	-1.823984	-0.832401	1.450286
1095	H	-2.433666	-1.083707	0.736325
1096	H	-0.971407	-1.166704	1.115562
1097	O	-1.492055	1.759462	1.388521
1098	H	-1.713510	0.798020	1.534673
1099	H	-2.012023	2.290176	1.999057
1100	O	2.011413	-1.133039	1.609806
1101	H	1.324913	-1.727485	1.256829
1102	H	2.354611	-1.526937	2.417478
1103	O	-2.330126	-1.337139	-1.244385
1104	H	-2.949756	-1.569042	-1.941848
1105	H	-2.015060	-0.411134	-1.414329
1106	O	1.350191	1.705827	-1.506466
1107	H	1.742576	2.508155	-1.863601
1108	H	1.382520	1.757740	-0.508863
1109	O	2.330971	-0.895195	-1.287439
1110	H	2.130982	0.017991	-1.561404
1111	H	2.788160	-0.829775	-0.437672
1112	O	1.271220	1.561837	1.098359
1113	H	0.344688	1.710457	1.365571
1114	H	1.520803	0.670255	1.399434
1115	O	-1.427800	1.162963	-1.399661
1116	H	-1.549909	1.578093	-0.528792
1117	H	-0.498669	1.329233	-1.640805

1118
1119 Cartesian coordinates of : W 9_14

1121	O	2.267671	1.348779	0.129228
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1122	H	2.571259	0.453173	-0.115925
1123	H	1.814074	1.249717	0.986249
1124	O	-1.343234	-2.029000	-0.198755
1125	H	-0.902960	-1.574874	-0.950029
1126	H	-2.173569	-1.562978	-0.041997
1127	O	-1.456057	1.663187	0.534826
1128	H	-0.947519	1.887851	-0.269714
1129	H	-2.149865	1.039765	0.274802
1130	O	0.370892	2.041654	-1.499113
1131	H	1.172422	1.871594	-0.918980
1132	H	0.546596	2.819584	-2.036513
1133	O	2.494608	-1.342239	-0.485696
1134	H	3.221377	-1.967565	-0.557460
1135	H	1.913334	-1.617421	0.287992
1136	O	0.819521	-1.790188	1.438332
1137	H	-0.031113	-1.972520	0.980487
1138	H	0.692324	-0.944776	1.902061
1139	O	0.210805	-0.751875	-2.065578
1140	H	0.208209	0.219436	-2.066215
1141	H	1.090220	-1.012850	-1.739812
1142	O	0.435874	0.906433	2.223932
1143	H	-0.343116	1.186553	1.673743
1144	H	0.366412	1.345472	3.076797
1145	O	-3.631809	-0.181647	-0.088581
1146	H	-4.342680	-0.174156	0.562018
1147	H	-4.051585	-0.166842	-0.956266

1148

1149

1150 Cartesian coordinates of the water decamer

1151

1152 Cartesian coordinates of : W10_ 1

1153

1154	O	0.947287	2.432659	0.980176
1155	H	1.299593	3.212959	1.418615
1156	H	1.599638	1.702254	1.094918
1157	O	-1.643879	1.391633	1.370656
1158	H	-0.767901	1.816657	1.336260
1159	H	-2.005506	1.427678	0.464891
1160	O	2.539231	0.251596	1.069692
1161	H	3.366165	0.146842	1.550117
1162	H	1.969366	-0.560020	1.263282
1163	O	-1.572458	-1.143559	1.961713
1164	H	-1.619038	-0.150803	1.833665
1165	H	-2.086712	-1.369854	2.742305
1166	O	-2.322308	0.976437	-1.301804
1167	H	-2.217095	-0.014992	-1.207728
1168	H	-3.128573	1.144464	-1.798318
1169	O	-1.940324	-1.555195	-0.807235
1170	H	-1.076249	-1.903470	-1.101670
1171	H	-1.946030	-1.625625	0.163684
1172	O	1.965377	-0.156706	-1.704578
1173	H	2.405003	0.043552	-0.861598
1174	H	1.365005	0.606939	-1.870385
1175	O	0.675120	-2.351566	-1.322664
1176	H	0.956588	-3.060974	-1.907930
1177	H	1.189787	-1.517942	-1.566609
1178	O	1.052918	-1.827538	1.385611
1179	H	0.151989	-1.645895	1.717938
1180	H	0.944795	-2.233088	0.504290
1181	O	0.273814	1.971688	-1.771536
1182	H	-0.660480	1.698184	-1.750215
1183	H	0.461430	2.367538	-0.905759

1184

1185 Cartesian coordinates of : W10_ 2

1186

1187	O	-0.892045	1.169440	2.136751
1188	H	-0.847396	1.454920	3.054144
1189	H	-0.878843	0.164704	2.115103
1190	O	-0.986205	1.429686	-1.956940
1191	H	-1.013256	1.832486	-2.829874
1192	H	-0.977380	0.429551	-2.068350
1193	O	3.654721	1.307148	0.092657
1194	H	2.700803	1.521260	0.079632
1195	H	4.097312	1.953025	-0.465012
1196	O	0.903244	1.457661	0.055841

1197	H	0.317701	1.639447	-0.706259
1198	H	0.354507	1.543796	0.860938
1199	O	-2.856058	1.225779	0.128698
1200	H	-2.307931	1.411832	0.912016
1201	H	-2.331477	1.506674	-0.642691
1202	O	-0.961746	-1.161696	-1.945337
1203	H	-1.724066	-1.453092	-1.413248
1204	H	-0.161425	-1.432481	-1.453952
1205	O	3.883562	-1.430351	-0.115492
1206	H	3.965825	-0.457806	-0.043480
1207	H	4.414094	-1.809386	0.590958
1208	O	-3.014545	-1.393171	-0.043256
1209	H	-3.098969	-0.401987	0.026549
1210	H	-3.896804	-1.775559	-0.048313
1211	O	-0.870395	-1.401664	1.768786
1212	H	-0.101670	-1.591381	1.195570
1213	H	-1.662397	-1.621329	1.245809
1214	O	1.130185	-1.322483	-0.143137
1215	H	1.161165	-0.346389	-0.077272
1216	H	2.064472	-1.611074	-0.160830

1217

1218 Cartesian coordinates of : W10_ 3

1219

1220	O	0.434211	2.037224	-1.363904
1221	H	0.815194	1.270458	-1.829462
1222	H	-0.536963	1.897805	-1.345244
1223	O	-2.247748	1.468881	-1.117337
1224	H	-2.440165	1.361398	-0.170722
1225	H	-2.486244	0.609792	-1.493512
1226	O	-0.015429	-2.097238	-1.042589
1227	H	-0.955894	-1.864796	-0.936910
1228	H	0.356276	-2.225957	-0.150674
1229	O	2.928345	-0.203431	0.238063
1230	H	2.682940	-0.224100	-0.705640
1231	H	2.640939	0.668848	0.567491
1232	O	1.573972	-0.383306	-2.211638
1233	H	1.858263	-0.669311	-3.084683
1234	H	0.935741	-1.065878	-1.855544
1235	O	1.481498	2.066933	0.980125
1236	H	1.754245	2.944309	1.264313
1237	H	1.052880	2.148473	0.067817
1238	O	-2.581640	0.294229	1.452349
1239	H	-3.164882	0.479899	2.194104
1240	H	-1.637559	0.268075	1.809552
1241	O	-2.711974	-1.350051	-0.688726
1242	H	-2.809233	-0.922188	0.189997
1243	H	-3.386766	-2.031710	-0.763478
1244	O	-0.151923	0.232097	2.284261
1245	H	0.407229	0.952685	1.931135
1246	H	0.327374	-0.599108	2.109376
1247	O	1.376865	-1.944116	1.383840
1248	H	2.076593	-1.344471	0.986959
1249	H	1.820602	-2.623997	1.899564

1250

1251 Cartesian coordinates of : W10_ 4

1252

1253	O	0.536093	2.446964	-0.019000
1254	H	0.910501	2.078390	0.800800
1255	H	-0.439248	2.356699	0.041746
1256	O	1.795070	0.876948	1.952818
1257	H	2.344256	0.413373	1.255881
1258	H	2.380759	1.144740	2.667301
1259	O	1.053419	-2.486990	-0.152236
1260	H	1.156693	-3.422718	-0.348344
1261	H	0.558363	-2.057657	-0.913978
1262	O	-2.551494	-0.497110	1.432017
1263	H	-1.613200	-0.771320	1.680873
1264	H	-3.132160	-0.777469	2.145641
1265	O	1.532710	1.078064	-1.957409
1266	H	1.854327	1.627972	-2.677929
1267	H	1.136737	1.683011	-1.252073
1268	O	2.917592	-0.397623	-0.026498
1269	H	2.633401	0.082634	-0.827131
1270	H	2.475850	-1.265255	-0.069864
1271	O	-0.130334	-1.165048	2.002191

1272	H	0.490672	-0.423873	2.136114
1273	H	0.280261	-1.748407	1.335195
1274	O	-2.763774	-0.523506	-1.268062
1275	H	-3.491789	-0.971418	-1.709279
1276	H	-2.829682	-0.712507	-0.306576
1277	O	-2.168192	1.962018	0.063224
1278	H	-2.442668	1.502007	-0.742872
1279	H	-2.368244	1.320732	0.765720
1280	O	-0.126812	-1.148339	-2.026751
1281	H	-1.047383	-0.894706	-1.831637
1282	H	0.388332	-0.327251	-2.151921

1283
1284 Cartesian coordinates of : W10_ 5

1285				
1286	O	-0.432537	0.428191	-1.863006
1287	H	-0.577748	1.266938	-1.393503
1288	H	-0.502059	-0.281409	-1.191554
1289	O	2.175733	-2.030140	-0.370547
1290	H	2.859374	-2.677232	-0.567763
1291	H	2.333341	-1.225330	-0.943315
1292	O	-1.051839	-0.950419	2.248610
1293	H	-1.478366	-1.254952	3.054844
1294	H	-1.643142	-0.259253	1.818305
1295	O	-0.621726	-1.901316	-0.327618
1296	H	0.286154	-2.238954	-0.427886
1297	H	-0.779330	-1.815198	0.630139
1298	O	-3.023313	-0.756139	-1.386241
1299	H	-2.509117	-0.285993	-2.059145
1300	H	-2.464161	-1.518506	-1.168048
1301	O	1.617336	-0.365059	1.816930
1302	H	1.891657	-1.082973	1.216805
1303	H	0.701828	-0.560105	2.099627
1304	O	1.917932	1.892973	0.621010
1305	H	2.552630	2.437556	1.097461
1306	H	1.805959	1.036310	1.144676
1307	O	2.325220	0.230836	-1.686473
1308	H	2.419320	0.931268	-1.018895
1309	H	1.410199	0.337659	-2.017156
1310	O	-0.587654	2.630488	-0.080281
1311	H	0.335265	2.502537	0.242084
1312	H	-0.708588	3.565119	-0.272747
1313	O	-2.467545	0.736733	0.906784
1314	H	-1.943536	1.504280	0.621856
1315	H	-2.802552	0.289053	0.100863

1316
1317 Cartesian coordinates of : W10_ 6

1318				
1319	O	0.000374	-0.899773	-2.082402
1320	H	0.000248	0.091031	-1.933191
1321	H	0.001339	-1.052654	-3.032153
1322	O	3.724898	-0.054825	0.054989
1323	H	4.445243	-0.163977	-0.571921
1324	H	3.094912	-0.819705	-0.070552
1325	O	-0.000133	0.847530	1.817404
1326	H	-0.779368	1.239239	1.382010
1327	H	0.779297	1.239325	1.382376
1328	O	-2.097187	1.972367	0.284929
1329	H	-2.536388	2.768059	0.599823
1330	H	-2.796587	1.269551	0.168176
1331	O	-1.908654	-1.908724	-0.282662
1332	H	-1.297707	-1.641187	-0.994122
1333	H	-1.351808	-2.026964	0.508646
1334	O	0.000001	-1.766152	1.763966
1335	H	-0.000118	-0.771176	1.862983
1336	H	-0.000193	-2.151247	2.645237
1337	O	0.000368	1.658038	-1.557576
1338	H	-0.780082	1.889216	-1.021275
1339	H	0.780518	1.888182	-1.020274
1340	O	1.908557	-1.907945	-0.281988
1341	H	1.351663	-2.026201	0.509327
1342	H	1.297595	-1.640452	-0.993496
1343	O	-3.724747	-0.055035	0.054764
1344	H	-3.094865	-0.819896	-0.070942
1345	H	-4.445922	-0.164844	-0.571063
1346	O	2.096582	1.971521	0.285329

1347	H	2.535210	2.768521	0.597689
1348	H	2.796540	1.269165	0.168696
1349				
1350	Cartesian coordinates of : W10_ 7			
1351				
1352	O	-3.367060	-1.303185	-0.191438
1353	H	-3.933942	-1.784188	0.417925
1354	H	-3.112688	-0.446799	0.250801
1355	O	-1.054192	-2.123124	-1.097670
1356	H	-1.976562	-1.912557	-0.781634
1357	H	-1.119972	-2.836494	-1.739833
1358	O	1.142817	2.252247	0.751403
1359	H	0.428743	2.564297	0.165706
1360	H	1.806316	1.832612	0.173122
1361	O	2.720447	0.683085	-0.961309
1362	H	3.400107	0.937375	-1.592760
1363	H	3.028179	-0.149188	-0.506086
1364	O	-0.032502	0.469493	2.239662
1365	H	0.480007	1.170898	1.738466
1366	H	0.091786	0.633939	3.179603
1367	O	-1.053212	2.393552	-0.977252
1368	H	-1.366224	3.016312	-1.639948
1369	H	-0.675942	1.597181	-1.451963
1370	O	-2.491058	0.909341	0.925476
1371	H	-2.173276	1.550628	0.263917
1372	H	-1.723925	0.735244	1.501347
1373	O	3.204820	-1.590859	0.228145
1374	H	2.292558	-1.805232	0.572315
1375	H	3.830406	-1.765243	0.936788
1376	O	0.747550	-1.948286	1.055943
1377	H	0.112822	-2.141963	0.342938
1378	H	0.424754	-1.149535	1.514798
1379	O	0.109916	0.285855	-1.968359
1380	H	1.039756	0.300217	-1.676532
1381	H	-0.273124	-0.572446	-1.705777

1382				
1383	Cartesian coordinates of : W10_ 8			
1384				
1385	O	1.868597	0.309666	1.757871
1386	H	1.000875	0.123016	2.159332
1387	H	1.770842	1.158916	1.288802
1388	O	-1.643623	-2.363747	1.306408
1389	H	-1.167854	-3.136455	1.622490
1390	H	-1.344311	-1.599096	1.840524
1391	O	-1.559996	-1.577062	-1.334354
1392	H	-1.630001	-1.929927	-0.423395
1393	H	-0.627385	-1.666942	-1.600506
1394	O	2.726281	-1.535347	0.101278
1395	H	2.435662	-0.851494	0.767150
1396	H	3.061637	-2.294811	0.584096
1397	O	1.177919	-1.395782	-2.016578
1398	H	1.597440	-1.783602	-2.790654
1399	H	1.789458	-1.535890	-1.244301
1400	O	-0.814883	-0.067144	2.577430
1401	H	-1.130845	0.139010	3.462878
1402	H	-1.114301	0.683675	1.975734
1403	O	0.549639	1.359711	-2.041029
1404	H	-0.424726	1.340903	-2.065981
1405	H	0.836143	0.428755	-2.096524
1406	O	-2.164594	0.916542	-1.530840
1407	H	-2.988359	1.080653	-1.998819
1408	H	-2.027335	-0.080462	-1.468011
1409	O	1.209287	2.545218	0.183065
1410	H	1.680594	3.373853	0.056068
1411	H	1.057184	2.133176	-0.716171
1412	O	-1.400644	1.871474	0.969251
1413	H	-0.562894	2.317411	0.747629
1414	H	-1.795685	1.591094	0.119643

1415				
1416	Cartesian coordinates of : W10_ 9			
1417				
1418	O	2.084652	1.867980	-1.000021
1419	H	2.146424	0.935793	-1.352652
1420	H	2.762166	2.395010	-1.434314
1421	O	2.407987	-1.640587	0.937804

1422	H	3.167715	-2.080797	1.330524
1423	H	2.364924	-0.713916	1.299515
1424	O	-0.373023	-1.815042	0.769583
1425	H	0.537279	-2.074335	0.995015
1426	H	-0.349068	-1.566532	-0.177608
1427	O	-0.733625	0.626006	1.821661
1428	H	-1.665114	0.852476	1.950901
1429	H	-0.691388	-0.326007	1.558845
1430	O	-3.021865	-1.486387	-0.390692
1431	H	-3.203305	-0.597087	-0.043724
1432	H	-2.523781	-1.948890	0.297073
1433	O	-0.711858	-0.855981	-1.831455
1434	H	-1.617857	-1.203958	-1.746302
1435	H	-0.778474	0.088576	-1.582146
1436	O	-0.664082	1.682334	-0.698901
1437	H	-0.508225	1.378064	0.221465
1438	H	0.178708	2.071265	-0.991614
1439	O	2.064933	0.880117	1.643605
1440	H	1.160019	1.006829	1.972212
1441	H	2.145257	1.407587	0.827559
1442	O	-3.152846	1.287933	0.388569
1443	H	-3.976953	1.779846	0.318353
1444	H	-2.508779	1.709758	-0.208969
1445	O	2.083619	-0.669520	-1.686893
1446	H	2.289062	-1.177812	-0.880807
1447	H	1.200262	-0.950709	-1.979415

1448

1449 Cartesian coordinates of : W10_10

1450

1451	O	-2.636116	0.074271	-1.154585
1452	H	-2.528021	-0.591851	-0.450958
1453	H	-1.804588	0.057554	-1.651782
1454	O	2.086547	-1.661222	0.777054
1455	H	1.591272	-2.308709	0.252161
1456	H	2.518357	-1.065450	0.141729
1457	O	2.901112	0.348673	-1.097492
1458	H	3.677192	0.439194	-1.658519
1459	H	2.837268	1.167783	-0.540976
1460	O	-1.935362	-1.804684	0.871618
1461	H	-1.247029	-1.302416	1.428677
1462	H	-2.577066	-2.195369	1.473081
1463	O	0.191138	-0.177902	-1.566555
1464	H	1.133649	0.034539	-1.692552
1465	H	0.162702	-1.124013	-1.329379
1466	O	-0.052201	-2.843960	-0.710776
1467	H	-0.254642	-3.573715	-1.303913
1468	H	-0.836996	-2.691728	-0.134199
1469	O	-0.074572	-0.533242	2.068096
1470	H	-0.125085	0.377560	1.720672
1471	H	0.773350	-0.899500	1.733616
1472	O	-0.174640	1.722083	0.450051
1473	H	-0.169810	1.075061	-0.286037
1474	H	-1.026993	2.203404	0.384972
1475	O	-2.747880	2.507392	0.040718
1476	H	-3.139683	3.223234	-0.466674
1477	H	-2.904562	1.670107	-0.449194
1478	O	2.408830	2.450048	0.443478
1479	H	2.755827	2.485540	1.340197
1480	H	1.430009	2.367126	0.516225

1481

1482 Cartesian coordinates of : W10_11

1483

1484	O	-1.342863	2.348073	0.552042
1485	H	-1.006825	1.681606	1.177608
1486	H	-1.815094	1.845336	-0.133798
1487	O	3.379023	-1.174533	-0.133491
1488	H	3.932151	-1.270025	0.646995
1489	H	3.000986	-0.268022	-0.107380
1490	O	-0.689046	-1.993236	1.345459
1491	H	-1.576301	-1.974305	0.929270
1492	H	-0.073753	-2.385975	0.702005
1493	O	1.202804	-2.650645	-0.638819
1494	H	1.386750	-3.473083	-1.102337
1495	H	2.070574	-2.225088	-0.431019
1496	O	1.824308	1.018193	0.039483

1497	H	1.284011	0.854006	0.840337
1498	H	1.755193	1.981420	-0.134544
1499	O	0.916721	3.535779	-0.321661
1500	H	0.018745	3.251243	-0.029824
1501	H	1.095955	4.395249	0.068457
1502	O	0.112610	-0.283127	-1.756356
1503	H	0.735245	0.268285	-1.240850
1504	H	0.345442	-1.200641	-1.533084
1505	O	0.035269	0.377456	2.037601
1506	H	-0.254777	-0.560337	1.801024
1507	H	0.167836	0.407413	2.989683
1508	O	-3.123318	-1.656950	0.128493
1509	H	-2.994671	-0.861096	-0.428786
1510	H	-3.895616	-1.498746	0.678680
1511	O	-2.322575	0.493153	-1.367254
1512	H	-2.729081	0.743522	-2.202723
1513	H	-1.390233	0.175943	-1.573682

1514

1515 Cartesian coordinates of : W10_12

1516

1517	O	-0.312653	0.591336	1.773418
1518	H	0.013631	1.304675	1.193320
1519	H	-0.710704	-0.103659	1.206116
1520	O	2.035005	-0.656634	2.082740
1521	H	2.376189	-0.822765	2.966658
1522	H	1.166880	-0.186034	2.168441
1523	O	-2.809311	1.479115	-0.079371
1524	H	-2.249441	1.371423	-0.863687
1525	H	-2.205209	1.504948	0.675586
1526	O	2.910422	0.888713	-0.116086
1527	H	2.740462	0.320460	-0.890826
1528	H	2.847247	0.317044	0.670141
1529	O	-1.306355	-1.325422	0.045536
1530	H	-2.265962	-1.490186	0.125080
1531	H	-1.189511	-0.707782	-0.702759
1532	O	0.842263	2.433097	0.007709
1533	H	1.734591	1.976681	-0.030733
1534	H	0.972431	3.385347	0.040513
1535	O	-0.491018	0.702924	-1.682366
1536	H	0.214855	0.207095	-2.135800
1537	H	-0.026457	1.431583	-1.227816
1538	O	1.243658	-2.349200	-0.055185
1539	H	1.623191	-1.973249	0.758051
1540	H	0.276547	-2.263801	0.044877
1541	O	-4.025488	-0.989230	0.058012
1542	H	-3.860920	-0.026432	0.059691
1543	H	-4.835296	-1.159644	0.545685
1544	O	1.846387	-0.815136	-2.084144
1545	H	2.269658	-1.263673	-2.822627
1546	H	1.644530	-1.498534	-1.382003

1547

1548 Cartesian coordinates of : W10_13

1549

1550	O	-0.814479	-0.179256	-1.853898
1551	H	-1.759830	-0.045859	-1.670860
1552	H	-0.355492	0.452283	-1.263374
1553	O	0.149201	1.527165	0.145723
1554	H	1.038762	1.918784	-0.028570
1555	H	0.232503	0.938244	0.920858
1556	O	-3.319254	0.208733	-0.567370
1557	H	-4.218838	0.226954	-0.906926
1558	H	-3.102725	1.114791	-0.232312
1559	O	-0.172094	-2.560012	-1.030663
1560	H	-0.379732	-1.685899	-1.473069
1561	H	-0.156052	-3.245674	-1.704695
1562	O	0.023393	-0.404849	2.140549
1563	H	-0.047807	-0.351239	3.098124
1564	H	-0.776501	-0.898367	1.796665
1565	O	-2.329323	2.541401	0.223741
1566	H	-2.510442	3.007338	1.044792
1567	H	-1.365165	2.333106	0.210216
1568	O	3.847169	-0.052651	-0.338787
1569	H	3.189810	-0.718803	-0.017153
1570	H	4.285756	-0.432559	-1.104992
1571	O	1.988721	-1.740344	0.591723

1572	H	1.345844	-2.144492	-0.018483
1573	H	1.449072	-1.329045	1.288317
1574	O	2.650709	2.335151	-0.366488
1575	H	3.156952	2.952224	0.168954
1576	H	3.165197	1.492879	-0.406420
1577	O	-1.925327	-1.703839	0.990114
1578	H	-1.455560	-2.240219	0.325734
1579	H	-2.525480	-1.116436	0.496037

1580

1581 Cartesian coordinates of : W10_14

1582

1583	O	0.844854	-0.009162	-1.867582
1584	H	0.478045	-0.910965	-1.800609
1585	H	1.797627	-0.090862	-1.697607
1586	O	-0.146340	-2.496604	-1.081905
1587	H	-0.956453	-2.258204	-0.532445
1588	H	-0.329111	-3.326060	-1.532843
1589	O	-2.431660	2.480762	-0.410882
1590	H	-2.390230	2.923284	-1.264029
1591	H	-1.508949	2.240561	-0.176769
1592	O	2.626984	2.371654	0.441713
1593	H	3.024835	1.525691	0.148934
1594	H	3.037914	3.072802	-0.072026
1595	O	-3.831697	0.149744	-0.274048
1596	H	-4.650712	0.285728	0.210354
1597	H	-3.391265	1.025062	-0.346598
1598	O	0.047715	1.497241	0.179589
1599	H	0.867905	2.010595	0.336723
1600	H	0.268424	0.928167	-0.607597
1601	O	-2.038975	-1.767820	0.507596
1602	H	-2.724748	-1.136443	0.201609
1603	H	-1.576326	-1.335007	1.245730
1604	O	-0.237045	-0.315360	2.114648
1605	H	-0.294344	0.048061	3.003499
1606	H	-0.153766	0.442604	1.478641
1607	O	1.767111	-1.820415	0.841825
1608	H	1.178190	-2.245317	0.188629
1609	H	1.172071	-1.377898	1.474363
1610	O	3.297993	-0.153558	-0.433190
1611	H	2.770534	-0.806914	0.118419
1612	H	4.188836	-0.506738	-0.518493

1613

1614

1615 Cartesian coordinates of the water undecamer

1616

1617 Cartesian coordinates of : W11_1

1618

1619	O	-2.327260	-2.021221	0.540895
1620	H	-2.880276	-2.785312	0.728148
1621	H	-1.530228	-2.327375	0.024525
1622	O	2.414622	-0.057430	-1.409115
1623	H	2.494639	-0.890576	-0.906448
1624	H	1.511181	-0.039296	-1.765915
1625	O	-1.165628	-0.032515	2.215152
1626	H	-1.625180	-0.769689	1.778781
1627	H	-1.550491	0.785725	1.858922
1628	O	-0.212196	-2.490543	-0.923679
1629	H	-0.162638	-1.750104	-1.548686
1630	H	0.629918	-2.487674	-0.423514
1631	O	-2.609980	0.201111	-1.067669
1632	H	-2.738078	-0.599340	-0.522361
1633	H	-2.656296	0.961914	-0.457452
1634	O	-2.089728	2.221605	0.746538
1635	H	-2.538790	3.029977	1.010104
1636	H	-1.251648	2.469065	0.267874
1637	O	0.086026	2.550206	-0.674289
1638	H	0.947691	2.485805	-0.220794
1639	H	0.073861	1.835574	-1.331908
1640	O	-0.334413	0.122116	-2.262172
1641	H	-0.485005	0.201351	-3.210781
1642	H	-1.245825	0.153537	-1.817090
1643	O	2.550184	1.838994	0.407230
1644	H	3.359801	2.355685	0.459053
1645	H	2.652138	1.164584	-0.317647
1646	O	1.532786	-0.238032	2.063856

1647	H	1.877931	0.600733	1.714682
1648	H	0.558004	-0.135828	2.173419
1649	O	2.145357	-2.102738	0.431424
1650	H	2.719806	-2.772303	0.814084
1651	H	1.921318	-1.418885	1.147634
1652				
1653	Cartesian coordinates of : W11_ 2			
1654				
1655	O	-1.444453	2.118191	1.036022
1656	H	-1.901152	2.697956	1.653696
1657	H	-0.993885	1.383251	1.577686
1658	O	1.750023	-2.355655	0.250313
1659	H	2.061204	-1.782754	0.974275
1660	H	0.780397	-2.405150	0.348076
1661	O	-0.925269	-1.674681	0.319839
1662	H	-0.806613	-1.051494	-0.425596
1663	H	-1.865273	-1.947198	0.301257
1664	O	-0.305063	0.089674	-1.779515
1665	H	0.484527	-0.366008	-2.125375
1666	H	-0.006595	0.984741	-1.534307
1667	O	0.398699	2.630128	-0.802838
1668	H	-0.278712	2.626253	-0.081707
1669	H	0.280891	3.434446	-1.317336
1670	O	-0.327611	0.173494	2.239413
1671	H	-0.596137	-0.598594	1.695541
1672	H	0.645836	0.139294	2.287119
1673	O	2.766810	1.157799	-0.316851
1674	H	2.710159	0.491988	-1.027374
1675	H	2.048826	1.795882	-0.469803
1676	O	-3.650874	-1.730343	0.124797
1677	H	-3.615090	-0.838881	-0.284505
1678	H	-4.311638	-2.245314	-0.345660
1679	O	2.216952	-1.056175	-1.955749
1680	H	2.755794	-1.527317	-2.598055
1681	H	2.090945	-1.649267	-1.155900
1682	O	-2.969417	0.683142	-0.942415
1683	H	-2.249814	0.469000	-1.555746
1684	H	-2.556652	1.217175	-0.240325
1685	O	2.432428	-0.178334	1.910162
1686	H	2.635240	0.391573	1.115775
1687	H	3.149938	-0.077495	2.542848
1688				
1689	Cartesian coordinates of : W11_ 3			
1690				
1691	O	-0.373329	0.313229	-1.745741
1692	H	0.389871	-0.148356	-2.140506
1693	H	-0.028603	1.176783	-1.453948
1694	H	1.948342	-1.628831	-1.351540
1695	O	2.083079	-0.967738	-2.095820
1696	H	2.571810	-1.402161	-2.801185
1697	H	-2.317515	0.653571	-1.503769
1698	O	-3.016921	0.832701	-0.856302
1699	H	-2.570866	1.319941	-0.142281
1700	H	1.988709	-1.929745	0.764659
1701	O	1.626094	-2.418581	0.003304
1702	H	0.657542	-2.414993	0.127210
1703	H	-0.886310	-0.910762	-0.456510
1704	O	-1.006105	-1.606861	0.220564
1705	H	-1.951491	-1.859494	0.191409
1706	H	1.019970	3.434929	-1.032309
1707	O	0.762610	2.623692	-0.583896
1708	H	-0.567096	2.509270	0.525818
1709	H	-1.685651	2.965481	1.528797
1710	O	-1.329466	2.200634	1.065537
1711	H	-0.570058	0.790778	2.082491
1712	H	-0.595310	-0.707089	1.708771
1713	O	-0.186281	-0.067655	2.330432
1714	H	1.382072	-0.271719	2.195549
1715	H	2.717401	0.401359	-0.994766
1716	O	2.769267	1.066030	-0.282125
1717	H	1.600857	2.081698	-0.411905
1718	O	2.331526	-0.500227	1.953526
1719	H	2.833571	-0.598916	2.767933
1720	H	2.753839	0.567691	0.559882
1721	H	-3.689392	-0.710855	-0.286554

1722	O	-3.735916	-1.627224	0.061722
1723	H	-4.398154	-2.102574	-0.446845
1724				
1725	Cartesian coordinates of : W11_ 4			
1726				
1727	O	2.995149	1.458813	-0.545548
1728	H	2.173630	1.955905	-0.410162
1729	H	2.752491	0.669988	-1.064239
1730	O	-2.668044	-1.964995	0.291400
1731	H	-2.465545	-1.383454	1.078251
1732	H	-3.310813	-2.627283	0.562273
1733	O	-0.004791	-1.829289	-0.511548
1734	H	-0.892090	-2.189939	-0.333166
1735	H	0.261383	-1.345488	0.305234
1736	O	-2.897555	0.307709	-1.344664
1737	H	-2.961783	-0.572180	-0.929032
1738	H	-2.125344	0.275476	-1.934409
1739	O	2.695453	-1.277642	-1.136048
1740	H	3.156866	-1.369652	-0.288256
1741	H	1.892994	-1.814209	-1.060144
1742	O	0.792881	-0.215294	1.521002
1743	H	1.736206	-0.308728	1.748758
1744	H	0.709696	0.606566	0.988347
1745	O	-0.244814	0.130947	-2.279778
1746	H	0.312914	0.059931	-3.061162
1747	H	-0.087864	-0.670598	-1.714731
1748	O	-1.936919	-0.252368	2.135443
1749	H	-0.968275	-0.276328	2.228708
1750	H	-2.156125	0.638421	1.806104
1751	O	0.217942	1.865455	-0.169727
1752	H	0.018013	1.397501	-1.005035
1753	H	-0.631111	2.226404	0.143763
1754	O	3.582094	-0.244940	1.413648
1755	H	4.333467	-0.155174	2.006561
1756	H	3.553645	0.543854	0.820054
1757	O	-2.462646	2.040293	0.578969
1758	H	-3.122462	2.734246	0.671096
1759	H	-2.729885	1.455235	-0.184026

1760				
1761	Cartesian coordinates of : W11_ 5			
1762				
1763	O	2.119000	-2.155238	-0.528396
1764	H	2.550478	-2.989033	-0.736532
1765	H	1.142755	-2.336143	-0.391925
1766	O	-1.999975	-0.964986	-1.795500
1767	H	-1.385090	-0.177101	-1.988107
1768	H	-2.290161	-1.313727	-2.644192
1769	O	-0.328136	2.655883	0.105564
1770	H	-0.893154	2.095564	0.738969
1771	H	-0.677683	3.552291	0.128683
1772	O	-1.734040	1.178383	1.641849
1773	H	-2.501658	0.781266	1.179538
1774	H	-1.227263	0.434358	2.021046
1775	O	-0.422117	-2.424923	-0.012779
1776	H	-0.552025	-2.004860	0.856541
1777	H	-1.013871	-1.978958	-0.649492
1778	O	-0.420134	0.996645	-2.193617
1779	H	0.525345	0.717664	-2.209658
1780	H	-0.478847	1.675077	-1.497364
1781	O	-0.212519	-1.013135	2.424763
1782	H	-0.246887	-1.397064	3.306220
1783	H	0.745464	-0.791292	2.228056
1784	O	2.226699	-0.478946	1.691695
1785	H	2.410885	-1.103339	0.964892
1786	H	2.317026	0.417197	1.319459
1787	O	2.278265	2.000755	0.359175
1788	H	1.356203	2.349547	0.306465
1789	H	2.854846	2.731459	0.602175
1790	O	-3.683091	-0.053930	0.156383
1791	H	-3.201168	-0.431429	-0.609439
1792	H	-4.262202	-0.740325	0.499131
1793	O	2.187309	0.287835	-1.928399
1794	H	2.261962	-0.611744	-1.563152
1795	H	2.474952	0.893840	-1.227196
1796				

1797 Cartesian coordinates of : W11_ 6

1798
1799 0 2.124847 1.511232 -1.599748
1800 0 -1.715123 -0.455678 -1.302191
1801 0 -1.891143 -0.001794 1.427314
1802 0 1.948239 1.647399 1.194080
1803 0 -0.538460 2.389524 1.240867
1804 0 2.355237 -1.234841 -1.131385
1805 0 0.107792 -2.549667 -1.294773
1806 0 -0.065025 -2.120603 1.494689
1807 0 2.307252 -1.069678 1.673497
1808 H 2.573557 -1.212183 -0.182212
1809 H 2.330042 -0.305295 -1.428542
1810 H 2.122595 0.734176 1.493334
1811 H 2.227952 1.688900 0.261303
1812 H -0.781688 -1.474465 1.632863
1813 H -0.146382 -2.444653 0.579202
1814 H -1.195196 -1.238893 -1.560381
1815 H -1.606357 -0.388603 -0.330992
1816 H 1.148903 1.731940 -1.683086
1817 H 2.605452 2.030258 -2.251376
1818 H 1.399474 -1.495194 1.697269
1819 H 2.843820 -1.474801 2.361280
1820 H 0.990493 -2.077725 -1.324419
1821 H 0.201136 -3.379586 -1.771771
1822 H -1.527431 0.902182 1.515946
1823 H -2.851550 0.065289 1.290999
1824 H -0.654889 3.191041 1.759994
1825 H 0.428891 2.125657 1.304418
1826 H -0.626177 2.313927 -0.669380
1827 O -0.427742 1.999403 -1.569679
1828 H -0.925075 1.163148 -1.669820
1829 H -3.608807 -0.312158 -0.859204
1830 O -4.192330 -0.146126 -0.099083
1831 H -5.057118 0.103671 -0.434136

1832

1833 Cartesian coordinates of : W11_ 7

1834
1835 O -2.661632 2.054311 -0.879218
1836 H -2.033927 2.236919 -0.159563
1837 H -2.095840 1.716417 -1.591108
1838 O 2.224305 -0.441331 1.589838
1839 H 2.367107 0.507013 1.415322
1840 H 1.357172 -0.519389 2.036949
1841 O -0.437790 1.693785 0.851045
1842 H 0.459732 2.074449 0.844414
1843 H -0.493447 1.114301 1.633084
1844 O -0.052618 -2.365738 -1.373436
1845 H -0.137927 -3.099635 -1.989143
1846 H 0.901409 -2.264296 -1.147922
1847 O -0.422582 0.433578 -1.627854
1848 H -0.441393 0.636533 -0.670677
1849 H -0.511644 -0.530553 -1.710906
1850 O -0.355646 -0.474829 2.572909
1851 H -0.618724 -0.697819 3.470619
1852 H -0.909203 -1.031179 1.936372
1853 O 2.299635 0.901527 -1.765990
1854 H 2.589206 -0.008877 -1.586690
1855 H 1.339570 0.817593 -1.941902
1856 O -3.751211 -0.314355 -0.189357
1857 H -4.656726 -0.272602 0.129063
1858 H -3.471269 0.600755 -0.428081
1859 O 2.472111 -1.720776 -0.633831
1860 H 2.382156 -1.273349 0.266967
1861 H 3.206695 -2.339498 -0.571264
1862 O -1.717318 -1.779576 0.838747
1863 H -1.209870 -2.130095 0.087356
1864 H -2.492812 -1.294718 0.477906
1865 O 2.302747 2.147517 0.528607
1866 H 2.388548 1.773065 -0.396247
1867 H 2.881188 2.912061 0.603773

1868

1869 Cartesian coordinates of : W11_ 8

1870
1871 O 0.205003 1.630134 -2.102936

1872	H	0.677538	0.805455	-2.319123
1873	H	0.769468	2.109053	-1.475309
1874	H	1.206255	-1.488065	-1.775906
1875	O	1.664524	-0.770859	-2.306160
1876	H	1.991585	-1.169608	-3.118139
1877	H	-1.240249	1.314819	-1.225820
1878	O	-1.933253	1.097861	-0.555395
1879	H	-1.660145	1.556072	0.258612
1880	H	1.078788	-2.477201	0.108694
1881	O	0.573001	-2.527459	-0.721560
1882	H	-0.355453	-2.335912	-0.484168
1883	H	-1.796213	-0.597041	-0.152323
1884	O	-1.832414	-1.517363	0.199586
1885	H	-2.767535	-1.749025	0.094445
1886	H	1.905110	3.435655	0.474080
1887	O	1.507593	2.585272	0.263739
1888	H	0.771289	2.432387	0.901411
1889	H	-0.942700	2.365507	2.577603
1890	O	-0.594679	1.888826	1.817579
1891	H	-0.481302	0.921112	2.093872
1892	H	-0.994686	-1.087522	1.793875
1893	O	-0.376451	-0.609036	2.379762
1894	H	0.505133	-1.000255	2.223386
1895	H	2.703897	-0.085182	-0.930860
1896	O	2.970369	0.188626	-0.033102
1897	H	2.563705	1.060073	0.121197
1898	O	2.045296	-1.679563	1.536439
1899	H	2.722444	-2.108819	2.067746
1900	H	2.481085	-0.954989	1.001033
1901	H	-3.686508	0.342701	-0.703520
1902	O	-4.277598	-0.411243	-0.534893
1903	H	-5.062638	-0.290772	-1.075251

1904

1905 Cartesian coordinates of : W11_ 9

1906

1907	O	-2.204544	-0.130844	-2.009193
1908	O	-1.891993	2.304239	-0.606763
1909	O	-2.477482	0.952806	1.546119
1910	O	-3.377443	-1.255651	0.069238
1911	O	0.459212	-0.979066	-1.571513
1912	O	0.652139	1.361370	-0.135761
1913	O	0.104455	-0.090593	2.022434
1914	O	-0.780995	-2.186937	0.639923
1915	H	-2.073728	0.796383	-1.740967
1916	H	0.416501	0.909397	0.720741
1917	H	-2.897202	0.129580	1.233259
1918	H	-0.392357	-1.956889	-0.225006
1919	H	-1.321447	-0.507702	-2.162070
1920	H	-0.105640	1.927908	-0.374632
1921	H	-1.665517	0.695164	2.014952
1922	H	-1.744794	-2.137242	0.527086
1923	H	-4.252992	-1.624897	-0.078353
1924	H	1.356930	-1.310649	-1.731548
1925	H	-2.341374	3.149011	-0.703189
1926	H	1.032723	-0.242854	2.279905
1927	H	-3.046857	-0.879546	-0.790246
1928	H	0.595396	-0.118151	-1.120890
1929	H	-2.193725	1.883274	0.250348
1930	H	-0.202160	-0.941987	1.614772
1931	H	4.027717	-1.588192	-1.500894
1932	O	3.256112	-1.137481	-1.144776
1933	H	3.472075	-0.186155	-1.085425
1934	H	2.894372	-1.091025	0.961994
1935	O	2.855931	-0.479216	1.712534
1936	H	3.252179	0.333132	1.364973
1937	H	2.321913	1.637082	-0.304770
1938	O	3.298615	1.491327	-0.343587
1939	H	3.715938	2.324732	-0.579276

1940

1941 Cartesian coordinates of : W11_10

1942

1943	O	3.059992	2.409763	-0.199074
1944	H	2.085567	2.452990	-0.264165
1945	H	3.356402	3.227869	0.209391
1946	O	-2.338145	-1.874905	0.281646

1947	H	-2.714440	-1.319433	-0.423425
1948	H	-1.457660	-2.147474	-0.034281
1949	O	0.300528	-1.840513	-0.644708
1950	H	1.220051	-2.190993	-0.709654
1951	H	0.174882	-1.230110	-1.392750
1952	O	0.552246	-0.169223	1.500039
1953	H	0.419415	-0.869206	0.821028
1954	H	-0.222732	-0.203748	2.087508
1955	O	0.338212	1.908290	-0.233724
1956	H	0.173032	1.447824	-1.076308
1957	H	0.468538	1.190149	0.429776
1958	O	-0.512488	0.230202	-2.377070
1959	H	-1.487855	0.243693	-2.250119
1960	H	-0.329788	0.332218	-3.316354
1961	O	-2.378997	1.791593	0.528041
1962	H	-1.467077	2.084748	0.337992
1963	H	-2.334244	1.238901	1.330471
1964	O	2.938150	-2.281111	-0.655232
1965	H	3.467263	-3.030390	-0.368597
1966	H	3.203602	-1.502698	-0.104667
1967	O	-2.099695	-0.305169	2.377022
1968	H	-2.272348	-0.985939	1.669444
1969	H	-2.570047	-0.568308	3.173554
1970	O	3.322394	-0.153386	0.919793
1971	H	2.501208	-0.111235	1.435846
1972	H	3.415123	0.727352	0.510455
1973	O	-3.041046	0.261846	-1.438678
1974	H	-2.874115	0.911002	-0.683770
1975	H	-3.883981	0.483678	-1.845814

1976

1977 Cartesian coordinates of : W11_11

1978

1979	O	0.014221	0.928736	1.120359
1980	H	0.675483	0.429381	1.636529
1981	H	-0.005342	0.522581	0.231057
1982	H	-1.741203	0.590100	1.778652
1983	O	-2.605217	0.145424	1.835664
1984	H	-2.415680	-0.755476	1.522744
1985	H	2.781887	-0.038278	1.398402
1986	O	2.213034	-0.487870	2.082442
1987	H	2.701419	-0.540486	2.908966
1988	H	1.400314	-1.862331	1.073355
1989	O	1.043620	-2.259667	0.260691
1990	H	0.064723	-2.204584	0.293714
1991	H	-2.129413	-2.900940	0.121450
1992	O	-1.703060	-2.045257	0.235861
1993	H	-1.971514	-1.471098	-0.550610
1994	O	3.354553	0.690830	0.033514
1995	H	3.173037	0.094691	-0.716083
1996	H	2.886194	1.524118	-0.146983
1997	O	1.451809	2.786789	-0.255333
1998	H	0.871769	2.385988	0.427151
1999	H	1.471536	3.738374	-0.117259
2000	O	2.258007	-1.172161	-1.746878
2001	H	2.621248	-1.789009	-2.389066
2002	H	1.802600	-1.696109	-1.020789
2003	H	0.937722	0.042677	-1.948751
2004	O	0.230340	0.659699	-1.676773
2005	H	0.619116	1.547522	-1.650234
2006	H	-3.016892	0.188004	-1.335699
2007	O	-2.341901	-0.434477	-1.678222
2008	H	-1.546040	0.085894	-1.883650
2009	H	-3.613706	0.881642	0.629185
2010	O	-3.992797	1.188320	-0.227527
2011	H	-4.948126	1.224417	-0.132479

2012

2013 Cartesian coordinates of : W11_12

2014

2015	O	-0.001298	0.518851	-1.397686
2016	H	-0.000046	-0.416036	-1.734243
2017	H	-0.002015	1.175080	-2.109266
2018	O	-3.759705	-0.116564	0.023627
2019	H	-4.356542	0.150090	-0.681728
2020	H	-3.147101	0.640981	0.190578
2021	O	0.001163	-1.355841	1.566933

2022	H	0.784693	-1.650709	1.067159
2023	H	-0.781863	-1.652102	1.067214
2024	O	2.167735	-2.234955	-0.014193
2025	H	2.651890	-2.990892	0.332928
2026	H	2.815156	-1.484341	-0.071676
2027	O	1.775241	1.665559	0.311634
2028	H	1.168383	1.151248	-0.264937
2029	H	1.350976	1.663075	1.188602
2030	O	-0.000391	1.120886	2.410555
2031	H	0.000077	0.148205	2.190221
2032	H	0.000100	1.209379	3.368128
2033	O	0.002024	-2.061866	-1.838501
2034	H	0.785184	-2.331781	-1.328320
2035	H	-0.781068	-2.333838	-1.329344
2036	O	-1.777650	1.664138	0.312688
2037	H	-1.353247	1.661997	1.189590
2038	H	-1.170500	1.150292	-0.263964
2039	O	3.760269	-0.110887	0.023019
2040	H	3.145940	0.645380	0.189893
2041	H	4.356201	0.156674	-0.682763
2042	O	-2.163670	-2.238605	-0.014452
2043	H	-2.646494	-2.995174	0.333146
2044	H	-2.812093	-1.488941	-0.071649
2045	O	-0.003839	3.299518	-1.481461
2046	H	-0.769523	3.194255	-0.897836
2047	H	0.762857	3.195285	-0.899027

2048

2049 Cartesian coordinates of : W11_13

2050

2051	O	0.994460	1.120920	2.175101
2052	H	1.774679	0.616962	1.897900
2053	H	1.039168	1.978132	1.700120
2054	O	0.731542	-2.610826	0.786168
2055	H	0.658648	-3.554871	0.956670
2056	H	0.630077	-2.458669	-0.210943
2057	O	-3.700873	-0.123572	1.417468
2058	H	-2.740215	-0.250995	1.566473
2059	H	-4.164704	-0.695601	2.034715
2060	O	-0.987372	-0.434750	1.391645
2061	H	-0.545644	-1.301179	1.375824
2062	H	-0.311124	0.205481	1.748388
2063	O	2.791043	-0.908220	1.151905
2064	H	3.524161	-1.203867	1.701016
2065	H	2.115270	-1.627361	1.146533
2066	O	0.531250	-1.968207	-1.686900
2067	H	1.334835	-1.468688	-1.909387
2068	H	-0.212919	-1.328894	-1.746357
2069	O	-4.020974	0.168813	-1.287341
2070	H	-4.075108	0.051065	-0.316203
2071	H	-4.488140	0.983278	-1.494472
2072	O	2.782763	-0.255105	-1.540674
2073	H	2.955663	-0.411396	-0.589659
2074	H	3.632788	-0.185572	-1.986052
2075	O	0.806901	1.845120	-1.710781
2076	H	-0.012315	1.314968	-1.676702
2077	H	1.533919	1.203829	-1.753608
2078	O	-1.272375	0.027055	-1.311325
2079	H	-1.222683	-0.053839	-0.333492
2080	H	-2.226354	0.094495	-1.522160
2081	O	1.216559	3.276664	0.519280
2082	H	1.028548	2.853228	-0.352557
2083	H	0.788060	4.136354	0.527583

2084

2085 Cartesian coordinates of : W11_14

2086

2087	O	2.621233	-1.565947	-0.115995
2088	H	3.149353	-2.367439	-0.190389
2089	H	2.105537	-1.635707	0.715925
2090	O	0.251510	-1.852326	-1.738271
2091	H	1.125250	-1.621469	-1.383550
2092	H	-0.215381	-2.306218	-1.014555
2093	O	1.406512	2.509952	0.248961
2094	H	2.147993	2.094769	-0.224086
2095	H	0.663321	2.606899	-0.379920
2096	O	-1.511012	0.011720	-2.443035

2097	H	-0.775637	-0.634259	-2.289060
2098	H	-1.762763	-0.047350	-3.369516
2099	O	-1.266783	-2.584514	0.538986
2100	H	-1.928803	-1.829079	0.343804
2101	H	-1.772916	-3.391187	0.676442
2102	O	-2.814073	-0.671493	-0.071062
2103	H	-2.730496	0.125997	0.497280
2104	H	-2.574871	-0.391314	-0.974682
2105	O	0.167714	1.129828	2.131198
2106	H	0.728182	1.647361	1.490580
2107	H	0.431630	0.200607	2.051344
2108	O	-2.234986	1.573694	1.337386
2109	H	-2.757559	2.059266	1.982041
2110	H	-1.318392	1.406840	1.730941
2111	O	-1.016626	2.495462	-1.093831
2112	H	-1.155063	1.722156	-1.664400
2113	H	-1.589385	2.359387	-0.321257
2114	O	0.815340	-1.703632	1.930491
2115	H	-0.000424	-2.099018	1.529865
2116	H	0.894839	-2.033515	2.831171
2117	O	3.530283	1.008569	-0.844477
2118	H	4.406556	1.225829	-0.513955
2119	H	3.336129	0.096956	-0.566832

2120

2121

2122 Cartesian coordinates of the water dodecamer

2123

2124 Cartesian coordinates of : W12_ 1

2125

2126	O	0.117467	1.902135	-0.244466
2127	O	-2.903878	-0.248582	-1.988489
2128	O	-2.687367	-1.798106	0.354448
2129	O	-0.116887	0.245340	1.901904
2130	O	-0.117559	-0.245368	-1.900564
2131	O	-2.686428	1.798849	-0.354771
2132	O	0.116830	-1.901971	0.245817
2133	O	-2.903586	0.248692	1.987983
2134	H	-0.105813	0.602907	-1.400440
2135	H	-1.780002	2.150262	-0.372362
2136	H	-1.781318	-2.150467	0.372993
2137	H	-2.914593	-0.585515	1.440360
2138	H	-2.832371	-1.455295	-0.546725
2139	H	-3.615439	-0.193270	-2.633354
2140	H	0.105568	1.403082	0.604483
2141	H	1.781224	0.372585	2.150251
2142	H	-1.018331	-0.338366	-2.257485
2143	H	-2.914819	0.585674	-1.441109
2144	H	0.104725	-1.402771	-0.603034
2145	H	-2.832687	1.456701	0.546417
2146	H	-0.104812	-0.602909	1.401636
2147	H	-1.017896	0.338053	2.258105
2148	H	1.017574	-2.258914	0.338538
2149	H	-3.615123	0.193213	2.632847
2150	O	2.903596	-1.988823	0.248256
2151	H	2.914244	-1.441162	-0.585907
2152	H	3.614964	-2.633845	0.192436
2153	H	2.915660	1.441368	0.585122
2154	O	2.687282	0.354526	1.797992
2155	H	2.832718	-0.546595	1.455300
2156	H	3.615390	2.633491	-0.194871
2157	O	2.904246	1.988169	-0.249406
2158	H	1.018517	2.258145	-0.337863
2159	H	2.832175	0.546260	-1.456053
2160	O	2.686358	-0.354848	-1.798640
2161	H	1.779853	-0.372728	-2.149793

2162

2163 Cartesian coordinates of : W12_ 2

2164

2165	O	-1.339276	2.286558	1.290348
2166	O	-2.712324	0.092414	1.523002
2167	O	-1.310580	-2.303126	1.290348
2168	O	1.276129	-2.395149	1.523002
2169	O	2.649855	0.016568	1.290348
2170	O	1.436195	2.302735	1.523002
2171	O	-1.436195	2.302735	-1.523002

2172	O	-2.649855	0.016568	-1.290348
2173	O	-1.276129	-2.395149	-1.523002
2174	O	1.310580	-2.303126	-1.290348
2175	O	2.712324	0.092414	-1.523002
2176	O	1.339276	2.286558	-1.290348
2177	H	-0.389465	2.287328	1.515889
2178	H	-1.786152	-1.480950	1.515889
2179	H	2.175617	-0.806378	1.515889
2180	H	-2.175617	-0.806378	-1.515889
2181	H	1.786152	-1.480950	-1.515889
2182	H	0.389465	2.287328	-1.515889
2183	H	-1.395986	2.510248	0.343527
2184	H	-1.475946	-2.464083	0.343527
2185	H	2.871932	-0.046165	0.343527
2186	H	-2.871932	-0.046165	-0.343527
2187	H	1.475946	-2.464083	-0.343527
2188	H	1.395986	2.510248	-0.343527
2189	H	-2.169592	0.935637	1.532870
2190	H	0.274511	-2.346740	1.532870
2191	H	1.895081	1.411103	1.532870
2192	H	-1.895081	1.411103	-1.532870
2193	H	-0.274511	-2.346740	-1.532870
2194	H	2.169592	0.935637	-1.532870
2195	H	-3.462048	0.222006	2.111586
2196	H	1.538761	-3.109224	2.111586
2197	H	1.923286	2.887218	2.111586
2198	H	-1.923286	2.887218	-2.111586
2199	H	-1.538761	-3.109224	-2.111586
2200	H	3.462048	0.222006	-2.111586

2201

2202 Cartesian coordinates of : W12_ 3

2203

2204	O	1.373770	1.649822	-2.009990
2205	H	1.925703	1.586631	-1.159039
2206	H	1.894771	2.137975	-2.655586
2207	H	-0.234146	2.113714	-1.656031
2208	O	-1.159676	2.288028	-1.357516
2209	H	-1.436530	3.120577	-1.752764
2210	H	-2.292408	0.782645	-1.471762
2211	O	-2.827382	-0.009549	-1.290611
2212	H	-2.285267	-0.779746	-1.552885
2213	O	-1.117520	-2.162881	-1.652106
2214	H	-1.282332	-2.915178	-2.228579
2215	H	-0.197638	-1.823154	-1.859566
2216	H	1.271313	-0.239451	-2.243414
2217	O	1.257338	-1.204301	-2.119482
2218	H	1.900407	-1.396202	-1.407531
2219	H	0.168038	1.585126	2.056724
2220	O	1.092018	1.346457	2.364618
2221	H	1.263168	1.839962	3.172467
2222	H	-1.262737	2.135844	0.512838
2223	O	-1.277974	1.921313	1.462471
2224	H	-1.957798	1.229175	1.572445
2225	H	-3.159109	-0.107672	0.293361
2226	O	-3.134802	-0.154375	1.292071
2227	H	-4.038934	-0.193030	1.617365
2228	H	-1.886224	-1.589974	1.404505
2229	O	-1.167232	-2.209488	1.194826
2230	H	-1.184958	-2.322096	0.228318
2231	H	1.194968	-0.534419	2.312235
2232	O	1.292429	-1.458990	2.023718
2233	H	0.390223	-1.773361	1.775488
2234	H	2.221304	1.430712	0.951294
2235	O	2.732963	1.310323	0.125736
2236	H	3.025153	0.377352	0.124977
2237	H	2.303011	-1.545018	0.869100
2238	O	2.934665	-1.449550	0.077795
2239	H	3.671237	-2.054891	0.203792

2240

2241 Cartesian coordinates of : W12_ 4

2242

2243	O	-1.116042	-0.644383	2.648576
2244	H	-2.314660	0.340502	1.691254
2245	H	-1.277426	-0.857072	3.572853
2246	H	-0.203150	-0.238010	2.589769

2247	O	1.235232	0.450726	2.383242
2248	H	1.203607	1.254344	1.834142
2249	H	1.931208	-0.113861	1.996970
2250	O	3.134737	-0.932435	0.863469
2251	H	4.037608	-1.154886	1.109169
2252	O	1.291743	-2.366990	-0.722683
2253	H	1.216100	-1.340939	-1.860861
2254	H	1.945461	-2.087265	-0.058681
2255	H	-1.154528	-1.968669	1.310515
2256	O	-1.116994	-2.496870	0.493845
2257	H	0.426896	-2.478689	-0.260248
2258	H	0.218459	2.669450	0.148083
2259	O	-1.305143	2.498279	-0.583986
2260	H	-1.717862	3.268675	-0.987763
2261	H	1.344044	3.522470	0.844978
2262	O	1.114942	2.630900	0.564780
2263	H	2.304339	1.648534	-0.520446
2264	H	3.165084	-0.213175	0.170225
2265	O	2.851133	0.952638	-0.924818
2266	H	2.316679	0.551015	-1.637118
2267	H	1.440073	-0.948172	-3.394803
2268	O	1.183191	-0.584459	-2.541644
2269	H	-0.422128	0.157399	-2.433195
2270	H	-1.272624	1.768821	-1.294783
2271	O	-1.286012	0.594335	-2.276410
2272	H	-1.919170	-0.088143	-1.982681
2273	H	-2.374270	1.483338	0.620778
2274	O	-2.878453	0.743573	1.002389
2275	H	-3.153733	-0.349899	-0.172594
2276	H	-1.839620	-2.169144	-0.067714
2277	O	-3.097149	-1.017083	-0.914706
2278	H	-3.989870	-1.282460	-1.154275

2279

2280 Cartesian coordinates of : W12_ 5

2281

2282	O	-1.388673	0.368102	-1.426778
2283	H	-0.861201	1.187689	-1.483877
2284	H	-0.803777	-0.393223	-1.675262
2285	O	0.242983	2.567185	-0.957538
2286	H	0.059586	3.492592	-1.146386
2287	H	0.184660	2.434045	0.036684
2288	O	-0.145815	-2.431467	1.049883
2289	H	-0.736253	-1.656341	1.240638
2290	H	-0.527162	-3.205341	1.475311
2291	O	-4.112330	0.203070	-1.359038
2292	H	-4.480895	-0.353661	-2.050724
2293	H	-3.153743	0.294178	-1.543930
2294	O	0.133538	-1.795937	-1.718629
2295	H	1.086980	-1.632252	-1.839450
2296	H	0.039971	-2.231199	-0.854229
2297	O	2.848234	-1.126513	-1.633760
2298	H	2.861213	-0.136937	-1.481208
2299	H	3.545130	-1.340829	-2.260912
2300	O	-4.292305	-0.215973	1.331291
2301	H	-4.392362	-0.085569	0.363801
2302	H	-4.842397	0.444616	1.761913
2303	O	2.533976	-1.620091	1.111129
2304	H	2.758026	-1.652550	0.163088
2305	H	1.630065	-1.976402	1.195903
2306	O	-1.563965	-0.191974	1.232074
2307	H	-2.512825	-0.208982	1.482416
2308	H	-1.557259	0.037137	0.271881
2309	O	2.761149	0.886453	1.781488
2310	H	2.697732	-0.100107	1.618175
2311	H	3.404929	1.031667	2.481259
2312	O	0.194103	1.952196	1.564473
2313	H	1.073245	1.605277	1.808117
2314	H	-0.443894	1.223524	1.684596
2315	O	2.799752	1.398447	-0.984585
2316	H	2.925265	1.409384	-0.018016
2317	H	1.959778	1.865292	-1.149871

2318

2319 Cartesian coordinates of : W12_ 6

2320

2321	O	0.241230	1.977215	0.314999
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2322	H	0.186916	1.458674	-0.521805
2323	H	1.185113	2.166355	0.463293
2324	O	-2.109410	3.400448	0.196557
2325	H	-2.098122	4.283825	-0.181843
2326	H	-1.181848	3.118866	0.314658
2327	O	2.607803	0.332894	-1.733775
2328	H	1.701370	0.431099	-2.069861
2329	H	2.706999	-0.591993	-1.442816
2330	O	3.008381	1.774344	0.423399
2331	H	3.764267	2.368859	0.421093
2332	H	2.975081	1.298370	-0.452097
2333	O	-0.238593	0.342090	-1.821785
2334	H	-0.188546	-0.561144	-1.450588
2335	H	-1.191796	0.580215	-1.764590
2336	O	0.034508	-2.011586	-0.375473
2337	H	-0.033798	-1.465221	0.442163
2338	H	0.952676	-2.333336	-0.422866
2339	O	-2.770358	0.975577	-1.013175
2340	H	-3.001588	0.408504	-0.258971
2341	H	-2.731386	1.884666	-0.662286
2342	O	-0.420297	-0.302061	1.698923
2343	H	-1.376989	-0.454192	1.805855
2344	H	-0.315742	0.596538	1.319977
2345	O	-3.100066	-0.900953	1.163868
2346	H	-3.885527	-1.000474	1.710415
2347	H	-3.001974	-1.725111	0.626788
2348	O	2.796147	-2.075601	-0.272477
2349	H	3.504541	-2.723905	-0.218127
2350	H	2.748593	-1.586551	0.594950
2351	O	-2.509328	-2.962729	-0.439526
2352	H	-1.542019	-2.822697	-0.515976
2353	H	-2.867922	-2.930394	-1.332090
2354	O	2.405726	-0.572935	1.847455
2355	H	1.470576	-0.542818	2.109694
2356	H	2.655181	0.328243	1.573119

2357

2358 Cartesian coordinates of : W12_ 7

2359

2360	O	0.001796	-1.216020	-2.056163
2361	H	0.004906	-1.498817	-2.975708
2362	H	0.001425	-0.205036	-2.033322
2363	O	-0.001662	-1.436350	1.959741
2364	H	-0.003395	-1.826067	2.839224
2365	H	-0.001543	-0.427491	2.058605
2366	O	4.647682	-1.212699	-0.141138
2367	H	3.702365	-1.458556	-0.107589
2368	H	5.121354	-1.834314	0.418621
2369	O	1.898250	-1.453236	-0.052076
2370	H	1.325157	-1.632165	0.719770
2371	H	1.334988	-1.555256	-0.844648
2372	O	-1.898515	-1.453140	-0.054995
2373	H	-1.335364	-1.555787	-0.847481
2374	H	-1.325449	-1.631684	0.717015
2375	O	-0.001319	1.130149	1.959881
2376	H	-0.784205	1.425548	1.455305
2377	H	0.782592	1.425795	1.457179
2378	O	4.811577	1.536049	0.022033
2379	H	4.917320	0.565434	-0.040325
2380	H	5.311904	1.919627	-0.703789
2381	O	-2.064007	1.341232	0.123260
2382	H	-2.126641	0.367233	0.061451
2383	H	-2.987687	1.662081	0.115451
2384	O	0.000983	1.338621	-1.724984
2385	H	0.782304	1.559201	-1.181004
2386	H	-0.781255	1.559762	-1.182603
2387	O	2.064246	1.341334	0.125311
2388	H	2.127082	0.367308	0.064386
2389	H	2.987741	1.662535	0.115580
2390	O	-4.648082	-1.212258	-0.143302
2391	H	-3.702786	-1.458243	-0.110216
2392	H	-5.121584	-1.833790	0.416697
2393	O	-4.811025	1.535868	0.023578
2394	H	-5.311548	1.920935	-0.701323
2395	H	-4.917078	0.565356	-0.040429

2396


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2397
2398 Cartesian coordinates of the water tridecamer
2399
2400 Cartesian coordinates of :    W13_ 1
2401
2402  0      -0.022876      -0.188871      -1.853416
2403  0      -2.846873      -0.052515      -1.852382
2404  0       2.111493      -2.577306       0.178770
2405  0       2.655079      -0.550291       2.058394
2406  0       2.616343      -1.081705      -1.920605
2407  0      -0.197358       1.886100      -0.040452
2408  0      -0.610060      -2.024067       0.079094
2409  0      -0.066849      -0.048575       1.871339
2410  0       2.159092       3.191227      -0.403821
2411  0      -2.869128       0.291714       1.839313
2412  0      -2.963417       2.098063      -0.044444
2413  0      -3.378046      -1.806889       0.031776
2414  0       3.454497       0.807815       0.003024
2415  H       0.059697       0.628159      -1.318022
2416  H       0.875167      -0.433195      -2.145922
2417  H      -3.283473      -1.198225      -0.752482
2418  H      -1.926143      -0.117848      -2.158563
2419  H       2.353212      -2.046997       0.960769
2420  H       1.147704      -2.702581       0.223772
2421  H       3.003736       0.032442       1.316555
2422  H       3.322476      -0.573393       2.750695
2423  H       2.478138      -1.740378      -1.182329
2424  H       3.170097      -1.495950      -2.589245
2425  H      -1.122478       2.192329      -0.087656
2426  H      -0.142392       1.278561       0.734261
2427  H      -1.552805      -2.265139       0.111717
2428  H      -0.490084      -1.442488      -0.705736
2429  H      -0.212289      -0.841076       1.306047
2430  H       0.841856      -0.136591       2.215709
2431  H       2.298996       4.009124       0.080725
2432  H       1.236142       2.903355      -0.247233
2433  H      -3.025912       1.478114       0.738060
2434  H      -1.956215       0.195264       2.161092
2435  H      -3.590762       2.815793       0.082973
2436  H      -2.938838       0.819233      -1.426406
2437  H      -4.151738      -2.361104      -0.106501
2438  H      -3.111767      -0.550616       1.412874
2439  H       3.285056       0.288352      -0.802837
2440  H       3.097435       1.707232      -0.145038
2441
2442 Cartesian coordinates of :    W13_ 2
2443
2444  0      -0.126309       1.211078       1.254587
2445  0       2.852836      -1.542204       1.678261
2446  0       3.273558      -1.079709      -1.067559
2447  0       0.717716       1.466397      -1.325982
2448  0       0.144429      -1.515915       1.034544
2449  0       2.610588       1.058563       1.846204
2450  0       0.526893      -1.218331      -1.639598
2451  0       3.454834       1.528901      -0.802148
2452  H       0.004770      -0.571691       1.267794
2453  H       1.666363       1.293292       1.881157
2454  H       2.441890      -1.321646      -1.509145
2455  H       3.498206       0.546943      -0.973457
2456  H       3.222616      -1.446901      -0.165738
2457  H       3.408438      -1.949588       2.349406
2458  H       0.101321       1.408415       0.317517
2459  H      -1.122138       1.722803      -1.774547
2460  H       1.002977      -1.770413       1.418636
2461  H       2.830522      -0.557136       1.846448
2462  H       0.339923      -1.433029      -0.696178
2463  H       2.958794       1.427875       1.013924
2464  H       0.755228       0.505763      -1.542824
2465  H       1.638670       1.781092      -1.323496
2466  H      -0.309094      -1.375051      -2.114170
2467  H       4.258908       1.929713      -1.145421
2468  0      -2.209862      -1.220048      -2.156277
2469  H      -2.391638      -1.593769      -1.239395
2470  H      -2.797256      -1.662463      -2.776384
2471  H      -2.574812       1.884410      -0.181069
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2472	O	-2.068089	1.527786	-1.661910
2473	H	-2.191986	0.594389	-1.926770
2474	H	-3.142354	2.947774	0.848350
2475	O	-2.780862	2.058404	0.785522
2476	H	-1.015982	1.577348	1.398411
2477	H	-3.032898	-1.515270	0.838276
2478	O	-2.487677	-2.092671	0.265400
2479	H	-1.612999	-2.145965	0.687860
2480	O	-3.851215	-0.263611	1.794305
2481	H	-4.796685	-0.256763	1.965938
2482	H	-3.595502	0.630759	1.492091

2483
2484 Cartesian coordinates of : W13_ 3

2486	O	0.438888	0.285200	-1.996330
2487	H	1.328161	-0.036147	-2.237475
2488	H	0.582132	1.174015	-1.613160
2489	H	2.935766	-1.373210	-1.115896
2490	O	3.070814	-0.680425	-1.826371
2491	H	3.746932	-1.000455	-2.431222
2492	H	-1.468103	0.125588	-2.305329
2493	O	-2.415847	0.078130	-2.095351
2494	H	-2.601390	-0.823218	-1.776449
2495	H	2.644712	-1.751785	1.021422
2496	O	2.527479	-2.243246	0.188421
2497	H	1.563117	-2.358764	0.097106
2498	H	-0.008496	-1.004354	-0.876652
2499	O	-0.143188	-1.724135	-0.221918
2500	H	-1.011006	-2.131020	-0.400948
2501	H	1.390976	3.491246	-1.076866
2502	O	1.136723	2.648885	-0.688123
2503	H	1.960557	2.224592	-0.300911
2504	H	-0.203563	2.525349	0.553072
2505	O	-0.861398	2.207936	1.197811
2506	H	-1.721199	2.187498	0.742667
2507	H	-0.224100	-0.773210	1.268959
2508	O	-0.210239	-0.223422	2.082049
2509	H	-0.413346	0.703411	1.790971
2510	H	3.339032	0.655230	-0.527773
2511	O	3.165575	1.300426	0.181415
2512	H	2.989654	0.789033	0.994171
2513	O	2.407540	-0.375259	2.312480
2514	H	2.766910	-0.384975	3.204745
2515	H	1.414777	-0.287650	2.380482
2516	H	-3.005221	-1.710679	0.330288
2517	O	-2.834960	-2.211054	-0.517865
2518	H	-3.427435	-2.967560	-0.553959
2519	O	-3.042726	-0.661583	1.583065
2520	H	-2.200548	-0.575402	2.061662
2521	H	-3.229052	0.210483	1.188953
2522	H	-2.969590	1.095654	-0.915090
2523	O	-3.258006	1.583347	-0.096725
2524	H	-4.024915	2.117927	-0.323242

2525
2526 Cartesian coordinates of : W13_ 4

2528	O	-1.251194	-3.031374	0.316528
2529	H	-1.409736	-3.969497	0.459670
2530	H	-0.260367	-2.900223	0.314505
2531	O	1.819943	2.440558	-0.877679
2532	H	1.175697	1.905519	-1.364767
2533	H	1.297658	2.909447	-0.204459
2534	O	-3.724996	0.377058	-0.054142
2535	H	-3.249993	-0.065950	0.710837
2536	H	-4.654762	0.464746	0.175765
2537	O	1.337415	-2.637108	0.278682
2538	H	1.702075	-2.313846	-0.564206
2539	H	1.756416	-2.100180	0.976472
2540	O	-2.257932	-0.817252	1.720165
2541	H	-1.993509	-1.691305	1.378614
2542	H	-1.424906	-0.311082	1.790771
2543	O	2.534953	-0.699109	1.921455
2544	H	3.042132	-0.232643	1.182546
2545	H	3.116780	-0.806299	2.679570
2546	O	3.561648	0.453566	-0.126061

2547	H	3.056672	1.272136	-0.325395
2548	H	3.375580	-0.135741	-0.876878
2549	O	-0.028002	0.262960	-1.310401
2550	H	-0.804623	-0.329523	-1.520875
2551	H	0.057467	0.251018	-0.329510
2552	O	-1.923009	2.388294	-0.755119
2553	H	-1.338428	1.793849	-1.253040
2554	H	-2.676151	1.827608	-0.484890
2555	O	-2.132608	-1.278549	-1.685832
2556	H	-1.970436	-2.035693	-1.093238
2557	H	-2.893412	-0.796880	-1.316034
2558	O	-0.163309	3.225567	1.001957
2559	H	-0.937989	3.038201	0.404731
2560	H	-0.329233	4.050470	1.467286
2561	O	0.150337	0.524828	1.445552
2562	H	0.986920	0.162337	1.802150
2563	H	0.156902	1.494307	1.554932
2564	O	2.154807	-1.146769	-1.972710
2565	H	1.334491	-0.599789	-1.884210
2566	H	2.260333	-1.382338	-2.899512

2567

2568 Cartesian coordinates of : W13_ 5

2569

2570	O	0.556453	1.238017	1.560983
2571	O	-2.109680	2.030049	1.525722
2572	O	-2.561267	-0.709006	1.224227
2573	O	0.119666	-1.422082	1.107787
2574	O	0.837697	1.629229	-1.129411
2575	O	-1.905319	2.207606	-1.076713
2576	O	-2.656077	-0.444824	-1.535484
2577	O	0.062318	-0.951345	-1.580297
2578	H	-0.268179	1.687526	1.818087
2579	H	0.346282	0.278120	1.513975
2580	H	-1.716604	-1.139505	1.446638
2581	H	-2.499699	0.217229	1.528228
2582	H	-0.970562	2.234323	-1.343708
2583	H	-2.278682	1.389032	-1.454907
2584	H	-0.863542	-0.999970	-1.879102
2585	H	0.289942	0.005297	-1.542632
2586	H	-2.667967	2.705292	1.922882
2587	H	0.952677	-1.861415	1.357806
2588	H	1.775956	1.683634	-1.384439
2589	H	-3.517496	-0.832906	-1.747737
2590	H	-2.082024	2.192696	0.537807
2591	H	0.108147	-1.387013	0.123609
2592	H	-2.594719	-0.571972	-0.563557
2593	H	0.819255	1.593823	-0.146655
2594	H	2.450211	1.061122	1.713357
2595	O	3.279661	0.615112	1.470866
2596	H	3.078342	-1.012978	1.465538
2597	H	3.505062	0.916582	0.571625
2598	O	3.538894	0.988225	-1.308753
2599	H	4.310558	1.221997	-1.833371
2600	H	3.333956	0.024545	-1.468279
2601	O	2.796021	-1.529169	-1.473134
2602	H	1.858175	-1.579198	-1.726651
2603	H	3.427708	-2.516215	1.837911
2604	O	2.836302	-1.969589	1.311774
2605	H	2.859550	-1.895675	-0.572482
2606	H	-4.212971	-1.494067	0.568300
2607	O	-4.780094	-1.656420	-0.203125
2608	H	-5.559985	-2.126728	0.102217

2609

2610 Cartesian coordinates of : W13_ 6

2611

2612	O	-2.695381	0.967865	1.164140
2613	O	-0.772159	2.780492	0.049911
2614	O	1.154668	-0.122290	2.453649
2615	O	-1.671297	-1.125792	2.408885
2616	O	-3.023647	-0.333819	-1.362834
2617	O	-1.270367	1.348433	-2.330454
2618	O	0.904771	-2.644313	-1.154752
2619	O	-1.589045	-2.330745	-0.094028
2620	H	-1.986859	1.581004	0.887466
2621	H	-0.421811	0.939489	-2.569720

2622	H	0.545385	-0.482246	3.110101
2623	H	-2.273685	-1.834851	-0.584845
2624	H	-3.020392	0.582156	0.332034
2625	H	-1.075151	1.922711	-1.562386
2626	H	0.603559	-0.061534	1.631306
2627	H	-1.733628	-2.168597	0.860359
2628	H	-2.242028	-1.362397	3.146916
2629	H	-3.809446	-0.345118	-1.918289
2630	H	-0.875032	3.734110	0.132429
2631	H	1.082993	-3.534554	-1.474836
2632	H	-2.045938	-0.282485	2.025116
2633	H	-2.358246	0.273945	-1.806003
2634	H	0.128414	2.565122	0.404755
2635	H	-0.011300	-2.650340	-0.794765
2636	H	2.325500	1.897071	0.426150
2637	O	1.692563	2.308636	1.041862
2638	H	1.640107	1.706743	1.802643
2639	H	2.123904	0.294075	-2.018590
2640	O	1.249742	-0.039744	-2.293878
2641	H	1.273114	-1.007834	-2.207794
2642	H	2.143609	-1.951747	0.134197
2643	O	2.798805	-1.453115	0.653855
2644	H	2.338336	-1.156227	1.463448
2645	H	3.258460	-0.126052	-0.149466
2646	O	3.350741	0.725233	-0.669677
2647	H	4.289176	0.914014	-0.767076
2648	O	-0.096343	0.061047	0.151325
2649	H	0.465189	0.154907	-0.640418
2650	H	-0.628628	-0.736469	-0.006752

2651

2652 Cartesian coordinates of : W13_ 7

2653

2654	O	-1.500785	2.408594	-1.262915
2655	O	1.072693	2.203370	-1.550610
2656	O	2.284202	-0.263903	-2.017202
2657	O	0.904543	-2.381619	-1.535322
2658	O	-1.853960	-2.134190	-1.294478
2659	O	-3.097376	0.140615	-1.472002
2660	O	-1.360495	2.483486	1.543218
2661	O	1.191342	2.051914	1.260911
2662	O	2.304713	-0.373747	2.086619
2663	O	0.850215	-2.319145	1.250834
2664	O	-1.918854	-2.170324	1.516585
2665	O	-2.960661	0.206521	1.337922
2666	H	-2.056048	1.634107	-1.475976
2667	H	1.791303	0.577441	-1.981808
2668	H	-0.904874	-2.199608	-1.518144
2669	H	1.555064	1.210038	1.595502
2670	H	-0.105967	-2.268786	1.442323
2671	H	-2.412233	0.986165	1.547828
2672	H	-1.625504	2.583477	-0.312582
2673	H	3.014609	-0.162368	-1.374343
2674	H	-1.927093	-2.372278	-0.352764
2675	H	1.349852	2.084828	0.299188
2676	H	0.935647	-2.457258	0.287019
2677	H	-3.207294	0.288796	0.398681
2678	H	0.071924	2.271673	-1.526913
2679	H	1.437176	-1.553747	-1.762297
2680	H	-2.605266	-0.732931	-1.504206
2681	H	-0.371770	2.316644	1.525384
2682	H	1.725942	-1.146072	1.784828
2683	H	-2.311462	-1.248568	1.546628
2684	H	1.394690	2.959430	-2.051481
2685	H	1.261977	-3.102819	-2.062719
2686	H	-3.855580	0.068686	-2.059597
2687	H	-1.522337	3.218965	2.141564
2688	H	2.578902	-0.559733	2.989942
2689	H	-2.416817	-2.721529	2.127646
2690	O	4.093554	0.085414	0.044452
2691	H	4.559549	0.915872	0.177464
2692	H	3.572567	-0.086308	0.854758

2693

2694 Cartesian coordinates of : W13_ 8

2695

2696	O	-2.120187	2.176997	1.132761
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2697	O	0.520863	1.406204	1.728495
2698	O	-1.780232	-2.259317	1.284005
2699	O	-3.455691	-0.259099	1.359995
2700	O	-2.131508	2.386465	-1.476338
2701	O	0.453186	1.428998	-1.087656
2702	O	-1.688407	-2.316431	-1.541646
2703	O	-3.225429	-0.209559	-1.439030
2704	H	-1.236484	2.088499	1.529694
2705	H	0.696621	-0.323852	-1.371641
2706	H	-2.825820	-1.034244	1.427668
2707	H	-2.878669	0.674849	-1.656448
2708	H	-2.173441	2.436515	-0.479623
2709	H	0.252089	1.469822	-0.131891
2710	H	-1.711145	-2.499009	0.341679
2711	H	-3.518707	-0.160797	-0.510527
2712	H	-4.204646	-0.438607	1.936512
2713	H	-2.537022	3.181813	-1.834179
2714	H	1.436431	1.712268	1.621057
2715	H	-2.039103	-2.980053	-2.143564
2716	H	-2.609200	1.363504	1.362183
2717	H	-0.310611	1.842607	-1.527351
2718	H	0.596115	0.436173	1.842217
2719	H	-2.278718	-1.510191	-1.601397
2720	H	1.744331	-1.641454	1.726551
2721	O	0.857716	-1.336217	1.489664
2722	H	-0.872691	-2.081451	1.588543
2723	H	0.870317	-1.338366	0.499404
2724	O	0.858301	-1.277444	-1.207271
2725	H	0.054709	-1.745392	-1.505222
2726	O	2.972381	1.371990	0.237073
2727	H	2.921583	0.394121	0.276227
2728	H	2.399459	1.627620	-0.503749
2729	H	4.223548	-1.224172	-0.181929
2730	O	3.309591	-1.400773	0.098991
2731	H	2.790707	-1.641386	-0.684697
2732	H	6.323101	0.545666	-0.263211
2733	O	5.437440	0.270986	-0.515452
2734	H	4.823053	0.983114	-0.265041
2735				
2736	Cartesian coordinates of : W13_9			
2737				
2738	O	0.341192	-1.935758	-0.717398
2739	O	0.844360	-1.081964	1.780958
2740	O	0.211330	2.166127	-0.784313
2741	O	0.219691	0.001665	-2.423943
2742	O	-2.379321	-2.392446	-0.475510
2743	O	-1.947452	-1.630057	1.944254
2744	O	-2.549176	2.195711	-0.555438
2745	O	-2.564025	-0.016189	-1.941838
2746	H	0.475717	-1.614010	0.210559
2747	H	-2.137653	-0.667590	2.031786
2748	H	0.204853	1.404374	-1.407617
2749	H	-2.633441	-0.855854	-1.445440
2750	H	-0.533847	-2.368637	-0.736720
2751	H	-1.007970	-1.728990	2.166294
2752	H	-0.711779	2.486096	-0.760928
2753	H	-1.708303	-0.046684	-2.400628
2754	H	0.845761	-0.123273	-3.145118
2755	H	-2.984194	-3.137467	-0.543192
2756	H	1.820527	-1.147441	1.835212
2757	H	-3.267430	2.789345	-0.795439
2758	H	0.308989	-0.775153	-1.793675
2759	H	-2.299139	-2.141060	0.498332
2760	H	0.678864	-0.123928	1.885147
2761	H	-2.654464	1.358189	-1.093345
2762	H	1.256439	2.199722	2.229441
2763	O	0.540728	1.675859	1.855766
2764	H	0.492371	1.872093	0.890665
2765	H	-1.356404	1.452586	2.271608
2766	O	-2.222525	1.083778	2.040818
2767	H	-2.463647	1.507124	1.197965
2768	H	3.703283	-1.101005	0.545685
2769	O	3.538288	-0.604235	1.365233
2770	H	3.386724	0.296325	1.040990
2771	H	2.264431	-1.782300	-1.272476

2772	O	3.058561	-1.236029	-1.371037
2773	H	2.767940	-0.315188	-1.276963
2774	H	3.620994	2.059620	-0.928985
2775	O	2.889611	1.574771	-0.531825
2776	H	2.081285	2.093242	-0.688971
2777				
2778				
2779	Cartesian coordinates of the water tetramer			
2780				
2781	Cartesian coordinates of : W14_ 1			
2782				
2783	O	-0.535473	0.014373	2.743867
2784	H	-0.510832	-0.197994	3.682314
2785	H	0.293190	0.554442	2.542693
2786	O	1.644819	1.263894	2.189844
2787	H	2.346922	0.619497	1.978480
2788	H	1.616894	1.902420	1.450764
2789	O	-0.319508	-0.550725	-1.748437
2790	H	-0.320757	-0.947291	-0.851294
2791	H	0.525909	-0.806896	-2.163863
2792	O	-3.262017	-2.031074	0.299952
2793	H	-3.924983	-2.727534	0.283737
2794	H	-3.281435	-1.556914	-0.583369
2795	O	3.386817	0.803586	-1.063557
2796	H	3.643775	0.408259	-0.211103
2797	H	2.805529	1.558434	-0.848981
2798	O	-0.524382	-1.835987	0.698136
2799	H	-0.506962	-1.254505	1.486663
2800	H	-1.438538	-2.168708	0.622137
2801	O	2.302842	-1.177076	-2.364213
2802	H	2.752202	-0.376237	-1.963253
2803	H	2.743028	-1.385880	-3.193371
2804	O	-3.206137	1.881508	-0.523947
2805	H	-3.907186	2.539452	-0.495729
2806	H	-3.184729	1.415618	0.360547
2807	O	-3.075883	0.439537	1.649737
2808	H	-3.258160	-0.474745	1.367187
2809	H	-2.202149	0.425243	2.083706
2810	O	2.128488	-2.499366	0.114204
2811	H	1.180773	-2.481588	0.342101
2812	H	2.195712	-2.270854	-0.830630
2813	O	1.608900	2.774978	-0.143631
2814	H	1.827375	3.707238	-0.236447
2815	H	0.726270	2.619771	-0.604327
2816	O	3.499847	-0.643547	1.331855
2817	H	2.994877	-1.413988	0.937527
2818	H	4.235822	-0.998576	1.839182
2819	O	-3.093798	-0.592983	-1.867360
2820	H	-2.154498	-0.631755	-2.125038
2821	H	-3.258089	0.329984	-1.599635
2822	O	-0.556802	2.168726	-1.393872
2823	H	-1.462855	2.271046	-1.051271
2824	H	-0.458805	1.215322	-1.599359
2825				
2826	Cartesian coordinates of : W14_ 2			
2827				
2828	O	-2.090249	2.266623	-1.623849
2829	O	-2.063561	-2.487603	-1.186253
2830	O	-2.146753	-2.026813	1.642945
2831	O	-1.993825	2.377572	0.969809
2832	O	-3.573034	0.136172	1.494875
2833	O	0.463777	1.237102	-1.516208
2834	O	0.459105	-1.470622	-1.140912
2835	O	0.434740	-1.028490	1.582472
2836	O	0.716531	1.701647	1.178466
2837	H	0.699495	1.613980	0.199039
2838	H	-0.364192	1.671136	-1.796272
2839	H	-1.080627	2.291925	1.295794
2840	H	-2.080555	2.416333	-0.630807
2841	H	-1.224088	-1.754002	1.823776
2842	H	0.451546	-1.191918	0.614994
2843	H	-0.290066	-2.061780	-1.347746
2844	H	-2.534764	-3.165117	-1.680862
2845	H	-2.954898	0.604024	-1.602706
2846	H	-2.474891	3.043418	-2.040865

2847	H	0.431426	-0.051836	1.651358
2848	H	1.643540	1.887596	1.408856
2849	H	0.309876	0.270485	-1.525355
2850	H	1.319458	-1.871201	-1.365137
2851	H	-3.060389	-0.714785	1.643678
2852	H	-2.134159	-2.415089	0.750539
2853	H	-4.321940	0.140994	2.098609
2854	H	-2.507604	1.624431	1.319360
2855	H	-3.639274	-0.027199	-0.360072
2856	O	-3.361323	-0.219037	-1.275260
2857	H	-2.559692	-1.627619	-1.313000
2858	H	2.337662	1.261188	-1.693850
2859	O	3.240292	1.012971	-1.426742
2860	H	3.298279	0.046200	-1.534625
2861	H	3.833448	-2.443499	-1.403847
2862	O	3.170487	-1.801698	-1.131989
2863	H	3.260508	-1.667774	-0.141775
2864	H	4.259886	2.145055	1.341107
2865	O	3.530590	1.554469	1.129995
2866	H	3.511513	1.431208	0.139992
2867	H	2.300762	-1.297477	1.722647
2868	O	3.225709	-1.235061	1.416613
2869	H	3.469854	-0.296526	1.515482
2870				
2871	Cartesian coordinates of : W14_ 3			
2872				
2873	O	-3.466183	0.984791	-1.218231
2874	H	-3.405037	0.002450	-1.278622
2875	H	-4.345707	1.243759	-1.509113
2876	O	-1.982383	-2.253268	1.015098
2877	H	-2.061045	-1.560933	1.699956
2878	H	-1.030093	-2.434921	0.916856
2879	O	0.714017	-1.986062	0.406162
2880	H	1.628815	-2.302742	0.306275
2881	H	0.768618	-1.161001	0.949730
2882	O	-0.788539	1.509121	-1.991239
2883	H	-0.562949	0.556253	-2.045696
2884	H	-1.757336	1.540967	-1.954625
2885	O	3.458325	-1.899880	-0.003136
2886	H	4.254500	-2.437735	0.034457
2887	H	3.567930	-1.132536	0.626295
2888	O	0.654502	0.232612	1.902147
2889	H	0.456656	1.001009	1.306119
2890	H	-0.115250	0.125186	2.487565
2891	O	2.462384	-0.157736	-1.986687
2892	H	1.602124	-0.447996	-2.325803
2893	H	2.824690	-0.897314	-1.465975
2894	O	2.936624	2.064777	-0.580460
2895	H	3.552634	2.637870	-1.047063
2896	H	2.719562	1.312952	-1.189749
2897	O	0.272024	2.314274	0.270101
2898	H	-0.088787	2.043702	-0.618978
2899	H	1.184876	2.599672	0.096032
2900	O	-0.228121	-1.178431	-2.002768
2901	H	-1.122585	-1.536351	-2.119353
2902	H	0.075704	-1.498920	-1.121615
2903	O	-1.986256	-0.082860	2.789350
2904	H	-2.220652	0.720196	2.242598
2905	H	-2.453157	-0.019405	3.627907
2906	O	-2.965469	-1.678007	-1.306438
2907	H	-3.601551	-2.353568	-1.562085
2908	H	-2.633201	-1.918168	-0.385393
2909	O	-2.370817	1.962087	1.208743
2910	H	-1.520026	2.381657	0.995413
2911	H	-2.772499	1.685701	0.364615
2912	O	3.425341	0.242635	1.512473
2913	H	3.415204	1.001840	0.900666
2914	H	2.554984	0.255952	1.948663
2915				
2916	Cartesian coordinates of : W14_ 4			
2917				
2918	O	-3.081332	-2.341690	0.855084
2919	O	-3.021316	-1.574099	-1.652592
2920	O	-0.490918	-1.384999	1.142429
2921	O	-1.122123	1.226051	1.593985

2922	O	-1.310512	1.659258	-1.076111
2923	O	-0.328861	-0.847816	-1.558282
2924	O	-4.019783	1.008237	-1.132109
2925	O	-3.772068	0.336017	1.402113
2926	O	1.560129	1.921772	1.952743
2927	O	2.163158	-0.590557	1.151889
2928	O	2.277436	0.029895	-1.438614
2929	O	1.370156	2.505316	-0.850135
2930	H	-0.772037	-0.481220	1.413631
2931	H	-1.275794	-1.954889	1.235384
2932	H	-2.098364	-1.442941	-1.930785
2933	H	-3.448839	-0.698788	-1.686493
2934	H	-0.997739	0.774744	-1.372559
2935	H	-2.260366	1.700467	-1.286855
2936	H	-3.632668	-0.628507	1.415104
2937	H	-2.963898	0.737682	1.764149
2938	H	-3.098810	-2.154459	-0.126732
2939	H	-3.569728	-3.155141	1.012839
2940	H	-0.298354	-1.148926	-0.624421
2941	H	-1.169695	1.512297	0.651708
2942	H	-4.034508	0.822521	-0.152362
2943	H	-4.856928	1.415316	-1.373982
2944	H	0.421220	2.527713	-1.056167
2945	H	1.443362	2.543168	0.118195
2946	H	2.079898	0.993456	-1.379572
2947	H	2.175215	-0.418000	0.171424
2948	H	1.367795	-1.128630	1.319658
2949	H	1.881081	1.002793	1.785151
2950	H	-0.328283	1.640970	1.973189
2951	H	0.599492	-0.727404	-1.831169
2952	H	2.139170	2.323806	2.607460
2953	H	3.212411	-0.097723	-1.702107
2954	O	4.820058	-1.332967	1.058086
2955	H	5.037673	-2.223045	1.349694
2956	H	3.877536	-1.182129	1.272060
2957	O	4.937783	-0.576083	-1.588348
2958	H	5.671825	0.012059	-1.786616
2959	H	5.044870	-0.871873	-0.660936
2960				
2961	Cartesian coordinates of : W14_ 5			
2962				
2963	O	0.731230	0.741526	-1.901672
2964	H	-0.162777	0.818881	-2.284033
2965	H	0.655108	1.189215	-1.031767
2966	O	-2.041489	0.779535	-1.831836
2967	H	-1.967759	-0.031380	-1.288505
2968	H	-2.119132	1.520405	-1.207409
2969	O	0.399827	-0.786702	1.630675
2970	H	0.487664	-1.257415	0.769977
2971	H	-0.468714	-1.033401	2.004528
2972	O	3.644519	-1.838844	-0.681686
2973	H	4.379089	-2.370594	-1.002292
2974	H	3.693098	-0.944809	-1.121764
2975	O	-3.699588	0.485536	1.203170
2976	H	-4.113767	0.181606	0.367371
2977	H	-3.189973	1.289426	1.004412
2978	O	0.856833	-1.792835	-0.856972
2979	H	0.871174	-0.940761	-1.348576
2980	H	1.769441	-2.131052	-0.884223
2981	O	-2.236799	-1.441042	2.099202
2982	H	-2.665229	-1.954195	2.790748
2983	H	-2.838318	-0.670868	1.859292
2984	O	3.334267	1.837497	0.908170
2985	H	3.361029	0.931512	1.334615
2986	H	3.976282	2.397168	1.355453
2987	O	3.509279	0.608229	-1.633145
2988	H	3.549602	1.211549	-0.868688
2989	H	2.640270	0.753829	-2.044808
2990	O	-1.945994	-1.777003	-0.661338
2991	H	-1.074783	-2.139160	-0.893035
2992	H	-2.038262	-1.878394	0.304268
2993	O	-1.964220	2.593839	0.372783
2994	H	-2.159450	3.531059	0.467640
2995	H	-1.015238	2.458515	0.592869
2996	O	-4.497965	-0.585643	-1.246579

2997	H	-3.918859	-1.363346	-1.235935
2998	H	-4.053895	0.015513	-1.863859
2999	O	3.183756	-0.607259	1.806419
3000	H	3.420194	-1.206382	1.074176
3001	H	2.252861	-0.791413	2.024369
3002	O	0.571817	1.723461	0.683067
3003	H	1.477028	2.041610	0.861995
3004	H	0.489528	0.850514	1.141116
3005				
3006	Cartesian coordinates of : W14_ 6			
3007				
3008	O	1.722689	-2.078612	-1.799812
3009	H	2.425850	-1.375903	-1.717324
3010	H	2.126335	-2.846265	-2.215934
3011	O	3.621359	-0.839649	1.502820
3012	H	2.766664	-1.337480	1.449631
3013	H	4.222940	-1.328210	2.072396
3014	O	3.510830	-0.237101	-1.251455
3015	H	3.773955	-0.403318	-0.329009
3016	H	3.207372	0.688104	-1.295277
3017	O	0.096609	0.635300	1.396088
3018	H	0.832510	1.158212	1.784901
3019	H	-0.784853	0.867792	1.780751
3020	O	2.393457	2.333924	-1.073212
3021	H	2.652313	3.114634	-1.572104
3022	H	1.427740	2.183684	-1.216530
3023	O	-3.721624	-1.166630	1.206923
3024	H	-2.924930	-1.755913	1.099959
3025	H	-4.424881	-1.682685	1.611920
3026	O	2.505139	1.766263	1.755440
3027	H	2.628671	2.129391	0.863188
3028	H	3.061679	0.970891	1.807418
3029	O	-1.574610	-2.486686	0.538059
3030	H	-0.754089	-2.553931	1.049263
3031	H	-1.318124	-2.007369	-0.278075
3032	O	-2.444618	1.263261	1.845545
3033	H	-3.000110	0.466109	1.779024
3034	H	-2.660384	1.803683	1.066511
3035	O	-3.528580	-0.141306	-1.407152
3036	H	-3.767516	-0.567303	-0.562689
3037	H	-2.769856	-0.635211	-1.760616
3038	O	-0.866744	-1.059188	-1.737713
3039	H	-0.072046	-1.514981	-2.066431
3040	H	-0.585481	-0.130288	-1.592587
3041	O	-0.156917	1.523626	-1.066335
3042	H	-0.989893	2.030363	-1.119783
3043	H	-0.084809	1.229572	-0.116409
3044	O	-2.803376	2.306147	-0.807862
3045	H	-3.373126	2.998972	-1.154915
3046	H	-3.157767	1.427082	-1.120554
3047	O	1.187697	-1.816983	0.980127
3048	H	0.727063	-0.952090	1.076261
3049	H	1.284296	-1.996453	0.025325
3050				
3051	Cartesian coordinates of : W14_ 7			
3052				
3053	O	2.687831	-0.999401	1.898990
3054	H	1.722002	-1.121153	1.856839
3055	H	2.839892	-0.036707	1.872615
3056	O	2.661869	1.622295	-1.194155
3057	H	2.761798	0.721366	-1.555066
3058	H	1.781634	1.930699	-1.466934
3059	O	-0.067361	-0.863105	1.380359
3060	H	-0.927186	-1.158173	1.732876
3061	H	-0.063637	0.119963	1.447607
3062	O	-0.131257	1.807713	-1.390609
3063	H	-1.037305	2.094440	-1.600656
3064	H	-0.131523	0.826497	-1.474782
3065	O	-3.893816	-2.230053	-0.045213
3066	H	-3.972736	-3.159017	-0.278581
3067	H	-3.474009	-1.760078	-0.818071
3068	O	-2.674844	1.541118	1.294194
3069	H	-2.789137	0.626139	1.612151
3070	H	-1.786313	1.822242	1.569622
3071	O	2.894609	1.778943	1.420855

3072	H	3.618631	2.343200	1.708701
3073	H	2.906181	1.752250	0.423678
3074	O	-2.756052	-1.183712	2.060434
3075	H	-3.223148	-1.665029	1.321357
3076	H	-3.184861	-1.429031	2.885871
3077	O	2.745133	-1.069192	-2.075854
3078	H	3.252083	-1.578564	-1.382929
3079	H	3.134672	-1.272199	-2.931775
3080	O	0.057203	-0.901856	-1.347020
3081	H	0.066367	-1.045016	-0.374094
3082	H	0.941045	-1.130225	-1.691341
3083	O	3.956423	-2.195112	-0.058537
3084	H	3.511824	-1.782509	0.733762
3085	H	4.072804	-3.130917	0.126743
3086	O	-2.680770	-0.897680	-1.957070
3087	H	-1.715310	-1.015267	-1.903049
3088	H	-2.846660	0.058858	-1.868361
3089	O	-2.911992	1.842906	-1.312438
3090	H	-2.904835	1.762582	-0.318353
3091	H	-3.650961	2.408945	-1.555220
3092	O	0.111704	1.846072	1.322619
3093	H	1.019981	2.050647	1.608062
3094	H	0.089256	1.974575	0.346901

3095

3096 Cartesian coordinates of : W14_ 8

3097

3098	O	-0.428929	1.937207	0.144296
3099	H	-0.360796	1.299257	0.887970
3100	H	0.431380	2.387656	0.047903
3101	O	2.200617	2.696540	-0.347180
3102	H	2.729848	2.341704	0.420413
3103	H	2.575013	3.547994	-0.592253
3104	O	-0.430787	-1.938690	-0.142652
3105	H	0.429024	-2.389983	-0.046126
3106	H	-0.361455	-1.300636	-0.886151
3107	O	-3.438056	-0.174391	1.998790
3108	H	-4.134740	-0.378188	2.629621
3109	H	-3.450359	-0.872745	1.285224
3110	O	3.444849	-1.550368	-1.648598
3111	H	3.748189	-1.957119	-2.464778
3112	H	2.974516	-0.708974	-1.896747
3113	O	-0.645908	-0.146629	1.889440
3114	H	-1.547719	-0.117973	2.254687
3115	H	-0.652493	-0.857488	1.206843
3116	O	2.199454	-2.696649	0.347290
3117	H	2.728981	-2.341766	-0.420059
3118	H	2.577458	-3.545401	0.596192
3119	O	-3.435136	0.176035	-2.001095
3120	H	-4.130515	0.380734	-2.633074
3121	H	-3.447721	0.874386	-1.287534
3122	O	-3.223585	1.825547	0.029679
3123	H	-3.382580	1.303737	0.837645
3124	H	-2.306737	2.147255	0.089072
3125	O	2.095962	-0.622430	2.289661
3126	H	1.143438	-0.452720	2.392423
3127	H	2.180449	-1.376365	1.678019
3128	O	2.098034	0.622374	-2.289910
3129	H	2.183527	1.376996	-1.679303
3130	H	1.145285	0.452847	-2.391130
3131	O	3.444130	1.549787	1.649487
3132	H	2.973134	0.708716	1.897393
3133	H	3.747500	1.956508	2.465659
3134	O	-3.225519	-1.824155	-0.031670
3135	H	-3.383033	-1.302285	-0.839880
3136	H	-2.308962	-2.146895	-0.089912
3137	O	-0.643351	0.145428	-1.887886
3138	H	-1.544770	0.117752	-2.254211
3139	H	-0.650063	0.856152	-1.205129

3140

3141 Cartesian coordinates of : W14_ 9

3142

3143	O	-0.333823	1.354013	1.418921
3144	H	0.524786	1.701422	1.758354
3145	H	-0.282592	0.377902	1.525933
3146	O	2.257393	1.895085	1.929462

3147	H	2.558022	0.996416	2.147334
3148	H	2.626314	2.097692	1.053380
3149	O	0.008001	-1.255473	-1.417291
3150	H	0.247397	-0.303124	-1.464503
3151	H	0.767556	-1.758803	-1.793184
3152	O	-3.628225	-0.696697	0.518991
3153	H	-3.354822	-0.863579	-0.400141
3154	H	-3.492313	0.253701	0.676039
3155	O	3.629818	-0.676091	-0.534471
3156	H	3.379160	-0.820578	0.395011
3157	H	3.472377	0.265884	-0.719307
3158	O	-2.308878	-2.239498	2.256833
3159	H	-2.714698	-3.100062	2.389665
3160	H	-2.893604	-1.714396	1.657068
3161	O	2.327570	-2.403845	-2.098320
3162	H	2.911898	-1.803100	-1.573774
3163	H	2.767365	-2.594609	-2.930756
3164	O	-2.283882	1.842827	-2.013595
3165	H	-2.665212	2.065387	-1.147756
3166	H	-2.553387	0.927155	-2.198019
3167	O	-2.854428	2.029689	0.786752
3168	H	-1.951889	1.921149	1.164853
3169	H	-3.321628	2.674886	1.326123
3170	O	0.037471	-1.361945	1.341229
3171	H	-0.001597	-1.486936	0.368221
3172	H	-0.736272	-1.831282	1.732769
3173	O	2.857570	2.039042	-0.870553
3174	H	3.303194	2.720304	-1.382890
3175	H	1.928754	1.971019	-1.193454
3176	O	2.572795	-0.922746	2.082716
3177	H	1.644271	-1.212278	1.910083
3178	H	2.938235	-1.499064	2.760891
3179	O	-2.564219	-0.996128	-2.086370
3180	H	-2.914131	-1.563595	-2.779764
3181	H	-1.617274	-1.240464	-1.940206
3182	O	0.276168	1.464931	-1.234480
3183	H	0.029255	1.488901	-0.280190
3184	H	-0.545819	1.744734	-1.700380

3185

3186 Cartesian coordinates of : W14_10

3187

3188	O	2.670280	0.263049	2.259491
3189	H	3.126314	0.709279	2.980130
3190	H	1.723599	0.198213	2.509208
3191	O	0.184922	-0.904202	-2.125763
3192	H	0.078578	0.082964	-2.134521
3193	H	0.294597	-1.166356	-1.177124
3194	O	-2.396441	-1.579298	-1.916555
3195	H	-2.870836	-1.875129	-2.699539
3196	H	-1.457828	-1.399670	-2.179147
3197	O	-3.148171	0.575304	-0.209228
3198	H	-2.952474	-0.138072	-0.843521
3199	H	-3.049285	0.199678	0.684700
3200	O	-0.016040	0.331246	2.159420
3201	H	-0.073733	1.252689	1.804549
3202	H	-0.910162	0.044660	2.423744
3203	O	0.174582	1.747992	-2.039996
3204	H	0.853226	1.840146	-1.349080
3205	H	-0.613730	2.225691	-1.726502
3206	O	-2.004280	-2.753562	0.643758
3207	H	-1.031652	-2.671295	0.594545
3208	H	-2.309965	-2.557993	-0.258832
3209	O	0.133307	2.815930	1.158352
3210	H	-0.614964	3.023623	0.567476
3211	H	0.933762	2.807017	0.614444
3212	O	3.209456	-1.900568	0.459467
3213	H	3.370077	-1.216277	1.127487
3214	H	3.388347	-1.508612	-0.411224
3215	O	-2.581185	-0.758974	2.215534
3216	H	-3.200381	-0.954649	2.925318
3217	H	-2.423763	-1.604045	1.699587
3218	O	2.356076	1.531544	-0.262984
3219	H	2.749177	0.940362	-0.928927
3220	H	2.510886	1.110264	0.601560
3221	O	2.919992	-0.592304	-2.068603

3222	H	3.421995	-0.609803	-2.889451
3223	H	1.986165	-0.808941	-2.292010
3224	O	-1.980559	2.859278	-0.653487
3225	H	-2.621122	3.538896	-0.882555
3226	H	-2.480593	2.011032	-0.474758
3227	O	0.519000	-1.709401	0.409778
3228	H	1.472644	-1.947210	0.484526
3229	H	0.373603	-0.934734	0.996443

3230
3231 Cartesian coordinates of : W14_11

3232				
3233	O	2.003405	-1.485623	-2.388507
3234	O	3.187154	-0.254299	1.515384
3235	O	0.509031	-0.129822	2.693368
3236	O	-0.469502	-1.048528	-1.261646
3237	O	-0.054783	-2.148970	1.105332
3238	O	2.022143	1.318187	-2.212869
3239	O	3.200038	2.095431	-0.016370
3240	O	0.670793	2.257744	1.135793
3241	O	-0.575842	1.616062	-1.145989
3242	H	1.078677	1.536651	-2.127652
3243	H	2.082102	0.354962	-2.362152
3244	H	-0.524760	-0.059114	-1.234581
3245	H	0.246404	-1.283978	-1.881128
3246	H	0.686281	1.542042	1.789660
3247	H	1.594963	2.410921	0.865698
3248	H	3.338028	0.561737	1.003596
3249	H	2.405734	-0.094991	2.065319
3250	H	2.301498	-1.887050	-1.516947
3251	H	2.390333	-1.999376	-3.103700
3252	H	-0.191466	1.882754	-0.273190
3253	H	-1.504949	1.904516	-1.130756
3254	H	2.830883	1.823992	-0.905817
3255	H	3.928950	2.704178	-0.168113
3256	H	0.313082	-0.969000	2.190074
3257	H	0.431413	-0.319427	3.634248
3258	H	-0.911530	-2.580637	1.239878
3259	H	-0.152607	-1.696083	0.221812
3260	H	1.788438	-2.730909	0.419443
3261	O	2.583966	-2.410867	-0.031857
3262	H	2.914315	-1.670860	0.528083
3263	H	-5.284093	-0.349059	-1.691109
3264	O	-4.822920	-0.329891	-0.848130
3265	H	-4.382085	0.538045	-0.775118
3266	H	-3.610839	-1.594714	-0.159570
3267	O	-2.715523	-1.856259	0.124592
3268	H	-2.149214	-1.701470	-0.651485
3269	O	-3.235166	1.913633	-0.270663
3270	H	-3.648391	2.729350	0.030247
3271	H	-2.850003	1.465678	0.531307
3272	O	-2.232837	0.402957	1.632081
3273	H	-1.340031	0.442665	2.002920
3274	H	-2.340789	-0.478867	1.214880

3275
3276
3277 Cartesian coordinates of the water pentamer

3278
3279 Cartesian coordinates of : W15_1

3280				
3281	O	-0.275273	-1.339172	-1.790495
3282	O	0.148872	-2.161311	0.747409
3283	O	-0.144050	2.180236	0.730897
3284	O	-0.080084	1.338379	-1.831655
3285	O	-3.044623	-1.440307	-1.749143
3286	O	-2.679568	-2.285209	0.659894
3287	O	-2.914624	2.225645	0.944626
3288	O	-2.886840	1.346821	-1.526497
3289	H	-0.193919	-1.651092	-0.856884
3290	H	-2.741437	-1.548921	1.312721
3291	H	-0.178290	1.882429	-0.210457
3292	H	-3.035010	0.387536	-1.643644
3293	H	-1.193047	-1.524766	-2.063144
3294	H	-1.773511	-2.620315	0.753091
3295	H	-1.043007	2.488403	0.947576
3296	H	-2.007889	1.534193	-1.895200

3297	H	0.793478	1.591770	-2.175946
3298	H	-3.760342	-1.898607	-2.199930
3299	H	1.065714	-2.483470	0.749990
3300	H	-3.621798	2.856635	1.109133
3301	H	-0.104115	0.350477	-1.826784
3302	H	-2.989345	-1.800449	-0.808303
3303	H	0.153980	-1.367099	1.334046
3304	H	-3.004866	1.905441	0.002812
3305	H	1.204476	0.053755	2.609031
3306	O	0.281468	0.044142	2.308989
3307	H	0.162649	0.838127	1.733078
3308	H	-1.639347	-0.131648	2.705257
3309	O	-2.554538	-0.189039	2.389946
3310	H	-2.757044	0.672484	1.982948
3311	H	2.844031	-1.808185	-0.508890
3312	O	2.970141	-2.174194	0.421878
3313	H	3.610831	-2.890014	0.361980
3314	H	3.158562	-0.875246	1.571221
3315	O	3.101791	-0.082101	2.153602
3316	H	3.845783	-0.113329	2.763053
3317	H	1.735918	2.467366	0.749915
3318	O	2.643853	2.198624	0.524519
3319	H	2.870052	1.458113	1.115668
3320	H	2.759720	1.842466	-1.062519
3321	O	2.704498	1.558578	-2.018848
3322	H	3.349581	2.069443	-2.517087
3323	H	1.577317	-1.382214	-2.175764
3324	O	2.509128	-1.225546	-1.941043
3325	H	2.669664	-0.267660	-2.049595

3326

3327 Cartesian coordinates of : W15_ 2

3328

3329	O	-2.941953	-1.896732	-0.009490
3330	H	-2.094549	-2.361786	0.250578
3331	H	-3.642627	-2.554564	0.043175
3332	O	-0.715729	-3.101391	0.702095
3333	H	-0.288976	-2.672488	1.467435
3334	H	-0.013575	-3.184763	0.035074
3335	O	1.275790	2.532818	1.782690
3336	H	0.897393	2.811115	0.898932
3337	H	1.765842	3.285292	2.128342
3338	O	1.762881	1.135379	-1.898006
3339	H	2.601162	0.712041	-1.636971
3340	H	1.372936	0.550467	-2.588319
3341	O	2.599921	0.031857	1.650782
3342	H	1.975727	-0.622085	2.009454
3343	H	2.171267	0.907064	1.710067
3344	O	0.475704	-0.795256	-3.340296
3345	H	-0.468012	-0.671401	-3.148361
3346	H	0.755800	-1.530201	-2.767235
3347	O	-0.690008	0.678373	2.341678
3348	H	-0.183616	1.476771	2.567455
3349	H	-0.436948	0.506164	1.395073
3350	O	0.285602	3.123535	-0.571574
3351	H	-0.641481	2.850269	-0.708151
3352	H	0.825595	2.653341	-1.231408
3353	O	-3.167247	0.703343	1.087213
3354	H	-2.477762	0.752892	1.773978
3355	H	-3.194898	-0.229864	0.803968
3356	O	-2.415618	2.260038	-0.891783
3357	H	-3.032597	2.983728	-1.041749
3358	H	-2.743963	1.746958	-0.099676
3359	O	3.631790	-0.580266	-0.692468
3360	H	4.592169	-0.632822	-0.693389
3361	H	3.342204	-0.351732	0.230758
3362	O	0.525229	-1.641337	2.779189
3363	H	0.640121	-2.018249	3.657391
3364	H	-0.010399	-0.816407	2.865114
3365	O	-1.977859	-0.244401	-1.999562
3366	H	-2.559814	-0.863496	-1.520849
3367	H	-2.347379	0.652046	-1.907881
3368	O	0.005803	0.006743	-0.116078
3369	H	0.660240	0.568198	-0.589606
3370	H	-0.738810	-0.089845	-0.753460
3371	O	1.347592	-2.251256	-1.020491

3372	H	0.957478	-1.474718	-0.570782
3373	H	2.302292	-2.073494	-1.010140
3374				
3375	Cartesian coordinates of : W15_ 3			
3376				
3377	O	-3.559054	0.665013	1.139562
3378	H	-2.838008	1.295553	1.314949
3379	H	-3.291396	-0.190799	1.521998
3380	O	-3.873714	0.256622	-1.425643
3381	H	-3.879216	0.469202	-0.448845
3382	H	-4.705018	0.554363	-1.806641
3383	O	2.584400	-1.996723	-1.666360
3384	H	2.972935	-2.701253	-2.194453
3385	H	2.673349	-2.252810	-0.703213
3386	O	1.123030	0.753762	1.415325
3387	H	0.728301	-0.149016	1.447030
3388	H	2.052468	0.664883	1.694013
3389	O	-1.207851	2.204626	1.114118
3390	H	-0.957354	3.118591	0.877478
3391	H	-0.409268	1.822596	1.522198
3392	O	0.125159	4.333545	-0.001374
3393	H	0.596993	5.136152	0.236121
3394	H	0.754380	3.726488	-0.436075
3395	O	-1.188239	0.978876	-1.393482
3396	H	-1.277028	1.371276	-0.498060
3397	H	-2.100559	0.851138	-1.710768
3398	O	3.832571	0.125089	1.420939
3399	H	4.652667	0.392932	1.845740
3400	H	3.900299	0.335580	0.444603
3401	O	-2.812972	-2.292065	-0.943942
3402	H	-3.270254	-1.508584	-1.301698
3403	H	-1.906173	-2.262427	-1.295115
3404	O	0.037476	-1.722592	1.300295
3405	H	-0.839722	-1.879792	1.694725
3406	H	-0.096714	-1.750889	0.322983
3407	O	-0.148065	-1.536866	-1.381791
3408	H	0.759497	-1.677337	-1.711917
3409	H	-0.386574	-0.588189	-1.470828
3410	O	3.707945	0.536368	-1.160557
3411	H	2.991484	1.176085	-1.327647
3412	H	3.401730	-0.311268	-1.532206
3413	O	1.349791	2.051514	-1.015333
3414	H	0.591361	1.810686	-1.573348
3415	H	1.220295	1.540582	-0.183968
3416	O	-2.726850	-1.976934	1.658879
3417	H	-2.822377	-2.200755	0.689461
3418	H	-3.232761	-2.622609	2.161868
3419	O	2.719118	-2.400735	0.920232
3420	H	3.196452	-1.633760	1.286505
3421	H	1.818238	-2.372619	1.288174

3422				
3423	Cartesian coordinates of : W15_ 4			
3424				
3425	O	3.390772	1.132442	-1.396963
3426	H	3.059933	0.218008	-1.658762
3427	H	4.144829	1.334157	-1.959941
3428	O	-0.313073	-0.469885	-2.171182
3429	H	-1.259645	-0.467444	-2.408551
3430	H	-0.067128	0.451417	-1.921198
3431	O	-3.194517	-0.221603	2.011419
3432	H	-3.249241	0.481163	1.293875
3433	H	-3.903019	-0.051611	2.639439
3434	O	-0.364946	-2.126792	-0.047615
3435	H	-0.299177	-1.531753	-0.833583
3436	H	0.462197	-2.637575	-0.000492
3437	O	-3.133361	-2.173656	-0.017171
3438	H	-2.207429	-2.469872	0.039237
3439	H	-3.288714	-1.649501	0.790572
3440	O	2.301319	-1.140154	2.208333
3441	H	2.711703	-0.289326	1.969949
3442	H	1.386551	-0.947492	2.479018
3443	O	-1.398273	3.422993	-0.072366
3444	H	-0.852249	3.303238	-0.863400
3445	H	-0.797401	3.200686	0.657180
3446	O	0.571141	1.921127	1.331780

3447	H	0.175602	1.075481	1.652588
3448	H	1.500240	1.929594	1.611714
3449	O	0.664907	1.920949	-1.372636
3450	H	1.600333	1.923611	-1.632887
3451	H	0.676492	1.852305	-0.389276
3452	O	-3.286217	1.419668	0.012442
3453	H	-2.667936	2.179640	-0.043147
3454	H	-3.236134	0.927604	-0.825167
3455	O	-0.432484	-0.466519	2.096821
3456	H	-1.365639	-0.372974	2.367586
3457	H	-0.451182	-1.064865	1.313602
3458	O	2.413395	-1.173993	-2.049261
3459	H	2.440968	-1.833168	-1.329238
3460	H	1.487012	-1.097415	-2.337720
3461	O	3.338242	1.337625	1.319142
3462	H	4.137807	1.713632	1.700150
3463	H	3.463545	1.297878	0.342177
3464	O	-3.094902	-0.521840	-2.056577
3465	H	-3.790434	-0.677691	-2.702804
3466	H	-3.191119	-1.208534	-1.335721
3467	O	2.311414	-2.825907	0.204054
3468	H	2.385391	-2.232896	1.005114
3469	H	2.806507	-3.631932	0.377916

3470

3471 Cartesian coordinates of : W15_ 5

3472

3473	O	3.180257	1.184374	1.816303
3474	H	3.638168	1.462454	2.615335
3475	H	3.764109	1.410604	1.034609
3476	O	3.134052	0.145522	-2.020781
3477	H	2.206489	0.447375	-2.037050
3478	H	3.100999	-0.798311	-1.779896
3479	O	2.565901	-1.572122	1.558274
3480	H	1.637570	-1.621601	1.843813
3481	H	2.843645	-0.647074	1.693787
3482	O	0.007919	-1.981313	-0.920319
3483	H	0.000985	-1.815140	0.049439
3484	H	0.867658	-2.392053	-1.120996
3485	O	0.432841	0.654685	-1.546438
3486	H	-0.355803	1.170705	-1.840258
3487	H	0.157762	-0.284473	-1.474817
3488	O	-2.782010	-2.099005	-0.901210
3489	H	-2.854606	-2.135788	0.069287
3490	H	-1.838686	-2.223285	-1.110428
3491	O	-3.744530	0.837175	1.099258
3492	H	-3.088610	1.556512	1.141611
3493	H	-3.978825	0.730703	0.158333
3494	O	-1.726545	2.794199	0.901047
3495	H	-0.841142	2.392537	1.071298
3496	H	-1.740513	3.665346	1.308622
3497	O	-1.841966	2.059114	-1.880011
3498	H	-2.605403	1.456569	-1.934973
3499	H	-1.910546	2.505426	-1.020512
3500	O	4.559799	1.554779	-0.350038
3501	H	4.062889	1.024281	-1.037847
3502	H	4.798426	2.395621	-0.749926
3503	O	2.766670	-2.432705	-0.922678
3504	H	3.357352	-3.184693	-1.027163
3505	H	2.786697	-2.159106	0.035303
3506	O	0.522901	1.349382	1.024973
3507	H	1.424084	1.464672	1.383654
3508	H	0.613410	1.133722	0.058810
3509	O	-0.210490	-1.215615	1.689421
3510	H	-1.131968	-1.390343	1.961554
3511	H	-0.107067	-0.246478	1.585768
3512	O	-2.949362	-1.523711	1.873267
3513	H	-3.511548	-1.902181	2.555867
3514	H	-3.289029	-0.604366	1.668424
3515	O	-3.899665	0.158100	-1.606373
3516	H	-3.478447	-0.732176	-1.433097
3517	H	-4.654237	0.017666	-2.186107

3518

3519 Cartesian coordinates of : W15_ 6

3520

3521	O	2.828693	0.759526	-1.543115
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3522	H	1.867754	0.601978	-1.596545
3523	H	2.934594	1.622830	-1.104375
3524	O	0.029674	0.214020	-1.312583
3525	H	0.015661	0.013608	-0.339583
3526	H	-0.011191	-0.657385	-1.760862
3527	O	-2.068567	-2.846931	-0.135310
3528	H	-1.546066	-2.735667	-0.949729
3529	H	-2.704306	-2.106232	-0.082930
3530	O	0.155761	3.038959	-0.816479
3531	H	1.012550	3.115498	-0.352034
3532	H	0.164291	2.172478	-1.251537
3533	O	3.650717	-1.067359	0.136426
3534	H	3.433576	-0.396516	-0.572876
3535	H	4.558855	-1.356443	0.003513
3536	O	-2.247253	3.259403	0.201788
3537	H	-1.299932	3.313640	-0.096646
3538	H	-2.602788	4.152337	0.232137
3539	O	2.486326	0.826052	1.897362
3540	H	1.557459	0.517442	1.843443
3541	H	3.018224	0.105677	1.516742
3542	O	1.683617	-3.008843	-0.197214
3543	H	1.161010	-3.086736	0.621984
3544	H	2.405546	-2.370868	-0.033168
3545	O	2.671713	2.854768	0.310709
3546	H	3.215513	3.579109	0.633632
3547	H	2.640537	2.137025	1.015831
3548	O	-0.030861	-0.158588	1.354640
3549	H	-0.870796	0.295729	1.631630
3550	H	-0.105890	-1.088516	1.647688
3551	O	-2.683519	1.090695	-1.529441
3552	H	-2.691914	1.949302	-1.068341
3553	H	-1.746757	0.822150	-1.576936
3554	O	-3.784358	-0.656647	0.055719
3555	H	-3.460935	-0.005667	-0.631724
3556	H	-4.717945	-0.822894	-0.107982
3557	O	-0.295794	-2.887903	1.748083
3558	H	-1.055609	-2.958125	1.095769
3559	H	-0.507349	-3.409348	2.527895
3560	O	-2.365024	0.997362	1.887803
3561	H	-3.025328	0.433421	1.450046
3562	H	-2.414926	1.867850	1.454533
3563	O	-0.034215	-2.429088	-2.041466
3564	H	0.107835	-2.879952	-2.879302
3565	H	0.693053	-2.709128	-1.405645

3566

3567 Cartesian coordinates of : W15_ 7

3568

3569	O	-3.402347	-1.839117	-1.429500
3570	H	-3.621352	-0.863814	-1.459033
3571	H	-4.017253	-2.303061	-2.005463
3572	O	-0.671931	-1.275927	-1.427251
3573	H	-1.540558	-1.671785	-1.624694
3574	H	-0.780837	-0.304375	-1.541601
3575	O	2.098213	-1.507142	-1.322169
3576	H	1.994059	-1.423191	-0.352056
3577	H	1.192574	-1.602633	-1.665327
3578	O	1.236882	2.775402	1.253856
3579	H	0.370913	2.389317	1.480155
3580	H	1.190363	3.036291	0.315901
3581	O	-3.861358	0.805665	1.533634
3582	H	-3.698253	-0.180479	1.563781
3583	H	-4.579109	1.010623	2.140208
3584	O	-0.429697	-1.337223	1.301914
3585	H	0.481219	-1.531197	1.588964
3586	H	-0.436436	-1.409458	0.320901
3587	O	1.317671	2.906922	-1.562033
3588	H	1.572384	3.627788	-2.145698
3589	H	2.051890	2.222703	-1.578363
3590	O	3.278838	1.167532	1.461930
3591	H	3.954411	1.546680	2.032617
3592	H	2.496168	1.794030	1.466372
3593	O	3.161864	1.083196	-1.369593
3594	H	2.845109	0.177900	-1.556263
3595	H	3.438676	1.077023	-0.435561
3596	O	2.341017	-1.428536	1.445849

3597	H	3.042983	-2.092191	1.332795
3598	H	2.762150	-0.560904	1.610690
3599	O	-3.198679	-1.720318	1.379681
3600	H	-2.247933	-1.806432	1.570951
3601	H	-3.316571	-1.989442	0.450208
3602	O	-1.126522	1.298186	1.399791
3603	H	-0.862608	0.356614	1.513262
3604	H	-2.068775	1.351066	1.644545
3605	O	3.988794	-3.080723	-0.035357
3606	H	4.409908	-3.920614	-0.235596
3607	H	3.486463	-2.801527	-0.819659
3608	O	-1.012279	1.428951	-1.322608
3609	H	-1.016903	1.485774	-0.340442
3610	H	-0.286447	2.007735	-1.624339
3611	O	-3.724733	0.752188	-1.282638
3612	H	-3.903995	0.964610	-0.348398
3613	H	-2.878102	1.180483	-1.502913

3614

3615 Cartesian coordinates of : W15_ 8

3616

3617	O	-2.788615	-2.115950	1.235428
3618	H	-1.828935	-1.914807	1.199649
3619	H	-3.020057	-2.266054	0.304964
3620	O	-0.087515	-1.158590	-1.869910
3621	H	0.768532	-1.622970	-1.935681
3622	H	0.051838	-0.206002	-2.133599
3623	O	1.729027	1.908116	1.728483
3624	H	1.862930	2.202576	0.808582
3625	H	0.771016	1.818751	1.865777
3626	O	3.858747	0.096711	-0.762511
3627	H	3.445980	-0.704703	-1.133967
3628	H	3.929504	-0.046616	0.199425
3629	O	3.496216	-0.021598	2.019139
3630	H	2.799446	0.691727	2.014457
3631	H	4.105439	0.173818	2.737224
3632	O	-3.739441	0.669880	-0.727956
3633	H	-3.872851	0.548559	0.229776
3634	H	-3.432704	-0.185242	-1.084285
3635	O	-0.298789	-1.056819	0.843407
3636	H	-0.223419	-1.048351	-0.138302
3637	H	-0.463619	-0.127498	1.104192
3638	O	-3.554004	0.242040	2.048035
3639	H	-3.342022	-0.716512	1.854225
3640	H	-4.201509	0.267488	2.758844
3641	O	-1.086642	1.519608	1.529149
3642	H	-1.926520	1.238343	1.937446
3643	H	-1.336972	2.021162	0.728502
3644	O	2.115871	-2.318822	1.205388
3645	H	2.703218	-1.675122	1.640108
3646	H	1.221642	-1.928769	1.283881
3647	O	2.447740	2.267887	-0.966662
3648	H	3.032118	1.452259	-0.959940
3649	H	2.978063	3.000019	-1.296387
3650	O	0.172840	1.417108	-2.332180
3651	H	-0.581089	1.888445	-1.933077
3652	H	0.977238	1.785934	-1.920297
3653	O	-2.695277	-1.798332	-1.621770
3654	H	-1.737159	-1.667192	-1.816674
3655	H	-3.081169	-2.230164	-2.390271
3656	O	2.432392	-2.267187	-1.373654
3657	H	2.340886	-2.405007	-0.382100
3658	H	2.841967	-3.055096	-1.744138
3659	O	-1.968422	2.546030	-0.919929
3660	H	-2.707089	1.867162	-0.937770
3661	H	-2.347725	3.403217	-1.136214

3662

3663 Cartesian coordinates of : W15_ 9

3664

3665	O	3.147452	-2.029494	1.304223
3666	H	3.157000	-1.041407	1.370437
3667	H	3.884425	-2.373028	1.817945
3668	O	0.096221	0.603087	2.109182
3669	H	-0.770906	0.708073	2.538096
3670	H	0.142442	-0.331942	1.799429
3671	O	-3.085653	0.564729	-2.079567

3672	H	-3.101448	-0.382323	-1.808247
3673	H	-3.831590	0.712395	-2.669113
3674	O	0.013789	2.426123	0.087585
3675	H	0.102961	1.802122	0.842537
3676	H	0.867440	2.900084	-0.002425
3677	O	-2.754835	2.145503	0.261898
3678	H	-1.876852	2.551355	0.149338
3679	H	-2.940365	1.649627	-0.555762
3680	O	2.477223	0.715142	-1.552501
3681	H	1.645942	0.800006	-2.046561
3682	H	2.767655	-0.215543	-1.683697
3683	O	-2.429318	-1.908638	1.374233
3684	H	-1.499108	-2.131003	1.556078
3685	H	-2.604605	-1.050120	1.807761
3686	O	-0.024190	-1.785389	-1.425366
3687	H	-0.927586	-2.119039	-1.559768
3688	H	-0.078313	-0.823721	-1.642741
3689	O	0.356784	-1.942604	1.227753
3690	H	1.258647	-2.238244	1.443869
3691	H	0.292605	-1.913706	0.241996
3692	O	-2.841648	-1.992251	-1.177094
3693	H	-2.733151	-1.962402	-0.174746
3694	H	-3.459188	-2.704040	-1.373642
3695	O	-0.280755	0.838842	-2.039251
3696	H	-1.182427	0.911446	-2.390364
3697	H	-0.224551	1.446756	-1.260264
3698	O	2.761728	0.617139	1.211597
3699	H	1.978047	0.787294	1.759447
3700	H	2.474480	0.685916	0.275557
3701	O	2.814667	-1.995470	-1.537239
3702	H	1.884398	-2.242581	-1.662740
3703	H	3.034811	-2.216925	-0.616772
3704	O	-2.680275	0.664881	2.417802
3705	H	-3.327057	0.939207	3.075095
3706	H	-2.786010	1.256068	1.617648
3707	O	2.660537	3.220031	-0.242268
3708	H	2.876702	2.559420	-0.921745
3709	H	3.121790	2.903202	0.545464

3710

3711 Cartesian coordinates of : W15_10

3712

3713	O	-2.646813	-2.755705	-0.041875
3714	H	-2.949650	-2.257096	-0.818042
3715	H	-2.966313	-2.299958	0.751580
3716	O	-0.039030	-0.313653	-2.170300
3717	H	-0.024899	0.663389	-1.988169
3718	H	-0.056512	-0.786056	-1.300564
3719	O	3.371016	0.620502	-0.030981
3720	H	3.210752	0.071287	0.758112
3721	H	3.163818	0.076768	-0.813178
3722	O	-2.055153	2.956105	0.085795
3723	H	-2.656531	3.705437	0.125319
3724	H	-2.603629	2.120847	0.074535
3725	O	0.003030	2.318571	-1.725388
3726	H	0.797038	2.624977	-1.251001
3727	H	-0.757051	2.652147	-1.216375
3728	O	0.091001	2.329349	1.791703
3729	H	0.854746	2.636395	1.269419
3730	H	-0.700093	2.633962	1.311109
3731	O	2.424176	-2.765906	-0.022462
3732	H	1.448996	-2.686252	-0.061615
3733	H	2.723185	-2.356912	-0.850800
3734	O	0.073438	-0.275379	2.240159
3735	H	0.973415	-0.574447	2.464431
3736	H	0.112681	0.708430	2.080426
3737	O	-0.130484	-1.831164	0.020042
3738	H	-1.002010	-2.295486	0.016856
3739	H	-0.104343	-1.253792	0.815910
3740	O	2.735413	-1.197666	2.051364
3741	H	2.700491	-1.896265	1.337308
3742	H	3.381653	-1.478973	2.706459
3743	O	2.150808	2.907363	-0.015709
3744	H	2.673621	2.052801	-0.020535
3745	H	2.777981	3.636178	-0.026890
3746	O	-2.686455	-0.876356	-2.204284

3747	H	-3.157139	-0.822162	-3.041660
3748	H	-1.732596	-0.687991	-2.385470
3749	O	-2.547084	-0.972788	2.216409
3750	H	-1.600760	-0.791509	2.413919
3751	H	-3.025482	-0.909291	3.049017
3752	O	2.585447	-0.960519	-2.245754
3753	H	1.637071	-0.730684	-2.405691
3754	H	3.034111	-0.952773	-3.096621
3755	O	-3.320367	0.680158	0.056590
3756	H	-3.071693	0.123710	0.816930
3757	H	-3.152407	0.170026	-0.757194

3758
3759 Cartesian coordinates of : W15_11

3760				
3761	O	3.891983	0.886104	-1.101529
3762	H	3.810938	0.947661	-0.088973
3763	H	4.695916	1.345622	-1.363405
3764	O	-2.391788	-1.651039	2.012821
3765	H	-2.680412	-2.262589	1.274476
3766	H	-2.804507	-1.960414	2.825032
3767	O	2.998408	-1.810255	1.535381
3768	H	2.033648	-1.819581	1.662874
3769	H	3.153930	-2.054079	0.609342
3770	O	-3.206901	0.857796	1.006316
3771	H	-2.653210	1.593697	1.323804
3772	H	-2.918800	0.034965	1.442331
3773	O	-1.510889	3.079710	1.279034
3774	H	-1.764475	3.950190	1.600053
3775	H	-1.417063	3.130141	0.283065
3776	O	0.589142	-1.273265	-1.228769
3777	H	1.460274	-1.665508	-1.415880
3778	H	0.455040	-1.329547	-0.253052
3779	O	-3.141993	0.879409	-1.605524
3780	H	-4.014010	1.055562	-1.973280
3781	H	-3.243252	0.832662	-0.610719
3782	O	-3.074893	-3.056756	-0.067774
3783	H	-2.908134	-3.994596	-0.196870
3784	H	-2.709976	-2.573845	-0.864243
3785	O	3.342489	-1.769259	-1.336461
3786	H	3.664952	-0.839393	-1.373808
3787	H	3.918124	-2.303122	-1.892565
3788	O	3.523432	0.864609	1.426463
3789	H	3.422525	-0.094600	1.625116
3790	H	2.670968	1.272733	1.659547
3791	O	-2.056105	-1.678861	-2.044133
3792	H	-1.093261	-1.584006	-1.926148
3793	H	-2.429500	-0.777715	-2.033727
3794	O	0.276299	-1.142091	1.464233
3795	H	0.372292	-0.171026	1.579291
3796	H	-0.611301	-1.389876	1.787997
3797	O	1.152269	1.404176	-1.351744
3798	H	0.907491	0.456525	-1.446364
3799	H	2.114755	1.439927	-1.496956
3800	O	0.802738	1.543629	1.371352
3801	H	0.892187	1.607000	0.394445
3802	H	0.093073	2.166724	1.611352
3803	O	-1.217932	2.893895	-1.309984
3804	H	-0.346228	2.517785	-1.526725
3805	H	-1.882058	2.246274	-1.613453

3806
3807 Cartesian coordinates of : W15_12

3808				
3809	O	3.766086	-0.282379	-2.240972
3810	H	4.397942	-0.512429	-2.928722
3811	H	3.846203	-0.953156	-1.507603
3812	O	1.381263	0.074452	1.906752
3813	H	2.323004	0.156693	2.147533
3814	H	1.303275	-0.725380	1.331214
3815	O	3.763151	1.826346	-0.381806
3816	H	2.861495	2.190039	-0.383469
3817	H	3.840254	1.258855	-1.170784
3818	O	1.012875	-0.097191	-1.906068
3819	H	1.042137	0.720919	-1.362658
3820	H	1.882933	-0.172872	-2.337173
3821	O	0.980911	1.954272	-0.078995

3822	H	1.079361	1.381659	0.711690
3823	H	0.071126	2.301541	-0.035194
3824	O	-4.333352	-2.312956	0.379978
3825	H	-4.542460	-1.545675	-0.210880
3826	H	-4.820687	-3.072745	0.050302
3827	O	3.789132	-1.849366	-0.123194
3828	H	4.012518	-1.279420	0.634698
3829	H	2.897652	-2.198420	0.045454
3830	O	0.994934	-1.917576	0.134344
3831	H	0.932048	-1.362745	-0.676083
3832	H	0.097648	-2.254632	0.312094
3833	O	-4.528677	2.342391	-0.114835
3834	H	-4.802462	3.161135	-0.537423
3835	H	-3.569917	2.411145	0.063846
3836	O	-1.817388	1.930025	0.248313
3837	H	-1.746367	1.466612	1.102594
3838	H	-1.810412	1.217423	-0.431234
3839	O	-1.229772	0.272186	2.495764
3840	H	-0.250675	0.251786	2.560411
3841	H	-1.587361	0.338366	3.386949
3842	O	-4.567408	-0.218120	-1.253825
3843	H	-3.695212	-0.154558	-1.675269
3844	H	-4.736071	0.662807	-0.869415
3845	O	4.125307	0.280443	1.703589
3846	H	4.876842	0.508360	2.259220
3847	H	4.073622	0.944269	0.958079
3848	O	-1.746835	-0.177641	-1.508266
3849	H	-0.916920	-0.209213	-2.012225
3850	H	-1.687210	-0.875971	-0.818479
3851	O	-1.719962	-1.852573	0.660069
3852	H	-2.640685	-2.206708	0.620607
3853	H	-1.693738	-1.226194	1.405132

3854

3855 Cartesian coordinates of : W15_13

3856

3857	O	1.412454	1.794220	-1.205571
3858	H	0.664213	1.383958	-1.677684
3859	H	1.158271	2.732318	-1.103209
3860	H	-1.657108	0.227590	-2.291665
3861	O	-0.849930	0.363815	-1.777166
3862	H	-0.579247	-0.557517	-1.537643
3863	H	-0.479430	-2.653626	-0.547028
3864	O	-0.253195	-2.225281	-1.392144
3865	H	0.711935	-2.334394	-1.505038
3866	H	3.115028	-2.940481	-1.684609
3867	O	2.525565	-2.317862	-1.248372
3868	H	2.963881	-1.413641	-1.291081
3869	H	2.970727	0.762084	-1.426413
3870	O	3.603858	0.044868	-1.245019
3871	H	4.013353	0.278977	-0.388932
3872	H	-1.696020	-2.368206	1.345027
3873	O	-1.044320	-3.085047	1.157632
3874	H	-1.404796	-3.914103	1.485980
3875	H	-3.269752	-0.391476	1.096227
3876	O	-2.431411	-0.844643	1.332542
3877	H	-1.889250	-0.187556	1.811272
3878	H	-2.598086	-2.081877	-1.951074
3879	O	-3.067515	-1.370281	-1.497322
3880	H	-2.613580	-1.278234	-0.642615
3881	H	0.736109	-2.439917	1.450718
3882	O	1.581347	-1.969307	1.364149
3883	H	2.014392	-2.299807	0.556672
3884	O	-0.873903	1.189505	2.408161
3885	H	0.066625	1.038888	2.097235
3886	H	-0.848292	1.506768	3.315761
3887	H	1.476823	-0.317577	1.301493
3888	O	1.447745	0.676725	1.348176
3889	H	1.406755	1.028089	0.431687
3890	H	3.290790	0.900501	1.608508
3891	O	4.226404	0.828339	1.341072
3892	H	4.677900	1.621258	1.643102
3893	H	-1.476519	1.476687	-0.498034
3894	O	-1.900141	2.193662	0.019857
3895	H	-1.642938	2.025432	0.946275
3896	H	-0.828260	3.590381	-0.454805

3897	O	-0.021449	4.085908	-0.703715
3898	H	-0.294745	4.875747	-1.177874
3899	O	-4.340253	0.657273	0.085203
3900	H	-4.396349	0.166877	-0.747111
3901	H	-3.714490	1.387705	-0.065011
3902				
3903	Cartesian coordinates of : W15_14			
3904				
3905	O	-4.840001	-1.521135	-0.685421
3906	H	-4.786342	-1.161411	0.237328
3907	H	-5.589331	-2.121887	-0.733710
3908	O	-4.394996	-0.105535	1.524113
3909	H	-3.475164	-0.215589	1.815426
3910	H	-4.385680	0.678375	0.943367
3911	H	-3.361976	1.471475	-1.081789
3912	O	-4.295669	1.379320	-0.834177
3913	H	-4.621112	0.576122	-1.265114
3914	H	-0.764124	-0.722978	1.778652
3915	O	-1.594231	-0.471517	1.332289
3916	H	-1.775803	-1.163636	0.669127
3917	H	-1.352900	0.727788	-0.004310
3918	O	-1.463642	1.272259	-0.815802
3919	H	-0.624392	1.232413	-1.310235
3920	H	-2.089004	-0.737029	-1.501186
3921	O	-2.151123	-1.631137	-1.132588
3922	H	-3.108087	-1.836564	-1.109824
3923	H	-0.262437	-2.158174	-1.003044
3924	O	0.648122	-1.872558	-0.822979
3925	H	0.725076	-1.675551	0.139211
3926	H	1.854575	-1.481177	2.046250
3927	O	1.064618	-0.986280	1.737769
3928	H	1.344415	-0.058840	1.602002
3929	H	0.983260	-0.326891	-1.474843
3930	O	1.113702	0.637212	-1.642164
3931	H	1.991152	0.736457	-2.051136
3932	H	3.583284	-2.271042	0.969324
3933	O	3.374709	-2.361688	1.925501
3934	H	4.195807	-2.279569	2.417258
3935	H	3.677103	-1.164645	-1.158868
3936	O	3.482040	-2.035872	-0.773842
3937	H	2.575531	-2.256861	-1.038276
3938	H	4.591275	0.664617	-2.538978
3939	O	3.893643	0.587026	-1.880859
3940	H	4.124698	1.178056	-1.124427
3941	H	-1.242401	3.632516	1.613254
3942	O	-0.637471	3.347309	0.921829
3943	H	-1.163680	2.860191	0.263707
3944	H	0.847650	2.281722	1.101036
3945	O	1.526350	1.612084	0.882616
3946	H	1.346421	1.340801	-0.045693
3947	H	4.457485	2.967766	0.437401
3948	O	4.156574	2.058698	0.350858
3949	H	3.243702	2.018059	0.710937
3950				
3951				
3952	Cartesian coordinates of the water hexamer			
3953				
3954	Cartesian coordinates of : W16_1			
3955				
3956	O	-1.489233	1.526042	1.172281
3957	O	-1.282616	-1.187794	1.519976
3958	O	1.288587	1.584431	1.095128
3959	O	1.491408	1.103431	-1.590151
3960	O	1.287369	-1.586414	-1.098138
3961	O	1.491202	-1.105268	1.586995
3962	O	-1.491796	-1.529389	-1.176130
3963	O	-1.282562	1.184527	-1.524063
3964	O	4.264148	1.290611	-1.530203
3965	O	4.087690	1.487724	1.085220
3966	O	4.264286	-1.288982	1.533147
3967	O	4.087343	-1.485877	-1.082512
3968	H	1.301653	1.533348	0.112402
3969	H	0.402724	1.897572	1.344836
3970	H	-0.400304	-1.415366	1.858720
3971	H	-1.287749	-1.429639	0.565779

3972	H	1.300334	-1.535426	-0.115415
3973	H	0.401980	-1.900547	-1.348160
3974	H	-1.286265	1.425964	-0.569766
3975	H	-0.400726	1.412399	-1.863785
3976	H	-1.456677	0.575741	1.424483
3977	H	-2.401215	1.820641	1.348029
3978	H	1.455985	-0.123916	1.536138
3979	H	1.455664	0.122122	-1.539615
3980	H	-1.458119	-0.579268	-1.428762
3981	H	-2.404685	-1.822263	-1.349862
3982	H	3.180378	-1.732292	-1.332243
3983	H	4.243001	-0.591733	-1.437551
3984	H	4.277586	-1.462153	0.550256
3985	H	4.243616	0.593672	1.440355
3986	H	3.179959	1.732957	1.333462
3987	H	4.277316	1.463775	-0.547238
3988	H	2.406799	1.334062	-1.831546
3989	H	2.406118	-1.335901	1.830139
3990	H	4.955329	1.820735	-1.938124
3991	H	4.955511	-1.818959	1.941195
3992	H	-3.175428	-1.254967	1.784882
3993	O	-4.082101	-1.014674	1.527718
3994	H	-4.234639	-1.412014	0.650627
3995	H	-4.294576	0.607960	1.435655
3996	O	-4.273910	1.584890	1.230405
3997	H	-4.965130	2.014117	1.743449
3998	O	-4.082580	1.018053	-1.523611
3999	H	-3.176045	1.256739	-1.782747
4000	H	-4.233094	1.415966	-0.646444
4001	O	-4.277397	-1.581336	-1.226178
4002	H	-4.296776	-0.604295	-1.431073
4003	H	-4.971224	-2.008858	-1.737144

4004

4005 Cartesian coordinates of : W16_ 2

4006

4007	O	1.291806	-1.410095	1.314168
4008	H	1.298002	-1.500627	0.334358
4009	H	0.406337	-1.678021	1.613380
4010	O	4.256637	-1.493724	-1.343714
4011	H	4.271367	-1.522381	-0.345725
4012	H	4.951697	-2.072283	-1.671398
4013	O	-1.482461	1.321622	-1.414508
4014	H	-1.453808	0.342864	-1.505688
4015	H	-2.395087	1.589922	-1.625534
4016	O	-1.291765	1.410031	1.314120
4017	H	-0.406297	1.677956	1.613340
4018	H	-1.297968	1.500563	0.334311
4019	O	1.291759	1.410044	-1.313904
4020	H	0.406271	1.677933	-1.613102
4021	H	1.297983	1.500574	-0.334094
4022	O	4.087981	1.317733	-1.271969
4023	H	3.181340	1.524635	-1.556612
4024	H	4.247875	0.385400	-1.506515
4025	O	-4.088018	1.317741	1.271765
4026	H	-4.247922	0.385405	1.506295
4027	H	-3.181435	1.524675	1.556560
4028	O	1.482447	-1.321683	-1.414471
4029	H	2.395073	-1.589964	-1.625522
4030	H	1.453783	-0.342925	-1.505640
4031	O	-4.256693	-1.493694	1.343516
4032	H	-4.951806	-2.072210	1.671152
4033	H	-4.271373	-1.522345	0.345527
4034	O	-1.482492	-1.321710	1.414660
4035	H	-2.395157	-1.589963	1.625582
4036	H	-1.453809	-0.342956	1.505853
4037	O	4.256687	1.493762	1.343461
4038	H	4.951732	2.072374	1.671073
4039	H	4.271340	1.522405	0.345471
4040	O	-4.088039	-1.317680	-1.271936
4041	H	-4.247925	-0.385350	-1.506497
4042	H	-3.181425	-1.524620	-1.556628
4043	O	-4.256632	1.493778	-1.343685
4044	H	-4.271329	1.522433	-0.345696
4045	H	-4.951645	2.072409	-1.671344
4046	O	1.482507	1.321648	1.414710

4047	H	2.395179	1.589917	1.625585
4048	H	1.453834	0.342894	1.505907
4049	O	4.088077	-1.317677	1.271756
4050	H	3.181513	-1.524641	1.556587
4051	H	4.247973	-0.385339	1.506285
4052	O	-1.291800	-1.410109	-1.313964
4053	H	-0.406312	-1.677999	-1.613157
4054	H	-1.298017	-1.500644	-0.334154
4055				
4056	Cartesian coordinates of : W16_ 3			
4057				
4058	O	-1.495378	1.938826	0.008293
4059	O	-4.270186	1.999058	-0.157216
4060	O	-4.092927	0.016551	1.837128
4061	O	-1.287690	-0.003211	1.920787
4062	O	-1.287481	0.004179	-1.920000
4063	O	-4.092710	-0.016719	-1.837545
4064	O	-4.272382	-1.999307	0.156604
4065	O	-1.497224	-1.937775	-0.007728
4066	H	-2.405121	2.282620	-0.045411
4067	H	-1.478692	1.325049	0.776769
4068	H	-3.186207	0.078311	2.182703
4069	H	-4.248250	0.825202	1.315626
4070	H	-3.185863	-0.078693	-2.182533
4071	H	-4.248863	-0.825304	-1.316217
4072	H	-2.406807	-2.281979	0.045750
4073	H	-1.480433	-1.324109	-0.776214
4074	H	-4.970223	2.630815	-0.347128
4075	H	-0.402816	0.039482	2.320719
4076	H	-0.402164	-0.038246	-2.320125
4077	H	-4.972396	-2.631058	0.346381
4078	H	-4.281013	1.299040	-0.868421
4079	H	-1.288979	-0.786209	1.324800
4080	H	-4.282375	-1.299808	0.867874
4081	H	-1.288572	0.787151	-1.323988
4082	H	0.403494	2.321666	-0.038662
4083	O	1.288793	1.921487	0.003408
4084	H	1.289991	1.325298	0.786236
4085	H	1.479808	0.777504	-1.324699
4086	O	1.496621	0.008795	-1.938183
4087	H	2.406466	-0.045349	-2.281653
4088	H	1.288086	-1.323479	-0.786730
4089	O	1.286524	-1.919701	-0.003935
4090	H	0.401227	-2.319896	0.038016
4091	H	2.405765	0.045611	2.281885
4092	O	1.496121	-0.007122	1.937895
4093	H	1.478547	-0.775787	1.324429
4094	H	3.184398	-2.182956	0.078621
4095	O	4.091567	-1.838443	0.017302
4096	H	4.247143	-1.316858	0.825883
4097	H	4.972127	-0.348894	-2.629386
4098	O	4.271498	-0.158716	-1.998358
4099	H	4.281371	-0.869877	-1.298228
4100	H	3.187743	2.182614	-0.079318
4101	O	4.094008	1.836020	-0.017083
4102	H	4.249412	1.314192	-0.825510
4103	H	4.281528	0.867226	1.298419
4104	O	4.270850	0.156194	1.998682
4105	H	4.971649	0.345793	2.629695
4106				
4107	Cartesian coordinates of : W16_ 4			
4108				
4109	O	-1.494340	1.393214	1.336749
4110	H	-1.462590	1.499110	0.359336
4111	H	-2.406041	1.610087	1.603217
4112	O	1.494340	-1.393214	1.336749
4113	H	2.406041	-1.610087	1.603217
4114	H	1.462590	-1.499110	0.359336
4115	O	4.084168	1.354654	1.222870
4116	H	4.239689	0.431387	1.494659
4117	H	3.177935	1.573807	1.499615
4118	O	1.285222	1.322831	1.398947
4119	H	0.402966	1.622071	1.676096
4120	H	1.292103	0.342948	1.494551
4121	O	1.285222	-1.322831	-1.398947

4122	H	0.402966	-1.622071	-1.676096
4123	H	1.292103	-0.342948	-1.494551
4124	O	-4.084168	1.354654	-1.222870
4125	H	-4.239689	0.431387	-1.494659
4126	H	-3.177935	1.573807	-1.499615
4127	O	-4.279656	-1.451220	-1.390508
4128	H	-4.299229	-1.505538	-0.393618
4129	H	-4.976682	-2.016590	-1.736432
4130	O	4.279656	1.451220	-1.390508
4131	H	4.976682	2.016590	-1.736432
4132	H	4.299229	1.505538	-0.393618
4133	O	4.279656	-1.451220	1.390508
4134	H	4.299229	-1.505538	0.393618
4135	H	4.976682	-2.016590	1.736432
4136	O	-4.084168	-1.354654	1.222870
4137	H	-4.239689	-0.431387	1.494659
4138	H	-3.177935	-1.573807	1.499615
4139	O	1.494340	1.393214	-1.336749
4140	H	1.462590	1.499110	-0.359336
4141	H	2.406041	1.610087	-1.603217
4142	O	-1.494340	-1.393214	-1.336749
4143	H	-2.406041	-1.610087	-1.603217
4144	H	-1.462590	-1.499110	-0.359336
4145	O	-4.279656	1.451220	1.390508
4146	H	-4.299229	1.505538	0.393618
4147	H	-4.976682	2.016590	1.736432
4148	O	4.084168	-1.354654	-1.222870
4149	H	4.239689	-0.431387	-1.494659
4150	H	3.177935	-1.573807	-1.499615
4151	O	-1.285222	1.322831	-1.398947
4152	H	-0.402966	1.622071	-1.676096
4153	H	-1.292103	0.342948	-1.494551
4154	O	-1.285222	-1.322831	1.398947
4155	H	-1.292103	-0.342948	1.494551
4156	H	-0.402966	-1.622071	1.676096

4157

4158 Cartesian coordinates of : W16_ 5

4159

4160	O	-0.012247	1.334786	-1.428423
4161	H	-0.133902	0.370209	-1.569385
4162	H	-0.866642	1.768281	-1.618999
4163	O	2.611109	-2.278001	1.492167
4164	H	3.010175	-2.924582	2.082218
4165	H	3.199000	-1.465539	1.485282
4166	O	-4.108362	0.054253	-1.223427
4167	H	-3.627523	0.868823	-1.459339
4168	H	-4.314458	0.132080	-0.273624
4169	O	-2.564060	2.405669	-1.347201
4170	H	-2.544342	2.451543	-0.343039
4171	H	-2.872195	3.254509	-1.679293
4172	O	0.027179	-1.319778	1.396896
4173	H	0.890313	-1.732525	1.599640
4174	H	0.128872	-0.352795	1.540527
4175	O	4.087771	-0.152441	1.234654
4176	H	3.703369	0.713699	1.464340
4177	H	4.301099	-0.107423	0.284013
4178	O	-2.633644	-2.131009	1.357692
4179	H	-1.688588	-1.956960	1.527716
4180	H	-2.705044	-2.397808	0.423653
4181	O	2.432335	-2.222820	-1.336281
4182	H	1.497741	-2.024768	-1.534937
4183	H	2.462589	-2.474896	-0.395815
4184	O	-2.863751	-2.225202	-1.463549
4185	H	-3.326880	-2.844311	-2.035609
4186	H	-3.368869	-1.360754	-1.470461
4187	O	2.654103	2.130775	-1.252282
4188	H	1.731375	1.946294	-1.508901
4189	H	3.179936	1.355377	-1.525881
4190	O	2.828666	2.359226	1.329055
4191	H	3.217556	3.182111	1.640494
4192	H	2.803544	2.385928	0.325796
4193	O	0.210586	1.403127	1.301239
4194	H	0.197857	1.438503	0.316723
4195	H	1.052408	1.817184	1.567962
4196	O	-2.449411	2.243319	1.238969

4197	H	-1.533936	2.030783	1.499538
4198	H	-3.012761	1.497954	1.521858
4199	O	-4.091120	0.014799	1.584711
4200	H	-4.795195	-0.076765	2.233781
4201	H	-3.552456	-0.830523	1.591412
4202	O	4.098339	-0.234776	-1.569215
4203	H	3.465096	-1.011720	-1.575727
4204	H	4.801722	-0.422938	-2.197740
4205	O	-0.228956	-1.386532	-1.316452
4206	H	-1.085156	-1.779575	-1.572572
4207	H	-0.202995	-1.412567	-0.332040

4208
4209 Cartesian coordinates of : W16_ 6

4211	O	0.006672	1.345608	1.400691
4212	H	-0.190302	1.420251	-0.345552
4213	H	0.860330	1.783603	1.585870
4214	O	-4.102229	-0.023251	1.568362
4215	H	-4.812171	0.073425	2.210272
4216	H	-3.569072	0.825911	1.566565
4217	O	2.541266	2.442901	1.311839
4218	H	2.832513	3.301306	1.634346
4219	H	2.526376	2.474515	0.306709
4220	O	4.102273	0.023321	-1.568274
4221	H	3.569119	-0.825840	-1.566501
4222	H	4.812247	-0.073359	-2.210147
4223	O	-2.856235	2.180380	-1.504537
4224	H	-3.357886	1.313970	-1.502289
4225	H	-3.319583	2.789689	-2.086944
4226	O	-2.441337	-2.242967	1.271012
4227	H	-1.529622	-2.020563	1.536069
4228	H	-3.012243	-1.497366	1.538069
4229	O	2.441304	2.242991	-1.271027
4230	H	1.529609	2.020527	-1.536102
4231	H	3.012257	1.497415	-1.538048
4232	O	2.856275	-2.180348	1.504561
4233	H	3.357885	-1.313914	1.502339
4234	H	3.319620	-2.789636	2.086997
4235	O	2.658409	-2.127905	-1.321086
4236	H	1.713977	-1.962045	-1.503279
4237	H	2.720976	-2.379074	-0.382120
4238	O	-4.097547	-0.098787	-1.239119
4239	H	-3.614284	-0.916321	-1.458926
4240	H	-4.311354	-0.163406	-0.289961
4241	O	0.210509	-1.375989	1.328790
4242	H	0.125589	0.382237	1.553930
4243	H	1.070008	-1.754894	1.595093
4244	O	-2.658334	2.127941	1.321110
4245	H	-1.713907	1.961984	1.503247
4246	H	-2.720922	2.379104	0.382144
4247	O	4.097511	0.098868	1.239205
4248	H	3.614236	0.916400	1.458993
4249	H	4.311351	0.163488	0.290055
4250	O	-0.006669	-1.345755	-1.400792
4251	H	0.190309	-1.420400	0.345458
4252	H	-0.860340	-1.783731	-1.585956
4253	O	-2.541361	-2.442865	-1.311857
4254	H	-2.526448	-2.474475	-0.306729
4255	H	-2.832771	-3.301222	-1.634346
4256	O	-0.210500	1.375856	-1.328884
4257	H	-1.069983	1.754805	-1.595174
4258	H	-0.125579	-0.382385	-1.554035

4259
4260 Cartesian coordinates of : W16_ 7

4261				
4262	O	-2.569184	2.099626	1.580262
4263	H	-2.687139	1.317903	2.144292
4264	H	-3.158037	1.972707	0.813166
4265	O	2.580704	1.607925	-2.156668
4266	H	3.179676	0.851004	-2.028156
4267	H	2.683255	2.173384	-1.373971
4268	O	-0.063356	-1.716920	-0.835834
4269	H	0.006686	-0.836487	-1.281124
4270	H	-0.915361	-2.102294	-1.118832
4271	O	-2.592231	0.408514	-2.520035

4272	H	-1.652177	0.664260	-2.444919
4273	H	-2.619428	-0.559203	-2.419890
4274	O	2.581755	-2.496788	-0.469622
4275	H	1.643128	-2.394013	-0.716818
4276	H	2.620461	-2.393541	0.497182
4277	O	2.410584	2.761550	0.475993
4278	H	1.470194	2.539801	0.684756
4279	H	2.582172	3.649941	0.803208
4280	O	0.057190	-0.874581	1.722446
4281	H	0.931255	-1.144813	2.070226
4282	H	-0.029022	-1.283689	0.826341
4283	O	0.033489	0.811538	-1.760553
4284	H	-0.055264	1.257214	-0.891134
4285	H	0.919286	1.088893	-2.095081
4286	O	-3.981994	-1.204572	0.471870
4287	H	-3.481208	-1.074109	1.297234
4288	H	-4.242390	-0.315024	0.167432
4289	O	3.944583	0.504923	1.142166
4290	H	4.222954	0.207201	0.255772
4291	H	3.454728	1.338511	1.012566
4292	O	4.152343	-0.618115	-1.403840
4293	H	4.897348	-0.975102	-1.896533
4294	H	3.564517	-1.382925	-1.141495
4295	O	-0.026040	1.746777	0.838400
4296	H	-0.931534	2.045031	1.106670
4297	H	0.083377	0.865592	1.254552
4298	O	-4.125114	1.353924	-0.638415
4299	H	-4.865417	1.851271	-0.999018
4300	H	-3.542108	1.075015	-1.405815
4301	O	-2.682213	-2.253971	-1.538790
4302	H	-3.205756	-1.949295	-0.742948
4303	H	-3.107795	-3.040533	-1.893012
4304	O	2.685612	-1.508553	2.192517
4305	H	3.188479	-0.700601	1.872053
4306	H	3.140601	-1.852465	2.967068
4307	O	-2.410716	-0.531061	2.722058
4308	H	-1.473197	-0.739686	2.497430
4309	H	-2.585592	-0.875691	3.603157

4310

4311 Cartesian coordinates of : W16_ 8

4312

4313	O	-4.146619	1.145863	1.259770
4314	H	-4.167443	1.125069	0.262344
4315	H	-4.924539	1.620115	1.567699
4316	O	2.918229	1.038486	2.217571
4317	H	3.336411	1.460611	2.974412
4318	H	2.222430	1.670157	1.870505
4319	O	4.236245	-0.022861	0.031838
4320	H	4.069877	-0.978445	0.144632
4321	H	3.887498	0.414702	0.834611
4322	O	-0.889145	-1.283764	-1.375678
4323	H	-0.996589	-0.317143	-1.517302
4324	H	-1.765294	-1.682113	-1.533832
4325	O	-3.591895	-1.910900	-1.249478
4326	H	-3.611758	-1.893263	-0.246951
4327	H	-4.144607	-2.638252	-1.550293
4328	O	-3.943526	0.876192	-1.350854
4329	H	-3.077057	1.216691	-1.633872
4330	H	-3.929814	-0.083689	-1.520462
4331	O	-0.750272	-1.175758	1.399645
4332	H	-0.659658	-1.336901	0.438364
4333	H	0.127044	-1.374978	1.813902
4334	O	1.316127	2.667015	-1.627931
4335	H	1.566250	3.489353	-2.060638
4336	H	1.986765	1.984868	-1.877336
4337	O	-1.376585	1.418477	1.298433
4338	H	-2.318781	1.523782	1.522589
4339	H	-1.145811	0.467104	1.455457
4340	O	3.180118	-2.588125	0.128751
4341	H	3.578297	-3.457778	0.027266
4342	H	2.602224	-2.416971	-0.669879
4343	O	1.730406	-1.546547	2.323396
4344	H	2.154664	-0.675505	2.415628
4345	H	2.254585	-2.038922	1.667632
4346	O	3.062483	0.679679	-2.136811

4347	H	3.561667	0.449908	-1.283866
4348	H	3.717934	0.746783	-2.839082
4349	O	1.760878	-1.863948	-1.940398
4350	H	0.793347	-1.783311	-1.829635
4351	H	2.089852	-0.979851	-2.177636
4352	O	-1.203117	1.433221	-1.403556
4353	H	-1.247050	1.533418	-0.423061
4354	H	-0.427515	1.941009	-1.698211
4355	O	-3.485449	-1.600366	1.336224
4356	H	-2.544150	-1.608038	1.595144
4357	H	-3.814367	-0.703295	1.524899
4358	O	1.111730	2.637570	1.225111
4359	H	0.193792	2.355072	1.398402
4360	H	1.194962	2.735958	0.260307

4361

4362 Cartesian coordinates of : W16_ 9

4363

4364	O	-2.560247	1.120226	-1.253408
4365	H	-2.085497	1.933463	-1.500297
4366	H	-2.620955	1.129534	-0.275602
4367	O	4.031876	0.839030	-1.134040
4368	H	4.188376	0.960480	-0.179712
4369	H	3.172125	1.256064	-1.324911
4370	O	-1.710826	-1.466815	-1.587616
4371	H	-0.785828	-1.647600	-1.828695
4372	H	-1.808699	-0.491437	-1.597669
4373	O	-2.019565	-1.911582	1.079951
4374	H	-1.986048	-1.879865	0.095815
4375	H	-2.932604	-2.129851	1.325594
4376	O	3.509584	-1.893950	1.255956
4377	H	3.663088	-2.068066	0.309299
4378	H	2.554395	-2.012092	1.404965
4379	O	-0.828185	2.801352	1.394222
4380	H	-1.570812	2.222638	1.640019
4381	H	-0.020811	2.312569	1.638147
4382	O	3.801173	-1.731993	-1.541189
4383	H	4.438215	-2.124744	-2.145488
4384	H	3.993434	-0.752900	-1.471660
4385	O	-4.762861	-1.207578	1.265629
4386	H	-4.797007	-1.130449	0.281263
4387	H	-5.633677	-1.486258	1.563927
4388	O	-0.815317	3.300627	-1.185436
4389	H	-0.832437	3.243296	-0.189126
4390	H	-0.873848	4.228147	-1.433218
4391	O	4.101179	0.614538	1.673197
4392	H	4.790711	0.784251	2.322071
4393	H	3.967473	-0.374733	1.605116
4394	O	-4.483183	-0.926002	-1.397967
4395	H	-4.105874	-0.044090	-1.558833
4396	H	-3.798187	-1.529784	-1.722996
4397	O	-2.723429	0.729907	1.484238
4398	H	-2.260000	-0.134048	1.461766
4399	H	-3.638310	0.469570	1.679615
4400	O	1.060506	-1.258447	-1.535827
4401	H	1.949592	-1.601486	-1.743148
4402	H	1.125268	-0.279784	-1.584859
4403	O	1.366200	1.074654	1.507756
4404	H	1.093999	0.130909	1.546648
4405	H	2.306394	1.098278	1.767752
4406	O	1.299483	1.456586	-1.194875
4407	H	1.264414	1.415398	-0.212169
4408	H	0.662794	2.145186	-1.458023
4409	O	0.731125	-1.565714	1.166610
4410	H	-0.147029	-1.895072	1.423951
4411	H	0.747242	-1.546228	0.182846

4412

4413 Cartesian coordinates of : W16_10

4414

4415	O	2.910816	-2.367595	-1.321772
4416	H	2.003684	-2.129026	-1.582721
4417	H	3.472341	-1.603997	-1.548345
4418	O	-4.466731	-2.235416	1.371422
4419	H	-3.617877	-1.777158	1.546932
4420	H	-5.130042	-1.820497	1.930632
4421	O	-2.313438	-0.635532	-1.403998

4422	H	-2.489659	0.308038	-1.590011
4423	H	-3.133123	-1.151840	-1.569588
4424	O	3.001751	-2.601126	1.289744
4425	H	2.994544	-2.633699	0.290800
4426	H	3.329960	-3.444204	1.616384
4427	O	0.607394	-1.193384	1.419667
4428	H	1.333627	-1.816647	1.606024
4429	H	0.976140	-0.288188	1.534050
4430	O	4.320774	0.068833	-1.377609
4431	H	4.367984	0.081565	-0.379419
4432	H	5.188511	0.296879	-1.724023
4433	O	-2.434411	1.984221	1.358201
4434	H	-2.349558	1.025011	1.524641
4435	H	-2.696307	2.066788	0.423181
4436	O	-4.574138	-2.125905	-1.350123
4437	H	-4.661177	-2.239423	-0.378200
4438	H	-4.661502	-2.997688	-1.746221
4439	O	0.388857	-1.174821	-1.325327
4440	H	-0.546941	-1.113797	-1.597357
4441	H	0.380965	-1.255390	-0.345914
4442	O	1.767024	1.168752	-1.408320
4443	H	2.694138	0.964319	-1.629500
4444	H	1.257803	0.334320	-1.525954
4445	O	4.136969	-0.023821	1.237294
4446	H	3.858363	-0.930011	1.462141
4447	H	3.411787	0.563736	1.515292
4448	O	-2.136225	-0.803684	1.315840
4449	H	-2.128548	-0.780795	0.330569
4450	H	-1.244027	-1.092972	1.583170
4451	O	-0.204966	3.312299	1.570286
4452	H	-0.283469	4.069971	2.157625
4453	H	-1.080222	2.822466	1.581370
4454	O	-2.527882	2.124998	-1.463515
4455	H	-3.087709	2.649878	-2.044101
4456	H	-1.615255	2.537943	-1.472747
4457	O	-0.152038	3.186647	-1.252755
4458	H	0.596835	2.606129	-1.481142
4459	H	-0.045757	3.422645	-0.313418
4460	O	1.683752	1.304341	1.323263
4461	H	1.132398	2.050903	1.625730
4462	H	1.712026	1.364289	0.341733

4463

4464 Cartesian coordinates of : W16_11

4465

4466	O	2.899019	0.834377	-2.099270
4467	H	3.608645	0.734476	-1.427444
4468	H	2.413735	-0.008417	-2.036146
4469	O	2.942041	0.978168	2.156859
4470	H	3.255034	1.328716	2.996366
4471	H	2.259601	1.625299	1.796881
4472	O	-1.350584	1.285290	1.374398
4473	H	-2.289693	1.427758	1.594454
4474	H	-1.172027	0.329412	1.521412
4475	O	3.862335	-2.652593	-0.121233
4476	H	4.432256	-3.378300	-0.392610
4477	H	3.163192	-2.545907	-0.795629
4478	O	-0.874577	-1.409916	1.363280
4479	H	0.026660	-1.637082	1.653178
4480	H	-0.888423	-1.505450	0.384395
4481	O	1.906022	-1.466841	1.543245
4482	H	2.643671	-2.084391	1.421993
4483	H	2.278415	-0.636159	1.909586
4484	O	-3.675327	-1.534987	1.393828
4485	H	-2.743299	-1.708174	1.612986
4486	H	-3.799971	-1.820183	0.469985
4487	O	4.557534	0.160585	-0.024663
4488	H	4.141431	0.487937	0.791453
4489	H	4.513446	-0.808340	0.007862
4490	O	-1.189232	1.337348	-1.346149
4491	H	-1.204283	1.417343	-0.365994
4492	H	-0.422892	1.864633	-1.646476
4493	O	-1.097647	-1.382447	-1.363592
4494	H	-1.988069	-1.719168	-1.573357
4495	H	-1.127804	-0.408405	-1.508516
4496	O	1.137368	2.564109	1.201316

4497	H	0.230459	2.261624	1.388095
4498	H	1.192451	2.728792	0.239440
4499	O	1.652419	-1.543777	-1.246019
4500	H	0.742205	-1.729829	-1.538692
4501	H	1.578087	-1.301821	-0.301197
4502	O	-3.857543	-1.719498	-1.414126
4503	H	-4.505356	-2.147542	-1.981784
4504	H	-3.990631	-0.730316	-1.476802
4505	O	1.208806	2.697156	-1.591476
4506	H	1.913202	2.009650	-1.829302
4507	H	1.390955	3.493358	-2.100071
4508	O	-3.949373	0.893676	-1.345067
4509	H	-4.129953	1.150807	-0.422537
4510	H	-3.064831	1.242542	-1.557045
4511	O	-4.119744	1.045156	1.466517
4512	H	-4.043308	0.050795	1.527466
4513	H	-4.825034	1.329893	2.055276

4514

4515 Cartesian coordinates of : W16_12

4516

4517	O	-3.451373	1.321609	1.235661
4518	H	-3.657536	1.356652	0.283681
4519	H	-3.444910	0.376565	1.479561
4520	O	-3.506402	-1.454358	1.489896
4521	H	-4.134523	-1.909464	2.058902
4522	H	-2.640829	-1.960029	1.529571
4523	O	-1.386400	2.870150	1.547875
4524	H	-1.608637	3.601624	2.132068
4525	H	-2.177782	2.254541	1.525160
4526	O	3.800479	-1.386583	1.512043
4527	H	4.456108	-1.739606	2.120953
4528	H	3.891440	-0.392693	1.499470
4529	O	3.807567	1.220926	1.234618
4530	H	2.916642	1.558381	1.436135
4531	H	3.966067	1.410716	0.292672
4532	O	-1.289250	-2.932897	-1.489278
4533	H	-2.085148	-2.325292	-1.520545
4534	H	-1.484796	-3.691010	-2.048391
4535	O	-3.380802	-1.387051	-1.315523
4536	H	-3.358737	-0.443776	-1.562124
4537	H	-3.636128	-1.418153	-0.375329
4538	O	1.016682	-1.203134	1.410597
4539	H	0.989826	-1.241609	0.425139
4540	H	1.926564	-1.458420	1.652357
4541	O	-1.275294	-2.781886	1.352523
4542	H	-1.178334	-3.035187	0.416820
4543	H	-0.459784	-2.299725	1.588184
4544	O	3.557420	-1.509709	-1.323049
4545	H	3.842567	-0.603973	-1.531964
4546	H	3.792497	-1.653381	-0.389735
4547	O	1.022280	1.527369	1.410035
4548	H	0.213095	2.021438	1.648479
4549	H	0.878836	0.578665	1.616286
4550	O	-1.282411	2.843981	-1.291027
4551	H	-1.242303	3.059756	-0.341655
4552	H	-0.430809	2.417893	-1.503216
4553	O	0.898112	-1.292528	-1.301779
4554	H	1.823584	-1.572883	-1.492715
4555	H	0.245030	-1.961269	-1.584354
4556	O	-3.443275	1.404170	-1.574662
4557	H	-4.064589	1.845996	-2.161492
4558	H	-2.602543	1.947058	-1.565130
4559	O	3.793585	1.328622	-1.588591
4560	H	4.220361	1.902398	-2.231905
4561	H	2.815420	1.475021	-1.642712
4562	O	1.143974	1.420950	-1.304086
4563	H	0.910523	0.483535	-1.476428
4564	H	1.119708	1.499194	-0.319766

4565

4566 Cartesian coordinates of : W16_13

4567

4568	O	2.999768	-2.257908	-1.451449
4569	H	3.530924	-1.409650	-1.426820
4570	H	3.464489	-2.883285	-2.015372
4571	O	2.703991	2.202051	1.323891

4572	H	1.777016	2.032700	1.570231
4573	H	3.224044	1.426594	1.609130
4574	O	0.053376	-1.311547	1.367456
4575	H	-0.845284	-1.602344	1.598387
4576	H	0.058746	-0.335923	1.484136
4577	O	2.859904	2.392228	-1.261692
4578	H	2.828066	2.426891	-0.258242
4579	H	3.227986	3.223482	-1.576997
4580	O	0.378680	-1.362339	-1.382132
4581	H	1.238059	-1.767109	-1.607051
4582	H	0.288608	-1.445264	-0.408540
4583	O	0.280151	1.391593	-1.426916
4584	H	1.145005	1.814774	-1.591882
4585	H	0.397823	0.425885	-1.565242
4586	O	-2.498327	1.434830	-1.392606
4587	H	-2.568259	1.579233	-0.426887
4588	H	-1.610179	1.734143	-1.652800
4589	O	4.304394	-0.023927	-1.129069
4590	H	4.484747	0.030243	-0.172406
4591	H	3.859703	0.810653	-1.365282
4592	O	-5.217710	-0.112570	1.324104
4593	H	-5.239058	-0.066753	0.339929
4594	H	-6.128097	-0.192137	1.623888
4595	O	4.214832	-0.113548	1.677796
4596	H	4.903182	-0.252750	2.335322
4597	H	3.644228	-0.936379	1.651190
4598	O	-2.722126	-1.424949	1.200600
4599	H	-2.681583	-1.530104	0.221366
4600	H	-3.659977	-1.441117	1.450746
4601	O	2.695156	-2.208214	1.359856
4602	H	1.749989	-2.032652	1.520788
4603	H	2.779513	-2.455468	0.421400
4604	O	-2.753906	1.320864	1.366152
4605	H	-3.673544	1.451442	1.638820
4606	H	-2.659465	0.341128	1.378284
4607	O	-4.927893	-0.054392	-1.376975
4608	H	-4.431067	-0.838002	-1.656908
4609	H	-4.361449	0.688657	-1.640049
4610	O	0.018130	1.437496	1.286215
4611	H	0.036451	1.505766	0.302550
4612	H	-0.861908	1.733413	1.572295
4613	O	-2.398851	-1.315005	-1.494306
4614	H	-1.521501	-1.655401	-1.738437
4615	H	-2.313756	-0.337968	-1.542947

4616

4617 Cartesian coordinates of : W16_14

4618

4619	O	3.394639	-2.162216	-0.145484
4620	O	3.107394	2.177641	0.669244
4621	O	0.424086	1.813812	1.542179
4622	O	0.703429	-2.250914	0.507739
4623	O	1.042400	-0.675112	2.615994
4624	O	2.518803	-0.743398	-2.386012
4625	O	2.503484	1.842713	-2.086154
4626	O	-0.048154	1.661094	-1.072199
4627	O	-0.181215	-0.987484	-1.697076
4628	H	1.579733	-0.999971	-2.382277
4629	H	2.941846	-1.263077	-1.674515
4630	H	0.403220	-1.750857	-0.290492
4631	H	1.618478	-2.529326	0.309061
4632	H	0.184766	1.676897	-0.104928
4633	H	0.763807	1.915532	-1.555070
4634	H	2.997533	2.178797	-0.297415
4635	H	2.236278	2.383374	1.044962
4636	H	3.583840	-1.442778	0.540033
4637	H	4.140265	-2.770171	-0.150237
4638	H	-0.276851	-0.029053	-1.499712
4639	H	-1.057225	-1.336049	-1.951605
4640	H	2.599981	0.856330	-2.240694
4641	H	2.923766	2.299943	-2.820767
4642	H	0.623444	0.967671	1.989647
4643	H	-0.497710	2.045840	1.798792
4644	H	0.624832	-1.011731	3.414606
4645	H	0.837411	-1.300281	1.871792
4646	H	2.915083	-0.419430	2.230388

4647	O	3.664590	-0.314889	1.621303
4648	H	3.586084	0.601975	1.269108
4649	H	-1.122223	-2.767895	0.810245
4650	O	-2.084762	-2.642400	0.767820
4651	H	-2.319956	-2.631096	-0.178018
4652	O	-3.328247	-0.527176	1.756512
4653	H	-2.801982	-1.323887	1.476054
4654	H	-3.956204	-0.822681	2.423425
4655	H	-2.541548	2.431732	0.930047
4656	O	-2.259935	2.112902	1.802667
4657	H	-2.617321	1.212014	1.890220
4658	O	-2.771199	-1.937278	-1.872998
4659	H	-3.263001	-2.395355	-2.561054
4660	H	-3.299479	-1.134480	-1.591231
4661	O	-3.981280	0.143931	-0.887952
4662	H	-3.937366	0.000558	0.075520
4663	H	-3.579856	1.015610	-1.057662
4664	O	-2.565929	2.564537	-1.017451
4665	H	-1.615148	2.355827	-1.182391
4666	H	-2.779329	3.379917	-1.480882

4667

4668 Cartesian coordinates of : W16_15

4669

4670	O	-3.121113	-1.432154	1.445118
4671	H	-3.370501	-1.376216	0.505212
4672	H	-2.275731	-1.914524	1.479743
4673	O	3.868714	0.980964	0.068579
4674	H	3.473125	0.434142	0.810659
4675	H	4.810104	0.782219	0.039809
4676	O	2.780593	-0.455247	1.957619
4677	H	2.620818	-1.376348	1.671265
4678	H	1.929373	-0.105715	2.272304
4679	O	2.147604	-2.979720	0.949941
4680	H	2.096117	-2.877353	-0.055041
4681	H	2.628539	-3.789825	1.143626
4682	O	-0.417010	-2.021702	1.253059
4683	H	0.382641	-2.573969	1.340632
4684	H	-0.169540	-1.116281	1.557784
4685	O	-2.403550	2.509327	0.275295
4686	H	-2.603583	2.028209	1.100816
4687	H	-1.433609	2.634159	0.264424
4688	O	0.120756	0.487044	2.110684
4689	H	0.230117	1.127322	1.364841
4690	H	-0.714242	0.726237	2.550075
4691	O	2.723851	3.447395	-0.068273
4692	H	3.018566	4.107519	0.565343
4693	H	3.295260	2.658290	0.034366
4694	O	1.859200	-2.605326	-1.580749
4695	H	0.910186	-2.598350	-1.787221
4696	H	2.190787	-1.722220	-1.866030
4697	O	0.315415	2.197849	0.054404
4698	H	0.241879	1.670274	-0.773757
4699	H	1.122159	2.754879	0.000299
4700	O	-2.982887	1.363485	-1.955062
4701	H	-2.813432	1.825088	-1.070776
4702	H	-3.531037	1.953924	-2.481890
4703	O	-2.635776	0.895280	2.551177
4704	H	-3.196479	1.063805	3.314546
4705	H	-2.896240	0.007406	2.173689
4706	O	-3.588750	-1.201051	-1.355638
4707	H	-3.473932	-0.261436	-1.636429
4708	H	-4.400883	-1.528624	-1.754177
4709	O	-0.849319	-1.861261	-1.402791
4710	H	-0.732118	-1.928544	-0.425024
4711	H	-1.804452	-1.913129	-1.571323
4712	O	-0.209225	0.687907	-2.134465
4713	H	-0.392577	-0.243596	-1.870302
4714	H	-1.074303	1.040779	-2.401740
4715	O	2.544712	-0.052829	-2.238482
4716	H	1.726092	0.426288	-2.439459
4717	H	2.981175	0.405912	-1.499586

4718

4719 Cartesian coordinates of : W16_16

4720

4721	O	2.574821	-2.172508	1.399928
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4722	H	2.634126	-2.459965	0.472152
4723	H	1.630274	-1.979184	1.549306
4724	O	-2.563076	-1.438337	-1.326813
4725	H	-2.565874	-0.481630	-1.119308
4726	H	-2.683430	-1.898772	-0.477748
4727	O	-2.725210	-2.142551	1.415059
4728	H	-3.311857	-1.333295	1.512497
4729	H	-3.111333	-2.856485	1.931051
4730	O	0.258997	1.426538	-1.467626
4731	H	1.119709	1.828753	-1.692913
4732	H	0.196300	1.476112	-0.487150
4733	O	4.134108	-0.024399	-1.160153
4734	H	3.650586	-0.843761	-1.368344
4735	H	4.357774	-0.074456	-0.212283
4736	O	-0.083076	-1.368088	1.174420
4737	H	-0.035121	-1.408781	0.195748
4738	H	-0.961672	-1.722345	1.419768
4739	O	2.905505	2.259168	-1.492279
4740	H	3.402600	1.392790	-1.471864
4741	H	3.401634	2.870482	-2.044943
4742	O	-2.523826	1.364365	-1.261580
4743	H	-2.540477	1.837637	-0.408886
4744	H	-1.666073	1.582676	-1.664484
4745	O	0.155838	-1.279447	-1.602501
4746	H	-0.783217	-1.506678	-1.769282
4747	H	0.229602	-0.301139	-1.704228
4748	O	-2.441398	2.260249	1.389277
4749	H	-1.486235	2.032171	1.516323
4750	H	-2.607567	3.108412	1.811468
4751	O	2.569836	2.164100	1.352543
4752	H	2.758275	2.407882	0.429725
4753	H	3.188601	1.443459	1.571423
4754	O	2.573832	-2.383377	-1.440967
4755	H	2.793677	-3.102332	-2.041323
4756	H	1.653506	-2.091828	-1.644624
4757	O	4.183893	-0.131437	1.638248
4758	H	4.897245	-0.285911	2.264809
4759	H	3.576062	-0.925090	1.661645
4760	O	-5.062419	0.125662	-1.271266
4761	H	-4.430786	0.786596	-1.597051
4762	H	-4.714504	-0.710960	-1.611246
4763	O	-4.160638	0.009145	1.382153
4764	H	-4.618683	0.092266	0.520281
4765	H	-3.643074	0.823007	1.512473
4766	O	0.038532	1.359583	1.279321
4767	H	0.955503	1.684490	1.472295
4768	H	0.028673	0.386536	1.412611

4769

4770 Cartesian coordinates of : W16_17

4771

4772	O	3.277537	1.493021	1.456809
4773	H	3.498308	1.812465	0.564125
4774	H	2.307895	1.533122	1.543476
4775	O	-3.914621	-2.101849	-0.913100
4776	H	-4.189695	-1.185419	-1.178618
4777	H	-4.541906	-2.729665	-1.283776
4778	O	-3.181979	-1.307292	1.697838
4779	H	-3.436346	-1.809913	0.902895
4780	H	-2.207347	-1.362357	1.772205
4781	O	-4.071644	1.066988	1.391319
4782	H	-3.719837	0.131783	1.578340
4783	H	-4.794201	1.233482	2.004967
4784	O	-0.453335	-1.163298	1.309929
4785	H	-0.646932	-1.309455	0.356396
4786	H	0.361693	-1.691063	1.487250
4787	O	3.865601	1.748168	-1.301047
4788	H	4.514867	2.264680	-1.787283
4789	H	4.122342	0.783509	-1.362308
4790	O	0.471443	1.359209	1.226971
4791	H	0.120299	0.442042	1.356466
4792	H	-0.287492	1.955410	1.339248
4793	O	4.306667	-0.831467	-1.239639
4794	H	4.428841	-1.045619	-0.295387
4795	H	3.513009	-1.308722	-1.534372
4796	O	-4.280951	0.476057	-1.372380

4797	H	-3.487402	0.865239	-1.774731
4798	H	-4.337541	0.845629	-0.472737
4799	O	1.914064	-2.412948	1.150999
4800	H	1.931396	-2.186569	0.202509
4801	H	2.732379	-2.040050	1.518903
4802	O	1.150243	1.232331	-1.401375
4803	H	0.967450	1.352411	-0.441320
4804	H	2.036398	1.604356	-1.567010
4805	O	4.278990	-0.935107	1.560461
4806	H	5.013304	-1.022734	2.175307
4807	H	3.927017	-0.004966	1.629927
4808	O	1.582859	-1.492493	-1.504735
4809	H	0.727404	-1.871980	-1.757083
4810	H	1.411659	-0.525134	-1.486528
4811	O	-1.592633	1.379299	-1.626142
4812	H	-1.658859	1.881767	-0.792054
4813	H	-0.674516	1.506166	-1.926950
4814	O	-1.999374	2.672372	0.858891
4815	H	-2.787935	2.172942	1.181898
4816	H	-2.219419	3.609025	0.882756
4817	O	-1.239149	-1.384072	-1.300803
4818	H	-2.092477	-1.851629	-1.326170
4819	H	-1.442099	-0.440095	-1.462299
4820				
4821	Cartesian coordinates of : W16_18			
4822				
4823	O	3.372348	1.952821	-0.648731
4824	H	3.703174	1.181022	-1.140109
4825	H	3.488164	1.736201	0.292267
4826	O	-2.021550	2.660786	1.243442
4827	H	-2.654650	1.915647	1.225661
4828	H	-1.229407	2.356439	1.713294
4829	O	3.349953	-1.518287	0.812169
4830	H	3.671625	-1.350827	-0.092158
4831	H	2.539691	-2.048523	0.718001
4832	O	-2.818825	0.748281	-1.873180
4833	H	-3.264978	0.710430	-1.008907
4834	H	-2.371194	1.609058	-1.900171
4835	O	0.731169	1.739016	-0.881008
4836	H	1.670161	2.043309	-0.912086
4837	H	0.115504	2.423633	-1.207141
4838	O	-1.722706	-3.271099	-0.589288
4839	H	-2.084704	-4.111397	-0.886915
4840	H	-1.712619	-2.639415	-1.382956
4841	O	-3.794189	0.567127	0.777895
4842	H	-3.481739	-0.348262	1.042839
4843	H	-4.720792	0.638943	1.026841
4844	O	0.684810	-2.430718	0.492481
4845	H	-0.035608	-2.989977	0.141166
4846	H	0.326621	-2.017392	1.303150
4847	O	-0.387823	-1.041853	2.627705
4848	H	-0.109716	-0.127782	2.338885
4849	H	-0.121954	-1.156491	3.545218
4850	O	0.456741	1.297423	1.772707
4851	H	0.480053	1.405351	0.790381
4852	H	1.397082	1.316448	2.037456
4853	O	3.700773	-0.615935	-1.825505
4854	H	2.724083	-0.734806	-1.963921
4855	H	4.159911	-0.943448	-2.604605
4856	O	-2.843435	-1.750073	1.471462
4857	H	-2.562125	-2.344081	0.747976
4858	H	-2.048120	-1.571464	2.003399
4859	O	3.194504	0.838830	1.978201
4860	H	3.839550	0.911319	2.688512
4861	H	3.245651	-0.091480	1.620649
4862	O	1.064829	-0.802246	-1.712781
4863	H	0.923343	-1.325450	-0.893682
4864	H	0.831434	0.125869	-1.480842
4865	O	-1.499556	3.234297	-1.268019
4866	H	-1.729675	3.143472	-0.302182
4867	H	-1.738957	4.120298	-1.554826
4868	O	-1.542475	-1.579314	-2.508385
4869	H	-2.042486	-0.746651	-2.346757
4870	H	-0.603877	-1.322449	-2.511766
4871				

4872 Cartesian coordinates of : W16_19

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4873
4874  O      2.682594      0.122455      1.305039
4875  H      2.703065      0.083687      0.318484
4876  H      2.145220      0.930472      1.496350
4877  O     -4.150374     -1.431942     -1.469873
4878  H     -4.183389     -0.435366     -1.541672
4879  H     -4.819123     -1.799716     -2.055261
4880  O     -4.017670     -1.234712      1.338322
4881  H     -4.154772     -1.518285      0.415809
4882  H     -3.102969     -1.478101      1.567319
4883  O     -4.234478      1.369699      1.383207
4884  H     -4.250114      0.372243      1.453439
4885  H     -4.930834      1.723618      1.944281
4886  O     -1.223786     -1.359432      1.378119
4887  H     -1.217479     -1.460790      0.398845
4888  H     -0.388292     -1.746228      1.697809
4889  O      2.743612     -0.051811     -1.408918
4890  H      3.695411     -0.204806     -1.593608
4891  H      2.244873     -0.903080     -1.496957
4892  O      1.174367      2.348039      1.317833
4893  H      1.236408      2.561065      0.371419
4894  H      0.233328      2.179862      1.500207
4895  O      5.448831     -0.247842     -1.364743
4896  H      5.587955     -0.117887     -0.401997
4897  H      6.005207     -0.982695     -1.637986
4898  O     -3.986776      1.178324     -1.417584
4899  H     -4.164082      1.457924     -0.500730
4900  H     -3.068994      1.439772     -1.611305
4901  O      1.416435     -2.191748      1.664081
4902  H      1.920190     -1.336175      1.666236
4903  H      1.868328     -2.799985      2.256783
4904  O      1.432464      2.270831     -1.550852
4905  H      1.833293      2.920778     -2.136242
4906  H      1.966324      1.440724     -1.620289
4907  O      5.424793      0.149987      1.343271
4908  H      5.827309      0.923979      1.748049
4909  H      4.461581      0.201553      1.521203
4910  O      1.281128     -2.270413     -1.208159
4911  H      0.343273     -2.130433     -1.428346
4912  H      1.312784     -2.469065     -0.256809
4913  O     -1.194939      1.353792     -1.343755
4914  H     -1.233975      1.451923     -0.364591
4915  H     -0.355317      1.759617     -1.626747
4916  O     -1.452299      1.364419      1.362596
4917  H     -2.382101      1.582671      1.558199
4918  H     -1.351636      0.399598      1.525753
4919  O     -1.370111     -1.373220     -1.340575
4920  H     -2.286051     -1.612338     -1.573125
4921  H     -1.285735     -0.405950     -1.498582
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4922 Cartesian coordinates of : W16_20

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4924
4925  O      2.827281     -1.134032     -1.626327
4926  H      2.864195     -0.236195     -1.991315
4927  H      1.995644     -1.513772     -1.962056
4928  O     -2.869853      0.479236      0.233939
4929  H     -2.808618      1.126124     -0.498056
4930  H     -2.766582      0.954352      1.082401
4931  O     -2.063705      2.135873     -1.792714
4932  H     -1.387368      1.613367     -2.322007
4933  H     -2.577069      2.642690     -2.429875
4934  O     -0.736700      3.297941      0.435852
4935  H     -1.252961      3.042755     -0.349514
4936  H     -1.168178      2.885111      1.205135
4937  O      1.446459      1.803748      0.107831
4938  H      0.899189      0.979909      0.050328
4939  H      0.756356      2.501378      0.247728
4940  O      0.417335     -2.242641      1.693028
4941  H      1.392135     -2.179363      1.489947
4942  H      0.034941     -2.966019      1.166857
4943  O      0.133657     -1.766026     -2.188553
4944  H     -0.198927     -2.652983     -1.986180
4945  H     -0.040888     -1.256709     -1.362229
4946  O      2.886936     -1.605213      1.089711
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4947	H	2.963501	-1.413884	0.129603
4948	H	3.017488	-0.766383	1.559803
4949	O	-3.325253	-2.203757	-0.157384
4950	H	-4.056714	-2.312505	-0.771847
4951	H	-3.243663	-1.243680	0.014420
4952	O	2.286396	1.574244	-2.403952
4953	H	2.838688	2.260713	-2.789492
4954	H	2.076260	1.826947	-1.470285
4955	O	0.040744	0.057091	3.280529
4956	H	0.024811	-0.864298	2.967410
4957	H	0.944219	0.379814	3.102659
4958	O	2.562985	0.945187	2.371265
4959	H	3.197841	1.497794	2.836729
4960	H	2.266911	1.425815	1.559124
4961	O	-1.854633	1.673900	2.482036
4962	H	-2.285214	1.995047	3.280675
4963	H	-1.131256	1.046046	2.780900
4964	O	-1.021310	-3.646456	-0.325634
4965	H	-1.221554	-4.586919	-0.283129
4966	H	-1.881861	-3.172947	-0.261044
4967	O	-0.303911	0.813333	-3.192099
4968	H	0.616026	1.107724	-3.052079
4969	H	-0.290832	-0.157377	-3.113042
4970	O	-0.225116	-0.301658	0.030117
4971	H	-1.159854	-0.030883	0.134545
4972	H	-0.027177	-0.977817	0.732742

4973

4974 Cartesian coordinates of : W16_21

4975

4976	O	2.218515	-2.442352	1.243870
4977	O	3.432627	-0.012759	2.073631
4978	O	2.994531	-0.136274	-2.181527
4979	O	2.285457	-2.705931	-1.353871
4980	O	-0.397418	-1.497841	1.483740
4981	O	0.728456	0.847885	2.187594
4982	O	0.349367	0.753480	-2.176382
4983	O	-0.314180	-1.662820	-1.202730
4984	H	2.671244	-1.643026	1.569592
4985	H	0.882811	1.372772	1.366007
4986	H	2.823748	-1.075382	-1.969269
4987	H	-0.315013	-1.633190	-0.213569
4988	H	1.288056	-2.363474	1.519517
4989	H	1.618580	0.630192	2.508018
4990	H	2.145084	0.235916	-2.477940
4991	H	0.423540	-2.243267	-1.459180
4992	H	2.702916	-3.524198	-1.639604
4993	H	-1.348285	-1.498910	1.705425
4994	H	4.179666	-0.044744	2.679538
4995	H	-0.455656	1.206531	-2.487334
4996	H	2.335035	-2.668288	-0.355198
4997	H	-0.052827	-0.613241	1.753704
4998	H	3.724009	0.478777	1.270882
4999	H	0.052121	-0.116663	-1.815929
5000	H	4.766374	1.710036	-0.516634
5001	O	3.934268	1.304849	-0.253102
5002	H	3.631617	0.717669	-1.014864
5003	H	2.222444	2.256798	-0.134583
5004	O	1.252850	2.218352	-0.089117
5005	H	0.961907	1.679793	-0.863577
5006	H	-2.776564	0.231237	-1.657562
5007	O	-2.925974	-0.659745	-1.279216
5008	H	-2.138376	-1.189932	-1.493277
5009	O	-3.042738	-0.741796	1.497426
5010	H	-3.897378	-1.191232	1.581820
5011	H	-2.971388	-0.596335	0.529648
5012	O	-1.969320	1.733821	2.313277
5013	H	-1.095271	1.468159	2.638486
5014	H	-2.479470	0.913603	2.188216
5015	H	-1.956164	2.372639	-1.307921
5016	O	-2.189457	1.865539	-2.150907
5017	H	-2.727301	2.444344	-2.699815
5018	H	-0.482943	3.135716	0.034643
5019	O	-1.450730	3.072473	0.000388
5020	H	-1.723695	2.642856	0.845068
5021	O	-5.093559	-1.871649	0.009574

5022	H	-4.551431	-1.527263	-0.720070
5023	H	-5.958952	-2.089736	-0.345422
5024				
5025	Cartesian coordinates of : W16_22			
5026				
5027	O	-2.192930	-2.487008	-1.448983
5028	H	-1.323567	-2.103235	-1.665657
5029	H	-2.123478	-2.763472	-0.518431
5030	O	2.798064	-0.362949	1.346678
5031	H	2.631036	0.584998	1.563171
5032	H	2.774740	-0.365677	0.364145
5033	O	5.423161	-1.132012	1.293854
5034	H	6.006942	-0.641137	1.879299
5035	H	4.502911	-0.869105	1.513892
5036	O	-0.721192	1.572966	1.400437
5037	H	-1.644101	1.752555	1.663582
5038	H	-0.708693	1.646140	0.419348
5039	O	-4.098747	-0.780360	1.221301
5040	H	-3.401503	-1.438760	1.391093
5041	H	-4.334176	-0.870911	0.279425
5042	O	0.195138	-1.070345	-1.313584
5043	H	0.214160	-1.116776	-0.333602
5044	H	1.127113	-0.970742	-1.585437
5045	O	-3.486337	1.741480	1.558183
5046	H	-3.751179	0.779060	1.538528
5047	H	-4.086280	2.200827	2.153386
5048	O	2.017101	2.230754	1.497834
5049	H	2.069644	2.522743	0.571928
5050	H	1.068322	2.219282	1.710539
5051	O	0.118125	-0.994732	1.464096
5052	H	1.079072	-0.960917	1.652997
5053	H	-0.217776	-0.073391	1.581329
5054	O	1.865977	2.513516	-1.366005
5055	H	0.905786	2.324300	-1.488929
5056	H	2.087920	3.263580	-1.926407
5057	O	-3.273753	1.791566	-1.302533
5058	H	-3.474032	1.965634	-0.366750
5059	H	-3.686836	0.933415	-1.509531
5060	O	-1.966219	-2.656471	1.387588
5061	H	-1.980722	-3.412126	1.983129
5062	H	-1.133571	-2.155676	1.557695
5063	O	-4.229730	-0.852901	-1.577324
5064	H	-4.915421	-1.163686	-2.176192
5065	H	-3.457717	-1.484008	-1.642479
5066	O	5.394781	-0.893678	-1.421305
5067	H	5.737862	-1.682697	-1.850366
5068	H	5.543799	-1.002629	-0.456146
5069	O	2.792431	-0.147523	-1.417541
5070	H	3.725377	-0.390617	-1.607986
5071	H	2.678975	0.810109	-1.559012
5072	O	-0.620672	1.548087	-1.341918
5073	H	-1.586607	1.706727	-1.494521
5074	H	-0.449574	0.593067	-1.488265

5075

5076 Cartesian coordinates of : W16_23

5077

5078	O	-0.586807	2.764610	-0.171905
5079	H	-0.885160	2.662781	0.748939
5080	H	-0.071551	1.945142	-0.375471
5081	O	-0.749354	-2.577553	0.739384
5082	H	-0.492893	-1.811809	1.299482
5083	H	-0.019943	-3.220284	0.820868
5084	O	-1.692530	1.863489	2.324070
5085	H	-1.863094	2.386811	3.113500
5086	H	-2.540094	1.440701	2.055421
5087	O	-3.353693	-1.710151	0.207696
5088	H	-3.284569	-1.544959	-0.750849
5089	H	-2.562097	-2.213946	0.470391
5090	O	-2.987054	1.690505	-1.230770
5091	H	-3.406718	1.509115	-0.372089
5092	H	-2.172177	2.189920	-1.031158
5093	O	2.328939	-2.419227	-1.601965
5094	H	1.481744	-2.154224	-1.997447
5095	H	2.827114	-1.603348	-1.414760
5096	O	0.116885	-0.275730	1.919759

5097	H	-0.460761	0.385297	2.335227
5098	H	0.338060	0.085756	1.028251
5099	O	1.795319	-3.697913	0.640198
5100	H	2.174798	-4.581332	0.672191
5101	H	2.039746	-3.296123	-0.239605
5102	O	2.736749	-1.327112	1.920026
5103	H	2.516658	-2.240466	1.668148
5104	H	1.900715	-0.934355	2.222301
5105	O	-2.920295	-0.675810	-2.372401
5106	H	-2.914885	0.266381	-2.042402
5107	H	-3.485719	-0.711100	-3.149996
5108	O	3.299837	-0.054885	-0.414338
5109	H	3.745851	0.816003	-0.391581
5110	H	3.284543	-0.433904	0.494754
5111	O	1.736441	4.234669	-0.542382
5112	H	1.651504	4.753513	-1.347826
5113	H	0.857908	3.833996	-0.378185
5114	O	3.975763	2.608894	-0.362473
5115	H	3.173330	3.166581	-0.434650
5116	H	4.572053	3.065028	0.237773
5117	O	-3.842758	0.608246	1.256075
5118	H	-4.738761	0.597913	1.607226
5119	H	-3.642376	-0.323109	0.930154
5120	O	0.730505	0.501496	-0.586918
5121	H	1.715772	0.363418	-0.606478
5122	H	0.322275	-0.191842	-1.153189
5123	O	-0.369901	-1.628453	-1.823647
5124	H	-1.211784	-1.390236	-2.252791
5125	H	-0.593852	-2.057918	-0.969425
5126				
5127	Cartesian coordinates of : W16_24			
5128				
5129	O	2.293329	-2.608675	-1.072767
5130	H	1.433360	-2.140062	-1.180121
5131	H	2.198849	-3.487054	-1.455715
5132	H	2.460913	-2.390728	0.916829
5133	O	2.367797	-1.917577	1.757364
5134	H	3.082323	-1.247355	1.760788
5135	O	0.004402	-0.723902	1.540280
5136	H	0.814959	-1.230222	1.807950
5137	H	-0.811853	-1.305172	1.712504
5138	H	3.603430	-1.396057	-1.412625
5139	O	4.111540	-0.559854	-1.464249
5140	H	4.900581	-0.728430	-1.988940
5141	H	3.499865	0.911076	1.423725
5142	O	4.125523	0.175027	1.340016
5143	H	4.306082	0.069475	0.393039
5144	O	1.652436	1.586650	1.208188
5145	H	1.150634	2.417226	1.314137
5146	H	1.067987	0.863845	1.499619
5147	H	0.793365	-0.149044	-1.371593
5148	O	0.187584	-0.881643	-1.107559
5149	H	0.111502	-0.811011	-0.111919
5150	O	1.917640	1.186450	-1.464540
5151	H	1.946075	1.377381	-0.498781
5152	H	2.777869	0.797283	-1.698161
5153	H	-1.202135	0.789883	1.617325
5154	O	-1.825013	1.452912	1.271741
5155	H	-1.389122	2.321961	1.354984
5156	O	-0.165415	3.654050	0.910464
5157	H	-0.208535	4.585233	1.148511
5158	H	-0.159211	3.579069	-0.085740
5159	H	-1.982101	1.132761	-0.436903
5160	O	-1.971038	0.936300	-1.403408
5161	H	-1.297139	0.235710	-1.487039
5162	H	-0.875736	2.468586	-1.798605
5163	O	-0.146559	3.099492	-1.655684
5164	H	0.665221	2.610393	-1.873054
5165	H	-2.923857	-1.539451	1.751433
5166	O	-2.134759	-2.116515	1.682661
5167	H	-2.185862	-2.491608	0.781318
5168	H	-3.621203	0.573280	1.426156
5169	O	-4.141980	-0.241537	1.365029
5170	H	-4.384766	-0.345111	0.430640
5171	H	-3.508746	0.104875	-1.661247

5172	O	-4.200500	-0.575946	-1.507693
5173	H	-4.907840	-0.441035	-2.145722
5174	H	-1.424665	-2.092789	-1.392443
5175	O	-2.194034	-2.585173	-1.073209
5176	H	-2.977868	-2.083377	-1.353409
5177				
5178	Cartesian coordinates of : W16_25			
5179				
5180	O	-1.770035	-0.920294	1.359149
5181	H	-2.598784	-1.344199	1.664536
5182	H	-1.811594	-0.944518	0.378183
5183	O	1.768268	0.918146	1.359677
5184	H	2.596942	1.342068	1.665278
5185	H	1.810068	0.942713	0.378691
5186	O	2.175414	-4.076900	1.172555
5187	H	1.717866	-3.248959	1.422758
5188	H	2.928169	-4.174514	1.762475
5189	O	0.870220	-1.669230	1.408492
5190	H	1.294444	-0.802266	1.580773
5191	H	-0.083914	-1.551484	1.597092
5192	O	-0.871495	1.667949	1.409349
5193	H	-1.295778	0.801072	1.581547
5194	H	0.082553	1.549548	1.598119
5195	O	1.668399	0.870517	-1.408900
5196	H	0.801779	1.295068	-1.581820
5197	H	1.549910	-0.083553	-1.597426
5198	O	2.176435	-4.195123	-1.564761
5199	H	2.268908	-4.288524	-0.593667
5200	H	1.786508	-5.012105	-1.888326
5201	O	-0.919355	1.769119	-1.359575
5202	H	-0.943516	1.810931	-0.378626
5203	H	-1.342274	2.598150	-1.665317
5204	O	-1.669517	-0.870689	-1.409517
5205	H	-0.802999	-1.295393	-1.582530
5206	H	-1.550797	0.083434	-1.597738
5207	O	0.918627	-1.770497	-1.359808
5208	H	0.942875	-1.813381	-0.378926
5209	H	1.342618	-2.598737	-1.666562
5210	O	-2.173853	4.077451	1.172431
5211	H	-1.721063	3.247412	1.424426
5212	H	-2.928621	4.178474	1.759260
5213	O	-2.168461	4.199933	-1.564621
5214	H	-1.776784	5.016120	-1.888048
5215	H	-2.262656	4.293789	-0.593755
5216	O	4.078720	2.172344	-1.171047
5217	H	3.249498	1.718291	-1.423138
5218	H	4.180524	2.925082	-1.760354
5219	O	-4.080285	-2.172176	-1.173074
5220	H	-4.180989	-2.925577	-1.761737
5221	H	-3.250874	-1.718102	-1.424533
5222	O	4.195621	2.173648	1.565617
5223	H	4.290921	2.265696	0.594691
5224	H	5.010850	1.781470	1.890879
5225	O	-4.198353	-2.174195	1.564276
5226	H	-4.292711	-2.266188	0.593248
5227	H	-5.013871	-1.781834	1.888606
5228				
5229				
5230	Cartesian coordinates of the water heptadecamer			
5231				
5232	Cartesian coordinates of : W17_1			
5233				
5234	O	0.075583	-0.002006	-0.087261
5235	H	0.753442	0.549565	-0.534142
5236	H	-0.542975	-0.293591	-0.792066
5237	O	1.985099	1.401775	-1.511283
5238	H	2.341227	2.016556	-0.840708
5239	H	2.663336	0.712916	-1.651086
5240	O	-1.492076	-0.758380	-2.211853
5241	H	-2.412812	-0.794347	-1.884726
5242	H	-1.165216	-1.676688	-2.266779
5243	O	1.366365	-1.686728	1.624011
5244	H	0.763568	-1.900795	2.356695
5245	H	0.822907	-1.164887	0.993025
5246	O	-1.200254	0.800233	2.178941

5247	H	-0.738022	0.483984	1.371221
5248	H	-1.210189	0.036224	2.781032
5249	O	2.554309	2.681361	0.863525
5250	H	3.099655	3.425537	1.136891
5251	H	1.608205	2.891281	1.132979
5252	O	-0.399734	-3.204075	-1.572601
5253	H	0.566657	-3.100681	-1.318307
5254	H	-0.493201	-4.085953	-1.946651
5255	O	-3.764083	-0.750498	-0.679941
5256	H	-3.664456	0.138644	-0.210344
5257	H	-4.701547	-0.905152	-0.829381
5258	O	-1.578173	3.154123	-0.823674
5259	H	-1.171873	2.649758	-1.589980
5260	H	-1.867686	4.004163	-1.171045
5261	O	-3.337005	1.464419	0.552286
5262	H	-2.844784	2.116223	0.016888
5263	H	-2.745399	1.257280	1.303099
5264	O	-1.995175	-2.468618	0.661640
5265	H	-1.427024	-2.801259	-0.057155
5266	H	-2.693737	-1.926547	0.250597
5267	O	0.076760	3.160109	1.450210
5268	H	-0.479535	3.227939	0.649485
5269	H	-0.337508	2.470913	1.999723
5270	O	3.714568	-0.734711	-1.204325
5271	H	3.740416	-0.451836	-0.239918
5272	H	4.620027	-0.885179	-1.493330
5273	O	-1.035681	-1.873928	3.041291
5274	H	-1.461544	-2.168918	2.192971
5275	H	-1.397471	-2.408878	3.753697
5276	O	-0.476826	1.810161	-2.771524
5277	H	-0.834649	0.905377	-2.814547
5278	H	0.469436	1.723038	-2.556958
5279	O	3.482612	0.053457	1.253032
5280	H	2.798177	-0.523240	1.644146
5281	H	3.151510	0.970609	1.285601
5282	O	2.050439	-2.976395	-0.738504
5283	H	2.628972	-2.267245	-1.075519
5284	H	1.948273	-2.787213	0.212817

5285
5286 Cartesian coordinates of : W17_2

5287				
5288	O	-4.049076	-2.206063	0.155570
5289	H	-3.106825	-2.440754	0.224621
5290	H	-4.239034	-1.648258	0.932614
5291	O	1.294867	-0.283631	-1.874650
5292	H	1.280350	-0.987409	-1.187126
5293	H	0.396147	-0.249976	-2.247740
5294	O	-1.490945	0.052155	1.922840
5295	H	-1.441371	-0.749020	1.355027
5296	H	-2.392258	0.045827	2.292776
5297	O	-4.433618	1.378134	-0.093414
5298	H	-3.547774	1.782832	-0.168276
5299	H	-4.528731	0.802232	-0.872776
5300	O	1.439370	-2.008703	0.249318
5301	H	2.321492	-2.422736	0.260281
5302	H	1.436915	-1.305460	0.936331
5303	O	1.299366	0.185020	1.882317
5304	H	0.395725	0.233942	2.242352
5305	H	1.385570	0.903807	1.221526
5306	O	-4.247309	-0.707636	-1.992998
5307	H	-4.241367	-1.357244	-1.233524
5308	H	-4.872907	-1.025083	-2.651319
5309	O	4.102609	-0.630019	-1.827989
5310	H	4.382875	0.201336	-1.404959
5311	H	3.200320	-0.487454	-2.161213
5312	O	0.101982	3.904628	-0.185974
5313	H	0.876395	3.312961	-0.286343
5314	H	0.153560	4.578669	-0.869515
5315	O	-1.502977	-0.152458	-1.911329
5316	H	-2.402727	-0.327148	-2.243686
5317	H	-1.568996	0.664861	-1.365865
5318	O	1.874658	1.849880	-0.262472
5319	H	2.849471	1.908533	-0.230518
5320	H	1.651893	1.168963	-0.937709
5321	O	-1.292821	-1.994016	0.101492

5322	H	-0.398495	-2.372993	0.157306
5323	H	-1.306395	-1.417057	-0.695509
5324	O	-1.718339	1.887931	-0.125126
5325	H	-1.529948	1.391563	0.698639
5326	H	-1.163242	2.697125	-0.141441
5327	O	-4.287845	-0.122845	2.047807
5328	H	-4.433076	0.507833	1.284814
5329	H	-4.976377	0.037933	2.700048
5330	O	4.098071	-0.232451	1.895450
5331	H	4.177660	-1.110541	1.480765
5332	H	3.178823	-0.135873	2.198065
5333	O	4.166768	-2.407264	0.109712
5334	H	4.775246	-3.142636	-0.008238
5335	H	4.221072	-1.818967	-0.693794
5336	O	4.598431	1.465498	-0.025941
5337	H	4.500790	0.874749	0.775222
5338	H	5.339680	2.060164	0.122275

5339

5340 Cartesian coordinates of : W17_ 3

5341

5342	O	3.869819	-0.513164	-2.051108
5343	H	3.916774	0.439166	-1.847418
5344	H	2.922484	-0.737047	-2.062723
5345	O	-1.638179	-1.109745	-1.555362
5346	H	-2.513825	-1.381608	-1.884035
5347	H	-1.603385	-1.385011	-0.611233
5348	O	-4.222266	-1.839377	0.911665
5349	H	-4.476574	-0.994422	1.326650
5350	H	-3.296886	-2.001262	1.163150
5351	O	-4.754696	0.852737	1.551102
5352	H	-5.524033	1.246845	1.972928
5353	H	-4.777262	1.085567	0.580506
5354	O	1.320184	-1.287635	1.141498
5355	H	2.221391	-1.473268	1.466362
5356	H	1.365830	-1.216213	0.162821
5357	O	3.771746	2.135705	-1.074547
5358	H	3.803159	1.928699	-0.098985
5359	H	4.430239	2.813997	-1.253705
5360	O	5.258403	-1.925762	-0.330881
5361	H	5.447121	-2.801860	-0.678034
5362	H	4.771601	-1.417476	-1.037462
5363	O	-4.397439	-1.486117	-1.682265
5364	H	-4.414758	-1.724021	-0.712944
5365	H	-5.027306	-2.049344	-2.141676
5366	O	-1.446337	-1.510599	1.146699
5367	H	-1.573605	-0.573259	1.418468
5368	H	-0.525893	-1.740173	1.363085
5369	O	0.796891	1.333881	1.674900
5370	H	-0.109641	1.489570	1.988458
5371	H	0.901082	0.359247	1.584252
5372	O	-1.979677	1.131867	1.572401
5373	H	-1.956083	1.418103	0.631811
5374	H	-2.911414	1.192686	1.849545
5375	O	4.011013	-1.285735	1.865517
5376	H	4.446881	-1.585576	2.669019
5377	H	4.543877	-1.615832	1.087959
5378	O	-4.534796	1.252537	-1.032400
5379	H	-4.565286	0.375105	-1.456485
5380	H	-3.660400	1.625814	-1.237257
5381	O	3.598389	1.486207	1.464539
5382	H	2.693911	1.639702	1.784943
5383	H	3.807833	0.554020	1.662581
5384	O	1.116410	-0.713039	-1.539493
5385	H	1.007367	0.260761	-1.440073
5386	H	0.264618	-1.050528	-1.865538
5387	O	-1.751994	1.583451	-1.127516
5388	H	-0.909064	2.024777	-1.326555
5389	H	-1.643420	0.642954	-1.396302
5390	O	0.995109	1.956200	-0.990571
5391	H	1.889230	2.279253	-1.204301
5392	H	0.954785	1.879348	-0.011245

5393

5394 Cartesian coordinates of : W17_ 4

5395

5396	O	-0.437051	-1.026745	-2.002915
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5397	H	0.397607	-1.422373	-2.305993
5398	H	-0.661620	-1.485070	-1.156362
5399	O	2.614122	2.879902	1.101149
5400	H	2.585550	2.837678	0.101542
5401	H	3.027224	3.709102	1.359280
5402	O	2.145517	-2.236880	-2.052804
5403	H	1.926012	-2.657796	-1.158302
5404	H	2.421551	-2.947275	-2.640988
5405	O	1.450768	-3.220997	0.218245
5406	H	1.789010	-2.758835	1.010780
5407	H	0.478438	-3.159877	0.277446
5408	O	-3.834091	-1.882672	0.049705
5409	H	-4.635153	-2.402404	-0.063865
5410	H	-3.694230	-1.345569	-0.781042
5411	O	-3.256850	-0.144252	2.229151
5412	H	-2.384123	-0.439151	2.532997
5413	H	-3.554681	-0.782792	1.557872
5414	O	-2.785813	2.304783	1.118370
5415	H	-1.845735	2.405521	1.347967
5416	H	-3.067462	1.466880	1.551819
5417	O	3.706356	-0.091418	-1.536555
5418	H	4.568802	-0.175971	-1.955722
5419	H	3.179048	-0.886490	-1.791164
5420	O	-0.423984	-0.578225	2.265961
5421	H	0.427921	-0.952773	2.555269
5422	H	-0.226674	0.326699	1.930465
5423	O	-2.946113	2.220874	-1.440581
5424	H	-2.953548	2.286306	-0.429113
5425	H	-3.500443	2.925606	-1.788719
5426	O	-0.250833	1.624791	-1.498034
5427	H	-1.134782	1.997643	-1.681656
5428	H	-0.299994	0.664654	-1.717370
5429	O	3.573811	0.256576	1.284783
5430	H	3.690460	0.118609	0.327787
5431	H	3.300509	1.186429	1.394725
5432	O	-0.004767	1.895156	1.210633
5433	H	-0.034123	1.782846	0.232862
5434	H	0.834859	2.348615	1.404499
5435	O	-1.121388	-2.247679	0.300154
5436	H	-0.938349	-1.604277	1.030403
5437	H	-2.084224	-2.402220	0.281145
5438	O	-3.225242	-0.470038	-2.076227
5439	H	-2.331716	-0.705268	-2.375293
5440	H	-3.219968	0.494358	-1.912709
5441	O	2.396160	2.429736	-1.455533
5442	H	2.849001	1.589817	-1.645963
5443	H	1.452034	2.280242	-1.656548
5444	O	2.179881	-1.638706	2.407258
5445	H	2.730307	-0.896460	2.021140
5446	H	2.664624	-1.990044	3.160730

5447

5448 Cartesian coordinates of : W17_ 5

5449

5450	O	4.638817	0.302356	0.492281
5451	H	4.289726	-0.465569	1.030008
5452	H	5.526416	0.512144	0.796984
5453	O	0.095599	-2.110725	-0.000561
5454	H	-0.257128	-1.545520	-0.726129
5455	H	0.906911	-2.539457	-0.331800
5456	O	-0.166999	3.541778	-1.384107
5457	H	-0.220623	4.422751	-1.766679
5458	H	0.030853	3.637533	-0.411188
5459	O	2.159469	1.496407	0.537158
5460	H	3.118176	1.315089	0.552014
5461	H	1.836093	1.307856	-0.369089
5462	O	1.152864	1.129159	-2.013373
5463	H	0.762104	2.021293	-2.069396
5464	H	0.424570	0.499263	-2.167437
5465	O	-3.530843	-0.551506	2.108764
5466	H	-3.134761	-1.348023	1.652126
5467	H	-4.019373	-0.874819	2.872238
5468	O	3.438201	-1.685949	1.694526
5469	H	3.183173	-2.275834	0.962072
5470	H	2.606025	-1.381155	2.098876
5471	O	3.467427	-0.556190	-1.904733

5472	H	4.038441	-0.145184	-1.230910
5473	H	2.791704	0.097455	-2.150394
5474	O	-1.104145	-0.531935	-1.839413
5475	H	-1.502471	0.228187	-1.346375
5476	H	-1.861569	-1.046322	-2.170713
5477	O	-4.454512	0.315289	-0.412105
5478	H	-4.376987	0.086039	0.531950
5479	H	-3.774339	0.998130	-0.553533
5480	O	2.664668	-2.804471	-0.784652
5481	H	2.957703	-2.000335	-1.295159
5482	H	3.001500	-3.581409	-1.241202
5483	O	0.287474	3.405700	1.201425
5484	H	-0.379848	2.914094	1.708147
5485	H	1.082688	2.840652	1.191273
5486	O	-2.570978	-2.554354	0.708753
5487	H	-2.940285	-2.492497	-0.190877
5488	H	-1.604839	-2.612108	0.598206
5489	O	-1.341269	1.192978	2.042511
5490	H	-0.593607	0.569389	2.183295
5491	H	-2.148486	0.706603	2.296594
5492	O	-3.619262	-1.755350	-1.792032
5493	H	-4.271949	-2.167882	-2.365435
5494	H	-4.051611	-0.976514	-1.340020
5495	O	-2.001637	1.620293	-0.542286
5496	H	-1.565697	2.401221	-0.928353
5497	H	-1.686140	1.527217	0.389682
5498	O	0.874629	-0.432213	2.007415
5499	H	0.551860	-1.059947	1.322737
5500	H	1.365747	0.257526	1.511910

5501

5502 Cartesian coordinates of : W17_ 6

5503

5504	O	-3.839825	-0.874400	1.240070
5505	H	-3.879135	0.055033	1.538915
5506	H	-2.951054	-1.205274	1.462445
5507	O	1.683382	-1.535445	1.211501
5508	H	2.565464	-1.864588	1.461960
5509	H	1.654413	-1.554396	0.228325
5510	O	4.304526	-1.538640	-1.322232
5511	H	3.386234	-1.646706	-1.623865
5512	H	4.550154	-0.613753	-1.509840
5513	O	4.795448	1.231465	-1.248555
5514	H	5.556840	1.735518	-1.551026
5515	H	4.811816	1.207706	-0.250468
5516	O	-1.243120	-1.004077	-1.498024
5517	H	-2.166429	-1.094774	-1.797544
5518	H	-1.247880	-1.204215	-0.536662
5519	O	-3.740356	1.902588	1.494462
5520	H	-3.743400	2.047908	0.503885
5521	H	-4.376214	2.508067	1.887725
5522	O	-5.956388	-2.094675	-0.137845
5523	H	-6.643674	-2.693620	0.165022
5524	H	-5.406808	-1.863530	0.628517
5525	O	4.451256	-1.860895	1.273530
5526	H	4.476528	-1.835188	0.274997
5527	H	5.084375	-2.520661	1.572174
5528	O	1.526728	-1.212168	-1.510559
5529	H	0.626113	-1.394158	-1.828016
5530	H	1.635385	-0.233974	-1.522055
5531	O	-0.753029	1.677681	-1.307842
5532	H	0.162378	1.896772	-1.551590
5533	H	-0.870993	0.718697	-1.495853
5534	O	2.017145	1.454233	-1.213896
5535	H	2.948251	1.600805	-1.459994
5536	H	1.987512	1.477630	-0.230974
5537	O	-3.991887	-0.673792	-1.507353
5538	H	-4.799435	-1.165062	-1.717196
5539	H	-3.933512	-0.761645	-0.530013
5540	O	4.564823	0.952027	1.349817
5541	H	3.683279	1.244010	1.638344
5542	H	4.610321	-0.004095	1.535512
5543	O	-3.534286	2.053304	-1.107475
5544	H	-2.608801	2.188011	-1.373402
5545	H	-3.802109	1.190104	-1.476190
5546	O	-1.071851	-1.170332	1.257965

5547	H	-0.964130	-0.204654	1.418513
5548	H	-0.230406	-1.585448	1.512645
5549	O	1.773554	1.177536	1.506935
5550	H	0.919456	1.543973	1.792434
5551	H	1.676421	0.198178	1.521015
5552	O	-0.977071	1.547786	1.414861
5553	H	-1.858026	1.848699	1.701140
5554	H	-0.925328	1.727060	0.448238

5555
5556 Cartesian coordinates of : W17_ 7

5557				
5558	O	4.332795	0.121852	-1.954508
5559	H	3.897080	-0.648565	-2.347442
5560	H	3.605349	0.758537	-1.814739
5561	O	-0.939278	-1.155195	-1.577062
5562	H	-1.807088	-1.498638	-1.858394
5563	H	-0.884024	-1.346647	-0.614436
5564	O	-3.592729	-2.098390	0.875217
5565	H	-2.651586	-2.066696	1.130858
5566	H	-3.997558	-1.294858	1.249111
5567	O	-4.468568	0.534914	1.404340
5568	H	-5.278897	0.876846	1.793719
5569	H	-4.499451	0.705466	0.419697
5570	O	3.086991	-2.431218	0.281238
5571	H	3.873666	-1.871354	0.398844
5572	H	2.640206	-2.118231	-0.536251
5573	O	2.006286	1.281503	-1.041804
5574	H	2.070192	1.117409	-0.077081
5575	H	1.533620	2.125905	-1.156509
5576	O	4.930316	-0.289268	0.585284
5577	H	5.856670	-0.224656	0.836541
5578	H	4.862211	-0.101855	-0.388564
5579	O	-3.659379	-1.876691	-1.726631
5580	H	-3.702583	-2.073015	-0.746424
5581	H	-4.131257	-2.572260	-2.194336
5582	O	-0.916736	-1.408580	1.166246
5583	H	-1.104725	-0.478430	1.417368
5584	H	-0.090750	-1.674750	1.616745
5585	O	0.516774	2.784068	1.705660
5586	H	-0.289775	2.265058	1.883390
5587	H	1.274637	2.199721	1.876748
5588	O	-1.747954	1.174447	1.461876
5589	H	-1.757874	1.348292	0.491806
5590	H	-2.683344	1.104934	1.726708
5591	O	1.561893	-1.856748	2.263110
5592	H	1.715275	-2.389302	3.049451
5593	H	2.152128	-2.203377	1.520942
5594	O	-4.249445	0.811880	-1.190886
5595	H	-4.175119	-0.081912	-1.573337
5596	H	-3.398057	1.246689	-1.376575
5597	O	2.494470	0.707397	1.618442
5598	H	2.118260	-0.117718	1.982235
5599	H	3.439148	0.516866	1.468194
5600	O	1.826502	-1.318794	-1.913908
5601	H	1.688133	-0.381467	-1.673594
5602	H	0.925400	-1.636955	-2.089131
5603	O	-1.548415	1.509663	-1.232933
5604	H	-0.913287	2.238149	-1.351757
5605	H	-1.142401	0.661732	-1.513027
5606	O	0.365910	3.487340	-0.812856
5607	H	0.446193	4.424003	-1.014594
5608	H	0.414145	3.365637	0.177236

5609
5610 Cartesian coordinates of : W17_ 8

5611				
5612	O	3.541993	-0.843886	1.268558
5613	H	3.805927	-0.693806	0.343241
5614	H	3.064590	-0.043674	1.558887
5615	O	-3.246724	0.294104	2.136196
5616	H	-3.692935	0.518253	2.957823
5617	H	-3.295226	-0.694359	1.998820
5618	O	3.734096	-0.705252	-1.551605
5619	H	3.093959	-1.462881	-1.657794
5620	H	4.492761	-0.885529	-2.114991
5621	O	2.144499	1.531552	-1.127352

5622	H	2.816178	0.903137	-1.450924
5623	H	2.170077	1.491576	-0.142839
5624	O	-0.755853	-2.060947	-1.560870
5625	H	-0.634817	-2.242953	-0.600264
5626	H	-0.564688	-1.101803	-1.668062
5627	O	-0.407068	-2.344890	1.132996
5628	H	-0.358080	-1.379919	1.309169
5629	H	0.467442	-2.726033	1.343258
5630	O	2.245269	-3.100964	1.231441
5631	H	2.692720	-3.782959	1.741384
5632	H	2.762689	-2.248853	1.339229
5633	O	0.491421	3.830957	-0.738161
5634	H	-0.400081	3.540820	-0.996516
5635	H	1.119979	3.215673	-1.146928
5636	O	2.053156	-2.732495	-1.562163
5637	H	1.116137	-2.614203	-1.795762
5638	H	2.073730	-3.071650	-0.648600
5639	O	-3.385366	-1.766169	-1.363142
5640	H	-3.954317	-2.177124	-2.021394
5641	H	-2.442914	-1.974053	-1.597055
5642	O	-1.979901	2.771193	-1.752389
5643	H	-2.475708	3.295453	-2.388167
5644	H	-2.625216	2.189855	-1.271551
5645	O	-0.634724	0.370285	1.197985
5646	H	-0.722921	0.556048	0.238610
5647	H	-1.493101	0.559881	1.621671
5648	O	-3.486977	0.968480	-0.557047
5649	H	-3.576815	0.882995	0.408581
5650	H	-3.499222	0.064745	-0.920725
5651	O	-3.179632	-2.218764	1.428011
5652	H	-3.409654	-2.216592	0.481601
5653	H	-2.257272	-2.528946	1.474609
5654	O	1.898424	1.387687	1.583182
5655	H	1.877249	2.323447	1.875366
5656	H	0.971231	1.077286	1.629860
5657	O	1.319337	4.021992	1.843678
5658	H	1.793919	4.839849	2.014271
5659	H	0.951538	4.079216	0.933624
5660	O	-0.307968	0.605513	-1.536590
5661	H	-0.846794	1.311885	-1.934478
5662	H	0.627772	0.928053	-1.495784

5663

5664 Cartesian coordinates of : W17_ 9

5665

5666	O	-4.541691	-0.113207	0.075742
5667	H	-5.468191	-0.305932	0.247148
5668	H	-4.174946	-0.842535	-0.490026
5669	O	3.204189	1.687321	-1.711644
5670	H	3.607695	1.626988	-0.791929
5671	H	3.821932	2.169359	-2.270378
5672	O	-1.085793	0.027170	-1.142111
5673	H	-0.425696	0.754344	-1.184347
5674	H	-1.392877	-0.004747	-0.198453
5675	O	4.043061	1.361660	0.728978
5676	H	3.229439	1.433842	1.265665
5677	H	4.341669	0.439641	0.831810
5678	O	4.333251	-1.427067	0.590297
5679	H	5.096409	-2.010579	0.636452
5680	H	4.005642	-1.411865	-0.350914
5681	O	-3.201442	-1.826489	-1.443148
5682	H	-2.505209	-1.251571	-1.794413
5683	H	-2.723527	-2.572582	-1.029481
5684	O	3.208373	-1.162948	-1.770260
5685	H	2.322443	-1.566275	-1.788355
5686	H	3.107353	-0.211109	-1.949479
5687	O	0.622249	-2.103784	-1.183264
5688	H	0.077722	-2.904535	-1.080851
5689	H	-0.023918	-1.367977	-1.265810
5690	O	-3.170667	1.991299	-1.245728
5691	H	-2.548211	1.300338	-1.528512
5692	H	-3.844705	1.504698	-0.739623
5693	O	-2.090907	-0.016215	1.362282
5694	H	-1.823410	0.846372	1.781473
5695	H	-3.053521	0.000686	1.214577
5696	O	-1.119664	2.267358	2.269318

5697	H	-0.178047	2.020360	2.324619
5698	H	-1.190076	2.921743	1.552977
5699	O	-1.452611	3.713756	-0.172976
5700	H	-1.717484	4.634216	-0.264258
5701	H	-2.185161	3.156744	-0.547815
5702	O	-1.482601	-3.682882	-0.255905
5703	H	-1.293036	-3.294497	0.652080
5704	H	-1.700516	-4.612903	-0.141108
5705	O	1.629060	-1.549825	1.334582
5706	H	2.595164	-1.669667	1.353937
5707	H	1.352550	-1.767787	0.418041
5708	O	1.398350	1.209655	1.624039
5709	H	1.123004	1.466529	0.721689
5710	H	1.382948	0.229942	1.633131
5711	O	0.640737	2.093328	-0.904129
5712	H	1.489088	2.214749	-1.374514
5713	H	0.134978	2.922295	-0.824163
5714	O	-0.941643	-2.466398	1.970427
5715	H	0.009074	-2.273766	2.044238
5716	H	-1.386588	-1.596372	1.924596

5717

5718 Cartesian coordinates of :

W17_10

5719

5720	O	-2.127737	1.260289	1.563857
5721	H	-1.370453	0.863577	1.072964
5722	H	-2.624923	1.767796	0.894645
5723	O	-2.123155	-2.401142	-1.722415
5724	H	-1.974899	-2.691815	-0.774825
5725	H	-2.445831	-3.163502	-2.213115
5726	O	0.057528	0.148605	0.407995
5727	H	0.802374	0.761609	0.601944
5728	H	0.064659	-0.045923	-0.554737
5729	O	0.208411	-0.944192	-2.100404
5730	H	-0.626594	-1.445047	-2.175165
5731	H	0.911643	-1.601688	-1.931949
5732	O	3.997163	-0.977067	-0.271921
5733	H	3.889674	-0.944311	0.693822
5734	H	3.920426	-0.057880	-0.602536
5735	O	3.499139	1.625845	-1.012185
5736	H	4.134885	2.221410	-1.420503
5737	H	2.648936	1.646842	-1.572758
5738	O	0.915125	-2.245463	1.270739
5739	H	1.328669	-2.628892	0.473325
5740	H	0.569667	-1.366288	0.975265
5741	O	2.224478	-2.631053	-1.177119
5742	H	2.614321	-3.379922	-1.638357
5743	H	2.969632	-2.015317	-0.902865
5744	O	-1.808059	-2.951817	0.808806
5745	H	-2.363980	-2.325624	1.310327
5746	H	-0.897146	-2.868436	1.142646
5747	O	-3.505883	-0.975010	1.830107
5748	H	-4.064482	-1.067014	2.607808
5749	H	-3.025970	-0.105182	1.891233
5750	O	3.010300	-0.953875	2.388474
5751	H	2.251123	-1.543180	2.160714
5752	H	3.361466	-1.232556	3.239725
5753	O	-0.063435	3.296617	1.675962
5754	H	-0.755808	2.726693	2.043525
5755	H	0.778071	2.831959	1.812726
5756	O	-3.266571	2.137564	-0.819987
5757	H	-3.978999	2.719126	-1.101917
5758	H	-3.553594	1.201064	-0.989471
5759	O	-0.568656	3.048551	-1.059738
5760	H	-1.493173	2.755650	-1.113713
5761	H	-0.388176	3.245761	-0.118100
5762	O	1.311007	1.645847	-2.307235
5763	H	0.600268	2.198073	-1.889202
5764	H	0.916182	0.783700	-2.516386
5765	O	2.172359	1.564249	1.380586
5766	H	2.786457	1.763949	0.645388
5767	H	2.564433	0.841342	1.901276
5768	O	-3.951247	-0.408637	-0.927826
5769	H	-4.026641	-0.706875	-0.005165
5770	H	-3.368352	-1.053594	-1.368143

5771

5772 Cartesian coordinates of : W17_11

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5773
5774  O      -0.985759      2.440826      -2.049338
5775  H      -0.147179      1.948024      -1.972054
5776  H      -1.684392      1.763391      -2.052905
5777  O      -1.229707      4.289944      -0.213270
5778  H      -0.806654      5.101175      -0.507446
5779  H      -1.157257      3.625024      -0.954891
5780  O      -1.858501     -2.378364     -1.053539
5781  H      -2.771039     -2.617299     -1.281131
5782  H      -1.810178     -2.330453     -0.071531
5783  O      -2.374535      0.710375      1.216789
5784  H      -2.434151      0.773720      0.242878
5785  H      -1.942059      1.519148      1.549352
5786  O      4.010527      0.650681     -1.717070
5787  H      3.961337     -0.347463     -1.658985
5788  H      4.644340      0.883261     -2.402081
5789  O      -1.502315     -1.857009      1.596968
5790  H      -0.573841     -2.007033      1.843352
5791  H      -1.616984     -0.883311      1.561618
5792  O      -4.620416     -1.744479     -1.184847
5793  H      -4.631389     -1.634981     -0.202368
5794  H      -5.493831     -2.044665     -1.452930
5795  O      1.252531      1.232935      1.260532
5796  H      1.133358      1.240001      0.285229
5797  H      0.605041      1.855165      1.641082
5798  O      -2.643216      0.244736     -1.506488
5799  H      -3.556963     -0.054954     -1.642261
5800  H      -2.151024     -0.601537     -1.468987
5801  O      1.253236     -1.498282      1.544056
5802  H      1.248161     -0.517209      1.595762
5803  H      2.170417     -1.776526      1.722005
5804  O      -4.280808     -1.349346      1.450247
5805  H      -3.890600     -0.462512      1.543511
5806  H      -3.588265     -1.938100      1.786354
5807  O      4.015272      0.839191      1.091052
5808  H      3.122341      1.170995      1.299664
5809  H      4.140817      0.983849      0.135643
5810  O      1.251025      0.880294     -1.450766
5811  H      2.183185      0.981537     -1.722242
5812  H      1.063702     -0.084486     -1.483917
5813  O      -0.853690      2.936634      1.975380
5814  H      -1.026919      3.422049      2.787596
5815  H      -0.971072      3.565682      1.207826
5816  O      3.648143     -1.903007     -1.323175
5817  H      2.702075     -2.099916     -1.444014
5818  H      3.846883     -2.073522     -0.384184
5819  O      0.853897     -1.810229     -1.146169
5820  H      0.001356     -2.206245     -1.395539
5821  H      0.891783     -1.807382     -0.163014
5822  O      4.025861     -1.747534      1.462259
5823  H      4.128403     -0.754218      1.402533
5824  H      4.718249     -2.090142      2.035120
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5825
5826 Cartesian coordinates of : W17_12

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5827
5828  O      -3.160966      2.074442      0.635205
5829  H      -3.742682      1.507376      0.091903
5830  H      -2.927236      1.560420      1.429013
5831  O      2.553831      0.810902     -2.349043
5832  H      2.752036      1.505242     -1.695369
5833  H      1.580231      0.726546     -2.391836
5834  O      0.210689      0.054495      2.117065
5835  H      0.450736      0.973193      1.801127
5836  H      -0.687509      0.097285      2.498803
5837  O      2.525451     -1.268076      2.481284
5838  H      1.653533     -0.805663      2.505283
5839  H      2.757856     -1.490378      3.388152
5840  O      -3.813725     -1.457429      1.075874
5841  H      -4.285550     -0.919113      0.414144
5842  H      -3.278511     -2.086376      0.556026
5843  O      -0.224728      0.521588     -2.041796
5844  H      -0.517187      1.357076     -1.626975
5845  H      -0.095736     -0.130499     -1.318110
5846  O      -1.102538      2.841406     -0.726794
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5847	H	-1.278273	3.678154	-1.167770
5848	H	-1.927028	2.591239	-0.208032
5849	O	4.366687	0.124885	0.835439
5850	H	4.431149	-0.447190	0.048426
5851	H	3.778750	-0.323508	1.470081
5852	O	-2.520295	0.169024	2.657829
5853	H	-2.995457	-0.524805	2.113166
5854	H	-2.945410	0.191669	3.520925
5855	O	-2.123770	-2.806652	-0.686204
5856	H	-1.257930	-2.381265	-0.431272
5857	H	-1.967047	-3.748877	-0.801323
5858	O	2.322842	-2.732584	0.039890
5859	H	2.582186	-2.470437	0.938210
5860	H	2.975552	-2.347709	-0.575568
5861	O	-4.553417	0.297188	-0.977161
5862	H	-3.878134	-0.038093	-1.641218
5863	H	-5.376278	0.465060	-1.445842
5864	O	3.985126	-1.218112	-1.583956
5865	H	4.595280	-1.502303	-2.270880
5866	H	3.415744	-0.481767	-1.962488
5867	O	-2.723333	-0.727670	-2.503111
5868	H	-2.531799	-1.583376	-2.079067
5869	H	-1.871571	-0.249879	-2.542153
5870	O	0.869315	2.410232	1.176536
5871	H	1.755188	2.464651	0.771373
5872	H	0.230658	2.703161	0.499821
5873	O	3.346004	2.335021	-0.102006
5874	H	3.795706	1.541977	0.310275
5875	H	3.964718	3.071013	-0.069773
5876	O	0.032689	-1.432533	-0.135472
5877	H	0.887098	-1.943778	-0.150067
5878	H	0.038030	-0.928059	0.712390

5879

5880 Cartesian coordinates of : W17_13

5881

5882	O	-2.456563	-2.018501	-1.773221
5883	H	-2.515815	-2.512632	-0.935240
5884	H	-1.505451	-1.961471	-1.973942
5885	O	3.027630	-1.839559	-1.956302
5886	H	3.306503	-0.894406	-1.783847
5887	H	3.604706	-2.195295	-2.638676
5888	O	4.169849	-0.205489	1.423389
5889	H	3.702279	-1.075325	1.300829
5890	H	4.991176	-0.381177	1.892127
5891	O	-0.381996	4.196588	-1.040072
5892	H	-0.575737	4.922665	-1.639366
5893	H	-1.180640	3.640462	-0.996076
5894	O	2.925616	-2.453192	0.807245
5895	H	2.969426	-2.465011	-0.165322
5896	H	1.995412	-2.590252	1.056472
5897	O	-0.023073	0.756008	-0.799710
5898	H	0.142338	-0.114373	-1.228019
5899	H	0.761696	1.351645	-0.902275
5900	O	0.311376	-1.798234	-1.548284
5901	H	0.317450	-2.078717	-0.605538
5902	H	1.210916	-1.943748	-1.898585
5903	O	-2.263059	2.125127	-0.626953
5904	H	-2.993573	1.653266	-1.068370
5905	H	-1.466008	1.557644	-0.792327
5906	O	-3.975191	0.101632	-1.511360
5907	H	-4.710107	0.052536	-2.130285
5908	H	-3.372591	-0.671590	-1.708669
5909	O	3.777220	0.562045	-1.248176
5910	H	4.053044	0.457045	-0.318664
5911	H	3.216411	1.356265	-1.284939
5912	O	-2.608036	-2.905364	0.909441
5913	H	-3.100221	-2.064750	1.126654
5914	H	-3.126671	-3.637198	1.257595
5915	O	1.892268	2.577468	-0.673245
5916	H	2.049760	2.490709	0.299732
5917	H	1.305583	3.340523	-0.822985
5918	O	0.112985	-2.309475	1.141011
5919	H	-0.767926	-2.723907	1.202163
5920	H	0.017655	-1.432710	1.572163
5921	O	-2.588465	1.689078	2.000104

5922	H	-2.500796	2.005076	1.065447
5923	H	-2.836752	2.440968	2.546609
5924	O	2.278631	1.835821	1.876671
5925	H	1.473356	1.343084	2.115829
5926	H	2.999413	1.182219	1.887844
5927	O	-3.929700	-0.653433	1.208335
5928	H	-4.137087	-0.329788	0.312568
5929	H	-3.546154	0.105639	1.681531
5930	O	-0.111188	0.329972	1.869451
5931	H	-0.929192	0.732369	2.208280
5932	H	-0.118830	0.516289	0.900676

5933

5934 Cartesian coordinates of : W17_14

5935

5936	O	-2.650834	-2.195044	1.750019
5937	H	-2.634016	-2.839568	2.464019
5938	H	-1.708718	-1.962904	1.513360
5939	O	1.733099	-2.680915	0.100090
5940	H	2.589486	-2.529144	0.538334
5941	H	1.777231	-2.178436	-0.736906
5942	O	4.242330	-0.564950	-1.647729
5943	H	4.342004	-1.127388	-0.856885
5944	H	3.398618	-0.810624	-2.062122
5945	O	4.106877	1.866730	-0.672328
5946	H	4.254640	0.990446	-1.126983
5947	H	4.772738	2.487242	-0.982962
5948	O	-1.357457	-0.880121	-1.713803
5949	H	-1.749640	-0.029175	-1.994951
5950	H	-2.105361	-1.497541	-1.627517
5951	O	-3.613160	0.513097	1.775219
5952	H	-2.870552	1.131271	1.905714
5953	H	-3.296874	-0.378421	1.990347
5954	O	-3.600338	-2.367329	-0.802659
5955	H	-3.991498	-3.199020	-1.087242
5956	H	-3.355730	-2.463026	0.144508
5957	O	4.222221	-1.711166	0.919715
5958	H	4.950989	-2.116340	1.399288
5959	H	4.011951	-0.838398	1.360113
5960	O	1.455956	-0.868930	-1.998935
5961	H	1.377145	0.005259	-1.555848
5962	H	0.554806	-1.071818	-2.297797
5963	O	-1.081727	2.930645	-0.568317
5964	H	-1.716766	2.506349	-1.177340
5965	H	-0.199502	2.587203	-0.801645
5966	O	1.356010	1.569153	-0.708825
5967	H	1.237533	1.370423	0.248214
5968	H	2.259718	1.922923	-0.806383
5969	O	-4.566927	0.330130	-0.750287
5970	H	-4.480541	-0.629088	-0.874394
5971	H	-4.312640	0.485100	0.190763
5972	O	3.612641	0.660930	1.834591
5973	H	2.672157	0.797284	2.049965
5974	H	3.832423	1.267930	1.105532
5975	O	-2.779428	1.460463	-2.199537
5976	H	-3.118915	1.815033	-3.026900
5977	H	-3.556796	1.087721	-1.670799
5978	O	-0.370217	-1.312402	0.849017
5979	H	-0.670526	-1.014404	-0.038402
5980	H	0.415509	-1.906515	0.676005
5981	O	0.813826	0.918270	1.882698
5982	H	0.103377	1.526464	2.162981
5983	H	0.361664	0.076305	1.653922
5984	O	-1.519393	2.413205	1.941167
5985	H	-1.395027	2.674595	0.978829
5986	H	-1.776725	3.206143	2.422399

5987

5988 Cartesian coordinates of : W17_15

5989

5990	O	-0.760528	2.252577	0.528904
5991	O	-0.921488	-0.115417	1.895691
5992	O	1.978523	1.852819	0.366804
5993	O	1.908444	0.317283	-1.897264
5994	O	1.383246	-1.895948	-0.367384
5995	O	1.841204	-0.419897	1.895272
5996	O	-1.348404	-1.439037	-0.460260

5997	O	-0.814340	0.881696	-1.847519
5998	O	4.679001	0.073710	-1.955466
5999	O	4.724676	1.314909	0.359346
6000	O	4.550273	-1.051260	1.876715
6001	O	4.159997	-2.241067	-0.433728
6002	H	1.905371	1.412967	-0.510251
6003	H	1.159606	2.363155	0.489755
6004	H	-0.049649	-0.325387	2.270809
6005	H	-1.037821	-0.699151	1.111288
6006	H	1.469148	-1.458337	0.509234
6007	H	0.444099	-2.129696	-0.468515
6008	H	-0.721947	1.468065	-1.063404
6009	H	0.069968	0.809022	-2.244521
6010	H	-0.845699	1.472942	1.122849
6011	H	-1.616607	2.717247	0.566640
6012	H	1.938549	0.454148	1.455575
6013	H	1.743502	-0.546166	-1.456374
6014	H	-1.208369	-0.676254	-1.062830
6015	H	-2.310030	-1.615199	-0.467017
6016	H	3.210029	-2.417378	-0.546818
6017	H	4.407321	-1.594756	-1.120106
6018	H	4.467081	-1.599258	1.046340
6019	H	4.772084	0.617433	1.038524
6020	H	3.880649	1.779039	0.494839
6021	H	4.788309	0.616989	-1.124832
6022	H	2.826097	0.288378	-2.223056
6023	H	2.730819	-0.678200	2.196389
6024	H	5.404410	0.284567	-2.550813
6025	H	5.196259	-1.472629	2.451327
6026	H	-4.049170	-0.661400	0.595940
6027	O	-4.072754	-1.136431	-0.270372
6028	H	-4.857973	-1.707783	-0.289381
6029	H	-3.697582	1.302673	1.576780
6030	O	-3.691844	0.388082	1.910479
6031	H	-2.789344	0.218652	2.228389
6032	H	-3.853604	0.318927	-1.360328
6033	O	-3.600362	1.198770	-1.704653
6034	H	-2.709596	1.102727	-2.081829
6035	H	-3.588532	2.252763	-0.460997
6036	O	-3.481511	2.770547	0.388309
6037	H	-4.059536	3.537972	0.345249
6038	O	-6.420100	-2.734804	-0.309697
6039	H	-7.200626	-2.398230	-0.761432
6040	H	-6.729474	-3.170098	0.491169
6041				
6042	Cartesian coordinates of : W17_16			
6043				
6044	O	-2.406642	-0.685144	1.274492
6045	O	-2.684440	0.022734	-1.305254
6046	O	-0.773415	3.249972	0.666742
6047	O	-1.588176	1.447198	2.700124
6048	O	0.105414	-1.793875	0.927284
6049	O	-0.169425	-1.136264	-1.646945
6050	O	1.793340	2.157137	0.410745
6051	O	0.980614	0.367431	2.264165
6052	H	-2.459177	-0.373977	0.333635
6053	H	-1.125017	-0.981058	-1.755005
6054	H	-1.085953	2.711856	1.416794
6055	H	0.608992	-0.412786	1.784331
6056	H	-1.647467	-1.299732	1.306687
6057	H	0.233670	-0.246613	-1.792903
6058	H	0.195295	3.159282	0.644219
6059	H	0.239315	0.772250	2.743510
6060	H	-2.165197	1.693621	3.429381
6061	H	0.814904	-2.453977	1.039487
6062	H	-3.614554	-0.201151	-1.528145
6063	H	2.761787	2.118022	0.309726
6064	H	-1.997594	0.676951	2.233596
6065	H	0.075341	-1.581915	-0.041389
6066	H	-2.514208	0.962219	-1.518353
6067	H	1.564973	1.478326	1.088726
6068	H	-2.200926	3.348854	-2.092982
6069	O	-1.749062	2.606107	-1.680690
6070	H	-1.448681	2.903520	-0.775555
6071	H	-0.007503	1.903670	-2.188494

6072	O	0.781467	1.375789	-1.978937
6073	H	1.106719	1.696930	-1.105569
6074	O	3.275899	0.039473	-2.303006
6075	H	3.734486	0.446747	-1.546471
6076	H	2.517374	0.610239	-2.501998
6077	H	5.264324	1.383861	0.215063
6078	O	4.348913	1.113583	0.096851
6079	H	4.151935	0.401339	0.767727
6080	O	3.574350	-0.676915	1.855259
6081	H	3.309414	-1.545719	1.493044
6082	H	2.794374	-0.324923	2.314290
6083	O	2.574390	-3.028310	0.716834
6084	H	2.543096	-2.861379	-0.278967
6085	H	2.968523	-3.894204	0.859721
6086	H	2.762924	-1.605057	-2.011687
6087	O	2.322447	-2.456521	-1.781068
6088	H	1.384486	-2.306448	-1.981409
6089	O	-4.941389	-1.790524	1.082219
6090	H	-4.044856	-1.476745	1.317286
6091	H	-5.514683	-1.615152	1.833716
6092	H	-5.294897	-1.238409	-0.569330
6093	O	-5.243425	-0.851120	-1.468317
6094	H	-5.518097	-1.534453	-2.086658

6095

6096 Cartesian coordinates of : W17_17

6097

6098	O	4.386795	-1.227158	-0.893855
6099	H	3.791426	-0.766593	-1.558272
6100	H	5.122220	-1.613754	-1.378586
6101	O	0.171084	-1.963867	0.092868
6102	H	0.020035	-1.289451	0.789171
6103	H	0.253521	-1.412012	-0.726771
6104	O	-3.929688	-1.521478	0.897106
6105	H	-3.338209	-2.215533	0.551137
6106	H	-3.432642	-1.020403	1.567963
6107	O	-4.495893	0.099656	-1.070000
6108	H	-5.413867	0.074136	-1.357528
6109	H	-4.393117	-0.553772	-0.320612
6110	O	0.069945	0.239151	1.778584
6111	H	0.907991	0.138817	2.272845
6112	H	0.216020	0.930404	1.086596
6113	O	2.991965	2.460367	-0.842806
6114	H	3.503400	1.964602	-0.138447
6115	H	3.432278	3.302769	-0.990346
6116	O	2.761276	-2.378210	1.046604
6117	H	3.386265	-2.138970	0.335225
6118	H	1.879345	-2.429408	0.629121
6119	O	-2.129067	-3.180929	-0.447818
6120	H	-1.227832	-2.848981	-0.199424
6121	H	-2.096006	-4.142003	-0.470147
6122	O	-2.507550	0.303789	2.522175
6123	H	-2.656022	0.453774	3.460987
6124	H	-1.531407	0.299664	2.372185
6125	O	-1.573857	3.772657	-0.155462
6126	H	-2.365552	3.239336	0.111694
6127	H	-1.851971	4.372436	-0.852933
6128	O	-3.544741	2.162877	0.603521
6129	H	-3.919705	1.568047	-0.071289
6130	H	-3.249266	1.590576	1.332191
6131	O	2.596861	-0.405306	2.710583
6132	H	2.882204	-0.619879	3.604141
6133	H	2.688078	-1.236121	2.147418
6134	O	-2.374851	-1.150980	-2.484881
6135	H	-3.123358	-0.614102	-2.169965
6136	H	-2.414425	-1.975202	-1.972506
6137	O	4.252196	0.955519	0.867246
6138	H	4.509681	0.167542	0.353467
6139	H	3.723985	0.628551	1.618287
6140	O	2.831263	0.146471	-2.459843
6141	H	2.863329	1.056363	-2.114258
6142	H	1.886615	-0.096754	-2.498773
6143	O	0.122641	-0.238679	-1.967126
6144	H	-0.771410	-0.468784	-2.312674
6145	H	0.041661	0.602815	-1.469660
6146	O	0.340668	1.935182	-0.304767

6147	H	1.234437	2.297871	-0.464700
6148	H	-0.310062	2.681521	-0.302576
6149				
6150	Cartesian coordinates of : W17_18			
6151				
6152	O	0.584027	2.244341	-1.993553
6153	H	-0.231821	1.729938	-2.133895
6154	H	1.317169	1.601361	-2.010933
6155	O	4.204888	-2.911219	-0.416632
6156	H	4.390335	-3.396063	0.393314
6157	H	3.222972	-2.800691	-0.465243
6158	O	1.217298	-1.163112	1.955231
6159	H	0.271518	-1.107089	2.174859
6160	H	1.540909	-0.245219	1.902859
6161	O	2.266121	1.348812	1.267052
6162	H	1.787221	2.192373	1.155885
6163	H	3.211456	1.525437	1.443823
6164	O	-4.303644	-1.154110	1.874574
6165	H	-4.968919	-1.354963	2.539502
6166	H	-4.467052	-0.228615	1.535602
6167	O	-1.163953	-1.818155	-0.674403
6168	H	-0.269528	-2.188832	-0.794369
6169	H	-1.212341	-1.514129	0.259731
6170	O	-4.443698	0.218474	-1.867367
6171	H	-4.333577	-0.714952	-1.522398
6172	H	-5.110242	0.206724	-2.560631
6173	O	-1.712034	1.773952	0.738106
6174	H	-1.018972	2.450267	0.842146
6175	H	-1.649428	1.458776	-0.192394
6176	O	-1.698935	0.645053	-1.745095
6177	H	-1.461602	-0.280016	-1.509703
6178	H	-2.629015	0.621463	-2.038110
6179	O	-3.938102	-2.090544	-0.761172
6180	H	-2.983869	-2.269732	-0.843580
6181	H	-4.117979	-1.992611	0.191671
6182	O	2.492968	0.358711	-1.273739
6183	H	2.414364	0.707852	-0.355944
6184	H	3.444401	0.209334	-1.409250
6185	O	5.172150	-0.493999	-0.869039
6186	H	4.893121	-1.429775	-0.676042
6187	H	5.891891	-0.535364	-1.506560
6188	O	0.581144	3.352571	0.370046
6189	H	0.669248	4.310404	0.350968
6190	H	0.599601	3.024152	-0.577631
6191	O	-4.456777	1.215321	0.768279
6192	H	-3.594544	1.658540	0.863618
6193	H	-4.582522	1.066380	-0.186724
6194	O	1.615339	-2.170637	-0.497009
6195	H	1.485555	-1.880825	0.443578
6196	H	1.816507	-1.334527	-0.965065
6197	O	-1.547686	-0.738457	1.816770
6198	H	-1.596901	0.214375	1.583366
6199	H	-2.443096	-0.999687	2.098496
6200	O	4.998483	1.320804	1.240683
6201	H	5.588146	1.120637	1.973147
6202	H	5.186286	0.672627	0.534053

6203				
6204	Cartesian coordinates of : W17_19			
6205				
6206	O	2.382992	0.546656	-1.322542
6207	H	3.256949	0.155025	-1.518969
6208	H	2.264127	0.453657	-0.354423
6209	O	4.471942	-0.854107	1.347296
6210	H	3.842054	-0.155835	1.589131
6211	H	3.910776	-1.645018	1.226900
6212	O	-0.474991	-0.357555	2.150082
6213	H	-1.253259	-0.778307	2.548892
6214	H	-0.777638	0.517736	1.803858
6215	O	0.102293	-2.105356	0.167977
6216	H	-0.063966	-1.477568	0.910058
6217	H	-0.673585	-2.691940	0.141777
6218	O	2.076084	0.687107	1.474002
6219	H	1.876031	1.635825	1.594379
6220	H	1.381275	0.197259	1.943427
6221	O	4.710172	-0.904472	-1.296149

6222	H	4.847110	-0.810474	-0.318791
6223	H	5.568939	-0.886479	-1.727249
6224	O	1.262797	3.093845	-1.280734
6225	H	0.356928	2.884817	-1.565788
6226	H	1.791196	2.294151	-1.472128
6227	O	-1.179667	2.051563	1.203384
6228	H	-1.154708	2.003875	0.215401
6229	H	-0.490746	2.689370	1.463626
6230	O	-3.754755	0.993592	1.123747
6231	H	-3.596441	0.123127	1.531458
6232	H	-2.994460	1.551980	1.364783
6233	O	1.270806	3.357669	1.312025
6234	H	1.682536	4.157533	1.652160
6235	H	1.321352	3.377609	0.311469
6236	O	-3.052267	-1.545450	2.187295
6237	H	-2.948481	-2.148343	1.415643
6238	H	-3.629010	-1.984542	2.820377
6239	O	-2.703676	-1.452124	-2.138525
6240	H	-3.207349	-0.625534	-1.999099
6241	H	-1.820636	-1.194635	-2.452759
6242	O	-1.241336	1.799210	-1.468570
6243	H	-2.182535	1.759111	-1.711612
6244	H	-0.857333	0.911954	-1.680964
6245	O	-2.551431	-2.999357	-0.065604
6246	H	-2.660552	-2.418076	-0.880870
6247	H	-2.912678	-3.865067	-0.281210
6248	O	-0.048265	-0.539132	-2.022721
6249	H	0.006091	-1.123431	-1.229421
6250	H	0.867320	-0.213466	-2.120918
6251	O	-3.912744	0.967152	-1.493472
6252	H	-3.943347	0.979388	-0.494572
6253	H	-4.763508	1.274888	-1.820655
6254	O	2.870761	-2.727956	0.094821
6255	H	1.904803	-2.618112	0.069708
6256	H	3.223016	-2.420752	-0.752109

6257

6258 Cartesian coordinates of : W17_20

6259

6260	O	4.238700	-0.009849	1.282343
6261	H	4.169431	-0.219447	0.309208
6262	H	5.167703	0.095324	1.507671
6263	O	-1.629333	1.894883	1.357881
6264	H	-1.022019	1.149628	1.528966
6265	H	-1.066100	2.701847	1.368356
6266	O	2.022567	1.635115	-1.519060
6267	H	1.510256	2.380226	-1.873689
6268	H	2.046985	1.745355	-0.542950
6269	O	-3.985801	-0.511829	-1.030776
6270	H	-3.516174	-1.371781	-0.928574
6271	H	-4.793715	-0.692145	-1.521879
6272	O	0.050911	-0.409246	1.355060
6273	H	0.038068	-0.457441	0.373338
6274	H	-0.730342	-0.963261	1.668984
6275	O	2.009782	1.615195	1.231055
6276	H	2.879465	1.227011	1.448626
6277	H	1.346244	0.947433	1.485391
6278	O	2.318729	-2.027306	1.725733
6279	H	1.505100	-1.490111	1.781470
6280	H	3.064597	-1.409080	1.815276
6281	O	3.722689	-0.598579	-1.223743
6282	H	3.231436	0.126711	-1.641931
6283	H	3.172743	-1.403482	-1.259555
6284	O	-0.339829	-2.854387	-1.737836
6285	H	0.494272	-3.145055	-1.325826
6286	H	-0.199901	-1.895328	-1.867918
6287	O	-3.927727	0.297471	1.748538
6288	H	-3.361574	1.084288	1.802136
6289	H	-4.139566	0.177758	0.809435
6290	O	0.244337	3.814231	0.921535
6291	H	0.207654	3.850316	-0.048133
6292	H	1.050723	3.324105	1.150464
6293	O	-2.099507	1.559329	-1.247635
6294	H	-2.875091	0.988494	-1.391484
6295	H	-2.034689	1.706833	-0.268753
6296	O	-2.085570	-1.740897	1.986163

6297	H	-2.813118	-1.087167	2.064427
6298	H	-2.313437	-2.298344	1.221876
6299	O	-0.174369	3.403092	-1.921184
6300	H	-0.382011	4.130371	-2.516634
6301	H	-0.969540	2.832808	-1.875262
6302	O	-2.634100	-2.865961	-0.561563
6303	H	-1.727718	-2.938713	-1.001518
6304	H	-3.079184	-3.709430	-0.692694
6305	O	-0.001950	-0.178715	-1.408111
6306	H	-0.777199	0.419832	-1.475744
6307	H	0.780864	0.384733	-1.585458
6308	O	2.273936	-2.984238	-0.705832
6309	H	2.806841	-3.780995	-0.796801
6310	H	2.301265	-2.717766	0.258630

6311

6312 Cartesian coordinates of : W17_21

6313

6314	O	-1.912873	-2.198512	1.350743
6315	H	-1.128660	-1.661050	1.559794
6316	H	-1.567498	-2.979411	0.869792
6317	H	-2.565744	-1.780204	-0.426503
6318	O	-2.564220	-1.631471	-1.388395
6319	H	-3.263839	-0.961747	-1.538510
6320	O	-0.113263	-0.598864	-1.307278
6321	H	-0.998371	-1.010201	-1.485710
6322	H	0.548145	-1.353007	-1.291723
6323	H	-3.289636	-1.057318	1.657124
6324	O	-3.827001	-0.239094	1.696750
6325	H	-4.564600	-0.418398	2.289313
6326	H	-3.571814	1.238988	-1.252680
6327	O	-4.219023	0.534099	-1.095392
6328	H	-4.273825	0.422437	-0.132930
6329	O	-1.680019	1.843629	-1.181717
6330	H	-1.146802	2.624792	-1.428957
6331	H	-1.140748	1.069210	-1.409219
6332	H	-0.549796	0.497626	1.616265
6333	O	0.106709	-0.199464	1.382685
6334	H	0.010623	-0.310200	0.404281
6335	O	-1.785074	1.728329	1.553470
6336	H	-1.868817	1.822054	0.578995
6337	H	-2.592185	1.275769	1.852808
6338	H	1.107859	0.771741	-1.719180
6339	O	1.825816	1.421760	-1.609660
6340	H	1.439111	2.298235	-1.787725
6341	O	0.285083	3.758880	-1.368059
6342	H	0.326982	4.655943	-1.713504
6343	H	0.355976	3.800164	-0.374182
6344	H	2.262611	1.462001	0.108084
6345	O	2.352446	1.409709	1.086892
6346	H	1.639850	0.788054	1.341111
6347	H	1.199788	2.925237	1.415049
6348	O	0.444169	3.517118	1.246631
6349	H	-0.338122	3.098198	1.640550
6350	H	2.430915	-2.144359	-1.447425
6351	O	1.635097	-2.526186	-1.024105
6352	H	1.851412	-2.492012	-0.061162
6353	H	3.342632	0.075280	-1.812059
6354	O	3.715566	-0.787986	-1.579685
6355	H	4.156852	-0.670106	-0.722362
6356	H	3.820336	0.457992	1.283467
6357	O	4.400068	-0.331409	1.187873
6358	H	5.230229	-0.157977	1.642044
6359	H	1.547393	-1.492636	1.895797
6360	O	2.221462	-2.117140	1.590271
6361	H	3.073317	-1.648198	1.618446
6362	H	0.029351	-3.684342	-0.914696
6363	O	-0.894074	-3.825798	-0.649300
6364	H	-1.439867	-3.523352	-1.388179

6365

6366

6367 Cartesian coordinates of the water octadecamer

6368

6369 Cartesian coordinates of : W18_1

6370

6371	O	1.459768	-1.358165	1.379742
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6372	H	1.646104	-0.403167	1.541370
6373	H	2.284870	-1.840108	1.572283
6374	O	-2.007214	1.464484	-1.193067
6375	H	-2.059020	1.452545	-0.209047
6376	H	-1.324921	2.118913	-1.427557
6377	O	4.860868	0.698577	-1.261116
6378	H	4.890074	0.671630	-0.258931
6379	H	5.670260	1.113711	-1.573891
6380	O	-1.304038	-1.419378	1.255083
6381	H	-1.282930	-1.424441	0.272907
6382	H	-0.390296	-1.590961	1.547440
6383	O	4.685669	0.465171	1.330328
6384	H	3.857446	0.890058	1.620411
6385	H	4.593129	-0.484240	1.528884
6386	O	-0.073625	2.974965	1.582297
6387	H	-0.085771	3.255964	0.653475
6388	H	-0.893485	2.472175	1.728287
6389	O	-4.092251	-2.100213	-1.497130
6390	H	-4.577499	-2.831783	-1.890213
6391	H	-4.112052	-2.209415	-0.502971
6392	O	2.037491	1.286287	1.399040
6393	H	2.075108	1.384567	0.425522
6394	H	1.333840	1.913421	1.683698
6395	O	-4.010419	-2.090707	1.119917
6396	H	-4.420786	-1.253303	1.402725
6397	H	-3.081766	-2.054954	1.410660
6398	O	-4.933319	0.555505	1.352866
6399	H	-5.744202	0.928358	1.711482
6400	H	-4.949479	0.661403	0.359943
6401	O	3.990800	-1.982596	-1.322349
6402	H	4.394621	-1.117044	-1.513884
6403	H	3.057890	-1.913640	-1.591963
6404	O	-4.683579	0.641357	-1.258976
6405	H	-3.846927	1.089422	-1.475311
6406	H	-4.585843	-0.283393	-1.550433
6407	O	-2.221583	1.149779	1.498955
6408	H	-3.176203	1.089688	1.688306
6409	H	-1.861487	0.238710	1.576300
6410	O	0.217608	3.168179	-1.311925
6411	H	0.993515	2.581348	-1.461075
6412	H	0.352361	3.964894	-1.834262
6413	O	-1.469078	-1.194081	-1.489905
6414	H	-1.647446	-0.227953	-1.534087
6415	H	-2.300135	-1.644532	-1.729597
6416	O	2.164622	1.293743	-1.387420
6417	H	1.812033	0.382928	-1.521346
6418	H	3.126821	1.249526	-1.550436
6419	O	1.287769	-1.271870	-1.353038
6420	H	0.373303	-1.423087	-1.655040
6421	H	1.277083	-1.382652	-0.374470
6422	O	4.083316	-2.284448	1.286946
6423	H	4.102373	-2.286496	0.288824
6424	H	4.556978	-3.060802	1.600022

6425

6426 Cartesian coordinates of : W18_ 2

6427

6428	O	-5.015322	-0.335047	-1.464216
6429	H	-4.406392	-1.120975	-1.359074
6430	H	-5.757962	-0.610866	-2.009957
6431	O	-3.415954	1.954996	-1.754030
6432	H	-3.511567	2.347737	-0.871205
6433	H	-4.047790	1.214432	-1.793411
6434	O	-4.836757	0.259968	1.259186
6435	H	-5.098032	0.146234	0.326292
6436	H	-4.341160	1.097135	1.309744
6437	O	-3.410653	-2.331511	-0.931302
6438	H	-3.426500	-2.425708	0.037897
6439	H	-2.473067	-2.259295	-1.185275
6440	O	-3.256860	2.590305	1.055321
6441	H	-2.305257	2.359759	1.166780
6442	H	-3.412760	3.427960	1.502105
6443	O	-0.900126	1.023007	-1.629831
6444	H	-1.796431	1.374995	-1.850956
6445	H	-0.958835	0.045425	-1.607972
6446	O	-3.549482	-1.922530	1.870390

6447	H	-3.984081	-2.435216	2.558643
6448	H	-4.075178	-1.081406	1.732217
6449	O	-0.691108	-1.674643	-1.080176
6450	H	-0.672343	-1.562095	-0.103008
6451	H	0.197602	-1.971646	-1.338650
6452	O	-0.767492	1.574726	0.975109
6453	H	-0.741183	1.421738	-0.008229
6454	H	0.127308	1.864066	1.227876
6455	O	-0.927895	-1.114808	1.590396
6456	H	-1.000829	-0.139668	1.526821
6457	H	-1.798412	-1.456576	1.874170
6458	O	1.862051	0.995833	-1.643747
6459	H	1.878652	0.015345	-1.564578
6460	H	0.964364	1.231464	-1.939837
6461	O	2.102724	-1.671549	-1.059582
6462	H	2.069501	-1.566183	-0.082456
6463	H	3.020846	-1.913394	-1.276369
6464	O	1.844216	-1.051102	1.592170
6465	H	0.951595	-1.306872	1.883274
6466	H	1.833595	-0.071542	1.500186
6467	O	2.006643	1.617591	0.998183
6468	H	2.011928	1.503663	0.019020
6469	H	2.908852	1.887919	1.247473
6470	O	4.882316	-1.574805	-1.193649
6471	H	5.595472	-1.988674	-1.689000
6472	H	4.876453	-0.601044	-1.412417
6473	O	4.657801	1.025321	-1.514933
6474	H	4.787864	1.423578	-0.635116
6475	H	3.750441	1.244076	-1.788628
6476	O	4.644211	-0.995099	1.553180
6477	H	3.734951	-1.245846	1.790366
6478	H	4.824147	-1.388378	0.679537
6479	O	4.773648	1.610988	1.242517
6480	H	4.800952	0.636282	1.457201
6481	H	5.457551	2.050448	1.756641

6482

6483 Cartesian coordinates of : W18_ 3

6484

6485	O	-0.551287	-2.907618	-2.244428
6486	H	-0.676008	-3.613051	-2.886917
6487	H	0.436132	-2.840517	-2.051364
6488	O	2.705110	-0.710839	2.976609
6489	H	3.111508	-0.224493	2.210531
6490	H	3.396138	-0.862790	3.628461
6491	O	-0.973422	3.378857	-0.510196
6492	H	-1.002117	3.040483	-1.420364
6493	H	-1.782417	3.064809	-0.067616
6494	O	0.104368	0.040794	0.108740
6495	H	-0.355304	-0.034798	-0.757508
6496	H	0.574835	0.900465	0.156840
6497	O	3.232710	-0.257328	-1.806562
6498	H	4.045458	-0.208445	-2.320720
6499	H	2.716725	0.571615	-2.001648
6500	O	1.236453	-2.201564	1.120497
6501	H	1.764195	-2.004569	1.913554
6502	H	0.915167	-1.329608	0.800008
6503	O	-3.638588	-0.107213	-0.648371
6504	H	-3.646222	-0.760618	0.076255
6505	H	-3.654571	0.766532	-0.221670
6506	O	1.954601	2.020409	-2.044997
6507	H	1.076312	2.080414	-2.467882
6508	H	1.880726	2.440131	-1.174927
6509	O	-3.111516	2.219382	0.914537
6510	H	-3.680839	2.774100	1.457045
6511	H	-2.619484	1.601163	1.514186
6512	O	-1.247002	-3.277331	0.479750
6513	H	-0.379932	-3.063417	0.875060
6514	H	-1.121619	-3.226306	-0.486065
6515	O	-0.652853	2.030291	-3.001671
6516	H	-0.999656	1.117528	-2.834509
6517	H	-0.940541	2.307764	-3.876602
6518	O	-1.696933	0.320521	2.116657
6519	H	-1.089953	0.142282	1.358632
6520	H	-2.264447	-0.471005	2.180936
6521	O	0.742335	1.332558	3.151231

6522	H	1.362727	0.595454	3.291195
6523	H	-0.146308	0.942916	3.105476
6524	O	3.481331	0.652069	0.859919
6525	H	2.916283	1.434330	0.759091
6526	H	3.474947	0.200630	-0.004176
6527	O	-3.210901	-1.911528	1.465993
6528	H	-3.849086	-2.486826	1.898367
6529	H	-2.479652	-2.492375	1.095534
6530	O	1.242568	2.460515	0.732489
6531	H	0.467383	2.979061	0.415087
6532	H	1.081229	2.232136	1.679468
6533	O	-1.437887	-0.315973	-2.101571
6534	H	-1.233317	-1.241259	-2.345643
6535	H	-2.311510	-0.295438	-1.624191
6536	O	1.916159	-2.698395	-1.517580
6537	H	2.369709	-1.863232	-1.740637
6538	H	1.881541	-2.713915	-0.541651

6539

6540 Cartesian coordinates of : W18_ 4

6541

6542	O	2.911797	2.747643	-0.232579
6543	H	2.905200	2.155492	-1.037831
6544	H	3.586431	3.418874	-0.374726
6545	H	2.862928	1.870421	1.382295
6546	O	2.682269	1.433104	2.236411
6547	H	1.767361	1.659058	2.474796
6548	O	2.920684	-1.166597	2.475721
6549	H	2.911294	-0.173378	2.363147
6550	H	3.593777	-1.373672	3.131383
6551	O	2.685614	-2.670706	0.115507
6552	H	2.870087	-2.146661	0.918281
6553	H	1.769410	-2.985713	0.195174
6554	O	2.677203	1.232608	-2.358854
6555	H	2.863682	0.275867	-2.302940
6556	H	1.760363	1.317907	-2.670200
6557	H	2.908197	-1.966719	-1.335155
6558	O	2.916747	-1.561682	-2.248930
6559	H	3.591730	-2.020718	-2.758329
6560	H	1.032284	3.033804	-0.102476
6561	O	0.124240	2.686247	-0.053246
6562	H	0.071667	2.164369	0.783692
6563	H	-0.070203	0.401888	2.243811
6564	O	-0.128461	1.387017	2.283937
6565	H	-1.038178	1.596253	2.560449
6566	H	1.042454	-1.417464	2.653975
6567	O	0.133340	-1.285667	2.331359
6568	H	0.074836	-1.756335	1.464986
6569	H	-0.071570	-2.164058	-0.783932
6570	O	-0.124347	-2.685893	0.053022
6571	H	-1.032470	-3.033273	0.102135
6572	H	1.038354	-1.596197	-2.560589
6573	O	0.128607	-1.386921	-2.284216
6574	H	0.070314	-0.401797	-2.244124
6575	O	-0.133458	1.285685	-2.331463
6576	H	-0.074954	1.756439	-1.465151
6577	H	-1.042582	1.417459	-2.654064
6578	H	-1.769713	2.985559	-0.194941
6579	O	-2.685827	2.670336	-0.115126
6580	H	-2.870379	2.146471	-0.918002
6581	H	-2.908196	1.966181	1.335472
6582	O	-2.916582	1.561086	2.249220
6583	H	-3.591717	2.019825	2.758683
6584	H	-1.760162	-1.318407	2.670501
6585	O	-2.676964	-1.233009	2.359057
6586	H	-2.863270	-0.276171	2.303172
6587	H	-2.904834	-2.155096	1.037840
6588	O	-2.911695	-2.747120	0.232434
6589	H	-3.586080	-3.418558	0.374872
6590	O	-2.682300	-1.432910	-2.236600
6591	H	-1.767394	-1.658855	-2.474981
6592	H	-2.862965	-1.870231	-1.382490
6593	O	-2.920898	1.166775	-2.475675
6594	H	-3.593977	1.373925	-3.131330
6595	H	-2.911481	0.173542	-2.363229

6596

6597 Cartesian coordinates of : W18_ 5

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6598
6599 0      1.367841      2.608518      -1.054869
6600 H      0.694770      3.312104      -1.055953
6601 H      0.959167      1.864979      -1.556291
6602 O      0.005797      0.488828      -2.063027
6603 H      -0.127288      0.155105      -1.149552
6604 H      0.373399      -0.285636      -2.548926
6605 O      -3.904459      0.264065      -0.785082
6606 H      -3.337383      0.916838      -1.307737
6607 H      -4.803926      0.332823      -1.119657
6608 O      3.647149      0.575355      2.054651
6609 H      3.337128      -0.361957      1.913205
6610 H      4.337639      0.562581      2.723908
6611 O      -1.097046      3.911651      -0.581106
6612 H      -1.385557      4.829036      -0.618601
6613 H      -1.214103      3.603039      0.360835
6614 O      -0.210447      -0.148206      0.581392
6615 H      0.417753      0.472603      1.021282
6616 H      0.025621      -1.066670      0.834310
6617 O      1.054424      -1.878158      -2.798286
6618 H      1.908789      -1.829749      -2.334798
6619 H      0.499262      -2.506906      -2.306151
6620 O      2.830263      -1.824818      1.382764
6621 H      1.963646      -2.232267      1.547410
6622 H      2.996733      -1.866560      0.421914
6623 O      -2.351719      1.862990      -2.071640
6624 H      -1.548432      1.353495      -2.305101
6625 H      -2.025694      2.653089      -1.601881
6626 O      0.133359      -2.745512      1.340099
6627 H      -0.679263      -2.743942      1.877822
6628 H      -0.071492      -3.225872      0.513127
6629 O      -2.434407      -2.157649      2.404973
6630 H      -2.909068      -2.469624      3.181457
6631 H      -2.566544      -1.179189      2.339442
6632 O      -2.582142      0.406653      1.641951
6633 H      -3.263634      0.462624      0.944835
6634 H      -1.736168      0.227228      1.157385
6635 O      1.267700      1.860273      1.565580
6636 H      1.429683      2.212595      0.660770
6637 H      2.124731      1.585931      1.940982
6638 O      -0.680380      -3.499035      -1.195264
6639 H      -1.543165      -3.026371      -1.033412
6640 H      -0.899311      -4.362929      -1.559113
6641 O      -1.281036      2.950908      1.868618
6642 H      -1.873920      2.183462      1.957134
6643 H      -0.383252      2.626283      2.060772
6644 O      3.785662      1.148271      -0.711739
6645 H      3.876521      1.136642      0.257493
6646 H      3.138432      1.836754      -0.936693
6647 O      -2.887936      -2.321959      -0.419016
6648 H      -2.911661      -2.373441      0.550877
6649 H      -3.223747      -1.437817      -0.665081
6650 O      3.418415      -1.403752      -1.319304
6651 H      4.244918      -1.723239      -1.696293
6652 H      3.527104      -0.422424      -1.195268
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6653
6654 Cartesian coordinates of : W18_ 6

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6655
6656 O      0.478747      1.524390      1.645659
6657 O      0.272289      1.960485      -1.037595
6658 O      -2.242303      0.963211      1.630185
6659 O      -1.961414      -1.683881      0.980760
6660 O      -1.827218      -1.008166      -1.669013
6661 O      -2.482814      1.572342      -1.033927
6662 O      0.921711      -0.658745      -1.530389
6663 O      0.751847      -1.158766      1.192151
6664 O      -4.703899      -2.095695      1.118489
6665 O      -4.994886      0.489667      1.464690
6666 O      -5.207283      1.067038      -1.284061
6667 O      -4.590935      -1.466436      -1.625559
6668 H      -2.077074      0.000109      1.516907
6669 H      -1.416404      1.347691      1.970181
6670 H      -0.651900      2.149354      -1.272796
6671 H      0.457517      1.042990      -1.340078
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6672	H	-2.002423	-0.046069	-1.560792
6673	H	-0.907348	-1.090075	-1.973957
6674	H	0.589153	-0.227913	1.467273
6675	H	-0.075962	-1.643101	1.354058
6676	H	0.431322	1.810797	0.704582
6677	H	1.338196	1.828288	1.986713
6678	H	-2.461012	1.469386	-0.056601
6679	H	-1.927250	-1.568096	0.004318
6680	H	0.914848	-0.957564	-0.596034
6681	H	1.859989	-0.645272	-1.798281
6682	H	-3.653987	-1.543393	-1.874605
6683	H	-4.683828	-1.891827	-0.753669
6684	H	-5.053867	0.107964	-1.513219
6685	H	-5.201767	0.867379	0.590290
6686	H	-4.144444	0.872789	1.740326
6687	H	-4.892031	-1.140925	1.343165
6688	H	-2.828025	-2.082690	1.180240
6689	H	-3.420164	1.675487	-1.278404
6690	H	-5.324366	-2.647094	1.604378
6691	H	-5.950543	1.386096	-1.804658
6692	H	3.556207	0.864244	-1.415853
6693	O	3.620918	-0.118084	-1.468060
6694	H	4.523224	-0.373174	-1.750312
6695	H	3.152643	2.484609	0.079115
6696	O	3.044912	2.450674	-0.885924
6697	H	2.101005	2.592660	-1.064292
6698	H	3.502772	-0.548983	0.146675
6699	O	3.489497	-0.716920	1.127592
6700	H	2.632932	-1.141516	1.316661
6701	H	3.436474	0.907714	1.748683
6702	O	3.236084	1.859805	1.917355
6703	H	3.897183	2.196980	2.529748
6704	O	6.187755	-1.012358	-1.643975
6705	H	6.291248	-1.388319	-0.747288
6706	H	6.646437	-1.589748	-2.259682
6707	H	5.105428	-1.548289	1.222564
6708	O	6.014382	-1.826205	0.992855
6709	H	6.176704	-2.669321	1.424794

6710

6711 Cartesian coordinates of : W18_ 7

6712

6713	O	1.254277	-2.330930	-1.746236
6714	H	1.985814	-1.822969	-2.139482
6715	H	1.559648	-2.620799	-0.867882
6716	O	-1.881927	0.946685	1.689405
6717	H	-1.933305	-0.029818	1.546333
6718	H	-1.169512	1.086335	2.342674
6719	O	4.483058	1.131991	0.746162
6720	H	4.463969	0.141373	0.572609
6721	H	5.343878	1.350002	1.115876
6722	O	-1.083115	-1.127593	-1.435508
6723	H	-0.911460	-0.171672	-1.348514
6724	H	-0.220620	-1.578238	-1.635979
6725	O	4.352061	-1.362747	0.077164
6726	H	3.633599	-1.897948	0.468132
6727	H	4.191440	-1.348312	-0.884072
6728	O	0.348157	-1.871019	2.470036
6729	H	0.446747	-0.950321	2.775873
6730	H	-0.545126	-1.948244	2.089419
6731	O	-3.879736	1.827049	-1.635866
6732	H	-4.218323	1.660994	-0.708179
6733	H	-4.417098	2.518905	-2.032902
6734	O	2.165260	-2.872366	0.885036
6735	H	1.490678	-2.470798	1.506746
6736	H	2.322699	-3.771053	1.191589
6737	O	-3.776080	-0.964681	-2.064467
6738	H	-3.850904	0.000888	-2.163428
6739	H	-2.819513	-1.162002	-2.067929
6740	O	-4.725987	-1.581054	0.286667
6741	H	-4.450562	-1.423428	-0.663217
6742	H	-5.462127	-2.199998	0.287783
6743	O	3.405120	1.697352	-1.782353
6744	H	3.888584	1.688294	-0.935961
6745	H	2.551420	2.128999	-1.601930
6746	O	-4.525381	1.176514	0.807984

6747	H	-4.758078	0.229325	0.808025
6748	H	-3.721898	1.261225	1.351698
6749	O	-2.037764	-1.648685	1.021974
6750	H	-2.982750	-1.875509	0.951052
6751	H	-1.693276	-1.577678	0.096683
6752	O	0.452995	0.868529	3.178215
6753	H	1.119992	1.375534	2.625645
6754	H	0.582390	1.135663	4.093531
6755	O	-1.226515	1.620396	-0.840094
6756	H	-2.066481	1.860380	-1.277478
6757	H	-1.454880	1.463801	0.109973
6758	O	2.108033	2.206376	1.689612
6759	H	2.970642	1.808346	1.460791
6760	H	1.728615	2.542293	0.857777
6761	O	1.062482	2.965095	-0.837175
6762	H	0.178482	2.523193	-0.919455
6763	H	0.935749	3.898138	-1.036258
6764	O	3.495221	-0.815020	-2.539837
6765	H	3.412830	0.161157	-2.352213
6766	H	3.947467	-0.913201	-3.383093

6767

6768 Cartesian coordinates of : W18_ 8

6769

6770	O	1.785124	-3.713062	0.894242
6771	H	2.137602	-4.584946	1.097479
6772	H	1.698616	-3.643340	-0.098487
6773	O	-1.330252	-2.473802	-1.770967
6774	H	-2.281211	-2.324228	-1.894853
6775	H	-1.203731	-2.538357	-0.795256
6776	O	-0.764063	-2.507341	0.873869
6777	H	-0.036965	-3.122196	1.071612
6778	H	-0.429273	-1.611198	1.107484
6779	O	-0.203849	0.012472	-1.819212
6780	H	0.652214	-0.218287	-1.387024
6781	H	-0.612287	-0.852211	-2.039833
6782	O	0.012503	-0.094039	1.813281
6783	H	-0.871753	0.223824	2.101676
6784	H	0.397527	0.654974	1.308086
6785	O	-1.175142	3.342573	1.639906
6786	H	-1.733285	2.662717	2.053023
6787	H	-0.267751	2.990089	1.618467
6788	O	3.826005	1.248601	1.306347
6789	H	4.452155	1.555616	1.969920
6790	H	3.594197	0.326957	1.539842
6791	O	1.198169	2.114304	0.802516
6792	H	2.136260	1.998698	1.035121
6793	H	1.130404	2.264531	-0.166944
6794	O	-1.621289	3.772340	-0.917352
6795	H	-1.502425	3.713265	0.072383
6796	H	-2.035179	4.618512	-1.113417
6797	O	1.444409	-3.243180	-1.669029
6798	H	0.526072	-3.194692	-1.979924
6799	H	1.809568	-2.340784	-1.720388
6800	O	0.765323	2.602510	-1.841778
6801	H	0.393749	1.776795	-2.201750
6802	H	0.005097	3.201644	-1.716168
6803	O	-3.836540	-1.182929	-1.271465
6804	H	-3.472551	-0.274014	-1.202781
6805	H	-4.698705	-1.116402	-1.693717
6806	O	2.243593	-0.667544	-1.000448
6807	H	2.384689	-0.783179	-0.041057
6808	H	2.791400	0.096308	-1.292917
6809	O	3.493107	1.670483	-1.562375
6810	H	2.788097	2.304523	-1.767239
6811	H	3.833913	1.871865	-0.678897
6812	O	-2.529710	0.864769	1.980499
6813	H	-3.029182	0.041835	2.148253
6814	H	-2.557187	0.945522	1.002762
6815	O	-3.431514	-1.734033	1.549785
6816	H	-3.742633	-1.683233	0.631590
6817	H	-2.600495	-2.234290	1.504632
6818	O	2.528107	-1.160389	1.738691
6819	H	1.663353	-0.891211	2.102966
6820	H	2.477671	-2.127611	1.605327
6821	O	-2.391674	1.088377	-0.763700

6822	H	-2.387329	2.033762	-0.997642
6823	H	-1.509094	0.737842	-1.044809
6824				
6825	Cartesian coordinates of : W18_ 9			
6826				
6827	O	0.530441	0.628313	2.733415
6828	H	1.155562	1.139547	2.134046
6829	H	0.785116	0.781846	3.648373
6830	O	-2.001724	1.304387	-1.302023
6831	H	-1.758256	1.357855	-0.354093
6832	H	-1.435436	1.950994	-1.758925
6833	O	4.432790	-0.005900	-1.431538
6834	H	4.455226	0.102411	-0.441366
6835	H	5.289526	0.252692	-1.783807
6836	O	0.247448	-1.783569	1.468361
6837	H	0.334503	-0.960786	1.991493
6838	H	1.099112	-2.243199	1.593958
6839	O	4.142747	0.165991	1.181175
6840	H	3.547054	0.906192	1.380303
6841	H	3.709468	-0.657664	1.473991
6842	O	0.037957	3.814724	0.559957
6843	H	-0.015227	3.775193	-0.409368
6844	H	-0.747659	3.348235	0.892239
6845	O	-3.709122	-2.424041	-1.061839
6846	H	-4.206762	-3.240511	-1.163686
6847	H	-3.257777	-2.444548	-0.172751
6848	O	1.949148	1.959739	1.035946
6849	H	1.881579	1.550179	0.140800
6850	H	1.411665	2.784387	0.960889
6851	O	-2.560058	-2.185641	1.283652
6852	H	-1.592477	-2.164784	1.393190
6853	H	-2.931671	-1.377026	1.677255
6854	O	-3.960161	0.232146	1.820525
6855	H	-4.289949	0.256555	0.873791
6856	H	-4.718860	0.345342	2.400944
6857	O	3.149384	-2.502082	-1.143320
6858	H	3.709141	-1.765989	-1.446784
6859	H	2.236793	-2.274497	-1.410020
6860	O	-4.535824	0.230784	-0.719791
6861	H	-3.831401	0.754231	-1.141083
6862	H	-4.415368	-0.691151	-1.014333
6863	O	-1.671914	1.710530	1.422971
6864	H	-2.533993	1.360148	1.720294
6865	H	-0.994484	1.296081	1.989235
6866	O	0.126587	2.932467	-2.157226
6867	H	0.819993	2.237660	-2.066464
6868	H	0.268680	3.382533	-2.995560
6869	O	-1.656514	-1.187694	-2.509123
6870	H	-1.854988	-0.302240	-2.147081
6871	H	-2.369034	-1.771887	-2.196891
6872	O	1.810536	0.933693	-1.482659
6873	H	1.334993	0.055608	-1.443113
6874	H	2.737183	0.736142	-1.714901
6875	O	0.629525	-1.405495	-1.257353
6876	H	-0.213412	-1.444698	-1.789138
6877	H	0.377731	-1.507582	-0.315735
6878	O	2.971480	-2.404255	1.450983
6879	H	3.095632	-2.532448	0.462264
6880	H	3.455992	-3.107591	1.895139

6881

6882 Cartesian coordinates of : W18_10

6883

6884	O	-0.070102	2.062619	-1.477812
6885	H	-0.271447	1.842090	-0.538980
6886	H	0.322451	1.236918	-1.848088
6887	O	2.204736	-1.686270	2.102231
6888	H	2.353424	-2.249439	1.319370
6889	H	1.243142	-1.534502	2.164907
6890	O	-4.428984	-0.048511	0.915931
6891	H	-4.043789	0.838323	1.042011
6892	H	-4.453304	-0.197939	-0.047589
6893	O	1.294358	-0.202335	-2.013249
6894	H	0.787135	-0.948575	-1.630537
6895	H	1.970707	0.043653	-1.351848
6896	O	-3.927465	-0.461807	-1.815285

6897	H	-4.562010	-0.534633	-2.535078
6898	H	-3.467469	0.418702	-1.918067
6899	O	-3.080017	2.423633	0.969071
6900	H	-2.134566	2.209899	1.180861
6901	H	-3.332948	3.195913	1.483968
6902	O	3.769393	-1.641972	-2.069332
6903	H	4.043575	-0.813712	-1.637543
6904	H	3.015675	-1.365174	-2.613934
6905	O	-0.580092	1.598321	1.178628
6906	H	-0.546114	0.640742	1.410545
6907	H	0.238618	2.025568	1.538530
6908	O	3.516815	0.796617	-0.659070
6909	H	3.324190	1.728397	-0.866752
6910	H	3.656092	0.745062	0.307372
6911	O	1.763370	2.715361	1.796007
6912	H	2.055847	3.092232	0.948703
6913	H	2.411365	2.026820	2.031982
6914	O	-2.526111	-2.737124	-0.855337
6915	H	-2.982182	-1.998198	-1.298829
6916	H	-2.809020	-2.704078	0.075352
6917	O	3.530290	0.539557	2.087003
6918	H	4.272266	0.495571	2.697622
6919	H	3.035578	-0.333282	2.145629
6920	O	2.252763	3.300168	-0.955692
6921	H	1.365828	2.980234	-1.261332
6922	H	2.446119	4.122512	-1.415805
6923	O	-3.071941	-2.052379	1.864647
6924	H	-3.538513	-2.539028	2.550768
6925	H	-3.637276	-1.267753	1.603739
6926	O	2.612562	-3.226044	-0.253301
6927	H	3.105336	-2.686526	-0.926937
6928	H	3.080276	-4.062874	-0.167930
6929	O	-0.483242	-1.074011	1.643231
6930	H	-0.317796	-1.479456	0.760926
6931	H	-1.340379	-1.438972	1.938155
6932	O	0.057137	-2.269288	-0.730276
6933	H	-0.856182	-2.611662	-0.912533
6934	H	0.712158	-2.981618	-0.652044
6935	O	-2.858236	1.933617	-1.816252
6936	H	-3.053569	2.299853	-0.935810
6937	H	-1.895087	2.043721	-1.929949

6938

6939 Cartesian coordinates of : W18_11

6940

6941	O	4.364212	-0.713646	-1.401014
6942	H	5.149658	-1.022573	-1.861924
6943	H	3.680624	-1.425743	-1.445147
6944	O	2.307468	-2.351689	-1.112274
6945	H	1.575632	-2.770770	-1.584803
6946	H	2.015590	-2.232823	-0.184743
6947	O	1.772681	-1.847640	1.564789
6948	H	1.133195	-1.140942	1.749791
6949	H	2.659891	-1.439335	1.685511
6950	O	0.039686	-0.218168	-1.220917
6951	H	0.956970	0.060866	-1.431930
6952	H	-0.054631	-1.196889	-1.323647
6953	O	-0.188746	0.174007	1.379938
6954	H	-0.098376	0.058587	0.394495
6955	H	-0.740123	0.983607	1.487750
6956	O	-3.870588	0.695702	1.351445
6957	H	-3.448653	-0.127672	1.665288
6958	H	-3.256680	1.422750	1.552041
6959	O	0.624294	4.066536	0.919044
6960	H	0.620928	3.889712	-0.062783
6961	H	0.804646	5.002864	1.048320
6962	O	-1.658483	2.438429	1.148501
6963	H	-1.051756	3.185098	1.299251
6964	H	-1.725722	2.331089	0.172243
6965	O	-4.238681	0.380448	-1.202764
6966	H	-4.183429	0.550535	-0.213260
6967	H	-5.125226	0.617715	-1.493172
6968	O	2.354463	1.187533	-1.358271
6969	H	3.175375	0.725673	-1.604537
6970	H	2.419316	1.384326	-0.398733
6971	O	-1.796208	1.738795	-1.494450

6972	H	-1.222359	0.942191	-1.528577
6973	H	-2.702147	1.429988	-1.668501
6974	O	-0.478366	-2.838814	-1.297113
6975	H	-1.419574	-2.812186	-1.531802
6976	H	-0.433607	-3.239168	-0.393441
6977	O	2.169215	1.763434	1.329627
6978	H	1.406106	1.197622	1.549459
6979	H	1.829799	2.676471	1.380878
6980	O	0.548568	3.320621	-1.602213
6981	H	-0.312900	2.939328	-1.839005
6982	H	1.223838	2.642351	-1.785756
6983	O	-2.310733	-1.654077	1.562087
6984	H	-1.509526	-1.095680	1.521773
6985	H	-2.537658	-1.887036	0.643322
6986	O	-0.299479	-3.717982	1.254322
6987	H	0.533520	-3.349180	1.593677
6988	H	-1.014134	-3.263527	1.728186
6989	O	4.058951	-0.362094	1.434079
6990	H	3.723717	0.540678	1.548322
6991	H	4.363389	-0.432149	0.513128
6992	O	-3.250170	-2.186884	-1.101735
6993	H	-3.652370	-1.312926	-1.299165
6994	H	-3.968003	-2.828940	-1.107154

6995

6996 Cartesian coordinates of : W18_12

6997

6998	O	3.035511	-2.251176	1.678846
6999	H	3.732522	-2.633678	2.220660
7000	H	3.215589	-1.273428	1.619581
7001	O	3.633250	0.271907	1.207500
7002	H	3.165958	1.098371	1.414652
7003	H	3.823446	0.292366	0.251020
7004	O	3.796958	-0.003816	-1.570165
7005	H	3.396272	-0.912512	-1.533117
7006	H	4.611064	-0.081658	-2.077606
7007	O	-0.395320	-0.029217	1.161307
7008	H	-0.054874	-0.898021	1.466545
7009	H	-0.359556	-0.064756	0.173487
7010	O	-0.580505	-0.017896	-1.516967
7011	H	-0.339768	0.920817	-1.688165
7012	H	-1.560482	-0.089103	-1.568636
7013	O	-2.925719	2.468737	-1.329083
7014	H	-2.036279	2.642526	-1.682994
7015	H	-3.189501	1.580088	-1.616881
7016	O	-2.693910	-3.152093	-1.222495
7017	H	-2.682459	-3.099641	-0.229039
7018	H	-3.201929	-3.933313	-1.463345
7019	O	-3.260543	-0.369866	-1.307139
7020	H	-3.326820	-1.316497	-1.522724
7021	H	-3.345314	-0.302852	-0.330180
7022	O	-3.025211	2.835596	1.301266
7023	H	-3.051427	2.754339	0.310763
7024	H	-3.623877	3.548820	1.544043
7025	O	0.293445	-2.627216	1.468071
7026	H	1.222481	-2.684723	1.756799
7027	H	0.293309	-2.763595	0.495785
7028	O	-3.074200	-0.000693	1.408004
7029	H	-2.089678	0.056618	1.411023
7030	H	-3.378172	0.890490	1.645601
7031	O	2.477008	2.890673	1.323984
7032	H	1.511818	2.992348	1.462790
7033	H	2.916790	3.558866	1.859008
7034	O	0.080997	-2.654021	-1.288490
7035	H	-0.018291	-1.708134	-1.521674
7036	H	-0.789843	-3.047202	-1.480073
7037	O	-2.534784	-2.787033	1.396085
7038	H	-2.902565	-1.927647	1.660314
7039	H	-1.615196	-2.818932	1.711104
7040	O	-0.121604	2.645085	-1.489437
7041	H	0.821939	2.758863	-1.739135
7042	H	-0.131528	2.753505	-0.517416
7043	O	2.599669	2.588455	-1.547094
7044	H	2.756889	2.783495	-0.609285
7045	H	2.944724	1.691952	-1.698915
7046	O	2.881508	-2.456227	-1.150638

7047	H	2.972549	-2.582585	-0.189295
7048	H	1.982318	-2.739033	-1.386619
7049	O	-0.225209	2.642281	1.333372
7050	H	-1.132038	2.937699	1.535727
7051	H	-0.228783	1.668303	1.460766
7052				
7053	Cartesian coordinates of : W18_13			
7054				
7055	O	0.804840	1.198417	-1.525664
7056	O	0.642472	-1.524668	-1.191916
7057	O	-1.962194	1.289743	-1.435333
7058	O	-2.129841	1.440090	1.293543
7059	O	-1.960513	-1.290027	1.434783
7060	O	-2.132387	-1.441154	-1.293296
7061	O	0.808389	-1.204849	1.526149
7062	O	0.644996	1.520002	1.192228
7063	O	-4.903189	1.612243	1.202335
7064	O	-4.756303	1.199134	-1.387740
7065	O	-4.906132	-1.609749	-1.201085
7066	O	-4.754995	-1.196768	1.388106
7067	H	-1.962611	1.466056	-0.467321
7068	H	-1.078247	1.531792	-1.760125
7069	H	-0.245895	-1.813586	-1.462871
7070	H	0.651788	-1.537013	-0.207931
7071	H	-1.962073	-1.466848	0.466894
7072	H	-1.076947	-1.534377	1.759371
7073	H	0.651820	1.530036	0.208129
7074	H	-0.243225	1.808390	1.464294
7075	H	0.782310	0.215702	-1.531617
7076	H	1.707445	1.449050	-1.795473
7077	H	-2.107963	-0.473650	-1.469271
7078	H	-2.105604	0.472524	1.469041
7079	H	0.786679	-0.222249	1.532989
7080	H	1.709895	-1.456525	1.797719
7081	H	-3.848827	-1.379322	1.691032
7082	H	-4.909898	-0.245616	1.532641
7083	H	-4.925883	-1.547773	-0.204632
7084	H	-4.912584	0.248081	-1.531824
7085	H	-3.850130	1.380353	-1.690923
7086	H	-4.924424	1.550025	0.205513
7087	H	-3.042427	1.727867	1.478012
7088	H	-3.045416	-1.728236	-1.477268
7089	H	-5.591516	2.224364	1.478917
7090	H	-5.594613	-2.222114	-1.477196
7091	H	3.496721	-1.357492	0.514576
7092	O	3.571338	-1.285443	1.492629
7093	H	4.300944	-1.890504	1.692913
7094	H	3.596943	-0.560166	-1.570661
7095	O	3.428549	-1.472153	-1.261464
7096	H	2.510671	-1.688585	-1.503987
7097	H	3.603355	0.562922	1.571862
7098	O	3.430909	1.474327	1.262963
7099	H	2.511152	1.684926	1.503743
7100	H	3.495115	1.361674	-0.512746
7101	O	3.566771	1.287312	-1.490960
7102	H	4.291119	1.896980	-1.695903
7103	O	5.281734	-3.025675	0.167223
7104	H	6.049660	-3.509084	-0.148090
7105	H	4.814707	-2.678518	-0.610385
7106	H	5.906628	3.687728	0.120641
7107	O	5.293412	3.007953	-0.170276
7108	H	4.818499	2.683313	0.612141
7109				
7110	Cartesian coordinates of : W18_14			
7111				
7112	O	-1.336410	2.127102	1.521967
7113	H	-2.265952	1.869494	1.676301
7114	H	-0.797978	1.318711	1.646564
7115	O	2.849366	-1.089184	1.523806
7116	H	2.571458	-1.994746	1.751026
7117	H	3.242724	-1.144729	0.632502
7118	O	-3.597222	-1.601552	1.120479
7119	H	-2.742915	-1.998932	1.370982
7120	H	-3.681951	-1.778110	0.166544
7121	O	-1.314024	2.431680	-1.292172

7122	H	-2.189749	2.054660	-1.532594
7123	H	-1.342046	2.478727	-0.316091
7124	O	-3.882726	0.986845	1.483063
7125	H	-3.780401	-0.005198	1.447568
7126	H	-4.655597	1.174084	2.024910
7127	O	1.505668	-3.572883	1.612698
7128	H	0.557148	-3.295766	1.580160
7129	H	1.566417	-4.359909	2.163003
7130	O	2.920500	1.373507	-1.364432
7131	H	2.567096	2.216351	-1.711688
7132	H	3.056726	1.545968	-0.400351
7133	O	0.312712	-0.025778	1.287222
7134	H	1.227240	-0.297748	1.507365
7135	H	0.335938	0.119995	0.305383
7136	O	0.931820	3.601170	1.397248
7137	H	0.025512	3.282798	1.585815
7138	H	1.064546	4.408127	1.905162
7139	O	3.092357	1.765053	1.298281
7140	H	2.299129	2.275761	1.537394
7141	H	3.075944	0.926167	1.780895
7142	O	-0.671059	-2.161056	-1.574793
7143	H	0.125274	-2.730035	-1.657936
7144	H	-0.315738	-1.247098	-1.630047
7145	O	1.277117	3.586151	-1.500749
7146	H	1.212213	3.734753	-0.542692
7147	H	0.362398	3.425293	-1.780484
7148	O	3.716387	-1.176803	-1.188658
7149	H	3.519428	-0.264169	-1.494269
7150	H	4.623182	-1.369113	-1.448870
7151	O	-0.901246	-2.437634	1.187207
7152	H	-0.545998	-1.535567	1.368240
7153	H	-0.903843	-2.467908	0.205469
7154	O	0.353329	0.356236	-1.351315
7155	H	-0.239582	1.143199	-1.464841
7156	H	1.274974	0.663622	-1.485076
7157	O	1.781918	-3.304813	-1.239927
7158	H	1.824859	-3.555222	-0.302253
7159	H	2.443686	-2.603985	-1.363435
7160	O	-3.335731	-1.792718	-1.697438
7161	H	-3.858243	-2.266684	-2.351924
7162	H	-2.396287	-2.056210	-1.821106
7163	O	-3.671774	1.070328	-1.386211
7164	H	-3.576349	0.125400	-1.590847
7165	H	-3.931126	1.122798	-0.451001

7166

7167 Cartesian coordinates of : W18_15

7168

7169	O	-2.130264	-1.732624	1.359190
7170	H	-1.347632	-1.162365	1.471969
7171	H	-1.753502	-2.647776	1.420356
7172	H	-2.428678	-1.642130	-0.442626
7173	O	-2.387995	-1.461601	-1.405407
7174	H	-3.084837	-0.790698	-1.568955
7175	O	-0.061139	-0.248019	-1.430710
7176	H	-0.944481	-0.705697	-1.533422
7177	H	0.624894	-0.969102	-1.540051
7178	H	-3.466767	-0.587517	1.635614
7179	O	-3.950308	0.266680	1.593516
7180	H	-4.724718	0.185568	2.159564
7181	H	-3.393212	1.488830	-1.425138
7182	O	-3.999864	0.750093	-1.264953
7183	H	-4.171675	0.727087	-0.309626
7184	O	-1.516468	2.215676	-1.320769
7185	H	-0.953380	2.994445	-1.492487
7186	H	-0.984530	1.441462	-1.571350
7187	H	-0.610984	0.818431	1.434650
7188	O	0.021048	0.086013	1.228916
7189	H	0.001166	-0.002342	0.238073
7190	O	-1.786490	2.054675	1.400083
7191	H	-1.829845	2.174181	0.425578
7192	H	-2.627217	1.644472	1.672451
7193	H	1.301674	1.097716	-1.611398
7194	O	2.040878	1.696245	-1.408394
7195	H	1.706681	2.597999	-1.570341
7196	O	0.555764	4.059249	-1.227700

7197	H	0.678483	4.967786	-1.520077
7198	H	0.568878	4.046827	-0.231839
7199	H	2.410170	1.605863	0.361864
7200	O	2.393970	1.454432	1.331417
7201	H	1.583371	0.914205	1.447271
7202	H	1.271676	3.069209	1.614902
7203	O	0.553683	3.683361	1.383081
7204	H	-0.277203	3.281988	1.686978
7205	H	2.597329	-1.711133	-1.606758
7206	O	1.737846	-2.150578	-1.425022
7207	H	1.749333	-2.321417	-0.460465
7208	H	3.580402	0.385367	-1.541244
7209	O	3.920773	-0.509672	-1.390809
7210	H	4.203717	-0.551476	-0.462348
7211	H	3.623996	0.234160	1.601387
7212	O	4.093105	-0.625627	1.492358
7213	H	4.862812	-0.623987	2.070212
7214	H	1.129625	-1.455016	1.591475
7215	O	1.717101	-2.196907	1.372653
7216	H	2.617268	-1.887764	1.580052
7217	H	0.268437	-3.691578	1.418085
7218	O	-0.633720	-3.928438	1.156726
7219	H	-0.612842	-4.020353	0.181228
7220	H	-1.325267	-3.105210	-1.878303
7221	O	-0.625390	-3.720367	-1.611548
7222	H	0.216616	-3.340779	-1.906306

7223

7224 Cartesian coordinates of : W18_16

7225

7226	O	1.356792	-2.285491	-0.824521
7227	O	1.763540	-1.802333	1.860512
7228	O	1.954149	1.958915	-0.064586
7229	O	2.195492	0.012217	-1.877871
7230	O	-1.371576	-1.993656	-1.085510
7231	O	-1.078815	-1.743338	1.604467
7232	O	-0.771856	2.235017	-0.263935
7233	O	-0.609107	0.342991	-2.183981
7234	H	1.281641	-2.078778	0.131549
7235	H	-0.255451	-2.155208	1.911315
7236	H	1.970770	1.224983	-0.734313
7237	H	-0.805010	-0.541965	-1.789876
7238	H	0.465917	-2.524381	-1.131074
7239	H	-0.968844	-0.783617	1.805120
7240	H	1.084751	2.392843	-0.150890
7241	H	0.304093	0.319360	-2.510360
7242	H	3.156603	-0.035579	-2.014402
7243	H	-2.299731	-2.149971	-1.339893
7244	H	2.661278	-2.095958	1.611311
7245	H	-1.636777	2.684934	-0.296427
7246	H	1.925676	-0.867946	-1.511209
7247	H	-1.360121	-1.906679	-0.103754
7248	H	1.866175	-0.875184	2.145406
7249	H	-0.785194	1.560317	-0.984450
7250	H	2.771862	1.280578	2.950944
7251	O	2.035482	0.944592	2.430232
7252	H	2.104126	1.338586	1.527450
7253	H	0.101414	1.046333	2.550439
7254	O	-0.750811	0.906377	2.106193
7255	H	-0.700399	1.388953	1.248369
7256	O	-3.580729	1.109308	1.978865
7257	H	-3.641690	1.718417	1.221921
7258	H	-2.672552	1.180782	2.313129
7259	H	-4.107944	3.382902	-0.618281
7260	O	-3.501272	2.668324	-0.402799
7261	H	-3.566830	1.982644	-1.126205
7262	O	-3.419029	0.800713	-2.237746
7263	H	-3.731616	-0.080801	-1.950700
7264	H	-2.506611	0.687969	-2.548499
7265	O	-4.111848	-1.716278	-1.261120
7266	H	-4.123925	-1.650387	-0.254063
7267	H	-4.890065	-2.208303	-1.539508
7268	H	-3.887800	-0.553806	1.577107
7269	O	-3.903565	-1.499433	1.296790
7270	H	-3.067712	-1.873827	1.617777
7271	O	3.984769	-2.390147	0.259953

7272	H	3.380017	-2.737868	-0.411070
7273	H	4.392736	-1.603936	-0.139322
7274	H	5.792386	-0.206363	-1.651520
7275	O	4.941297	-0.082025	-1.219702
7276	H	4.971611	0.785594	-0.758179
7277	O	4.625825	2.326885	0.034374
7278	H	3.657680	2.459853	-0.033565
7279	H	5.049630	3.154401	-0.211193
7280				
7281				
7282	Cartesian coordinates of the water nonadecamer			
7283				
7284	Cartesian coordinates of : W19_ 1			
7285				
7286	O	0.225612	3.613654	0.974446
7287	H	0.937115	2.951895	1.232214
7288	H	0.441781	4.457227	1.382443
7289	O	-1.556236	-0.272286	3.290566
7290	H	-2.153098	-0.177100	4.039386
7291	H	-1.649449	0.536004	2.725236
7292	O	3.914178	-1.402677	-0.178208
7293	H	3.158882	-1.683483	0.381250
7294	H	3.615966	-1.548007	-1.091673
7295	O	-3.639084	1.501259	-0.195368
7296	H	-3.298586	1.725497	-1.080669
7297	H	-3.901843	0.563012	-0.225899
7298	O	-0.048876	-0.073836	-0.056900
7299	H	-0.523365	0.537664	0.547185
7300	H	-0.705450	-0.366822	-0.724327
7301	O	1.274093	-0.204145	3.350959
7302	H	0.319958	-0.256092	3.530698
7303	H	1.472676	-0.985906	2.804394
7304	O	1.565569	-1.902074	1.165675
7305	H	0.971314	-1.260569	0.712765
7306	H	1.133516	-2.763082	1.028301
7307	O	0.116216	-2.719753	-2.171707
7308	H	-0.578149	-2.058969	-2.348649
7309	H	0.969873	-2.276791	-2.333084
7310	O	1.843414	1.706226	1.553821
7311	H	1.650022	1.065689	2.282450
7312	H	2.771052	1.595215	1.282669
7313	O	-2.297521	-2.264079	1.434027
7314	H	-1.958245	-1.648458	2.110037
7315	H	-1.547781	-2.764064	1.056666
7316	O	1.911560	1.126085	-1.490788
7317	H	2.723405	1.383548	-1.015236
7318	H	1.291177	0.769255	-0.810279
7319	O	-3.900883	-1.289948	-0.337847
7320	H	-4.702477	-1.818827	-0.391301
7321	H	-3.319006	-1.684274	0.383490
7322	O	-1.837035	-0.744016	-2.066803
7323	H	-2.668303	-1.021561	-1.633169
7324	H	-1.992876	0.141285	-2.451323
7325	O	4.175754	1.163384	0.149913
7326	H	4.193129	0.164031	0.061621
7327	H	5.081160	1.480352	0.211580
7328	O	-0.262068	-3.734926	0.196558
7329	H	-0.403071	-4.685450	0.150342
7330	H	-0.112529	-3.404317	-0.737813
7331	O	-1.606608	1.632138	1.471756
7332	H	-1.145053	2.491181	1.431703
7333	H	-2.409859	1.670896	0.883225
7334	O	2.470762	-1.226970	-2.628100
7335	H	2.269544	-0.299894	-2.339967
7336	H	2.769733	-1.191063	-3.542198
7337	O	-2.225859	1.940868	-2.583935
7338	H	-2.536864	2.401189	-3.369407
7339	H	-1.392636	2.412669	-2.274494
7340	O	-0.055276	3.103032	-1.773281
7341	H	0.720095	2.516940	-1.857787
7342	H	-0.033443	3.415697	-0.848637
7343				
7344	Cartesian coordinates of : W19_ 2			
7345				
7346	O	3.964854	2.427435	-0.226541

7347	H	3.888564	1.913383	-1.090803
7348	H	4.430973	3.249447	-0.406628
7349	O	1.326430	1.968160	0.410034
7350	H	0.720601	2.720780	0.591120
7351	H	2.238290	2.309139	0.320093
7352	O	0.907417	0.473689	-1.906228
7353	H	0.975922	1.063422	-1.125563
7354	H	0.915171	-0.430784	-1.529053
7355	O	-5.180178	1.399076	0.449517
7356	H	-5.927850	1.908069	0.776541
7357	H	-5.075981	0.586448	1.022776
7358	O	3.660738	0.902388	-2.286759
7359	H	2.706826	0.715057	-2.385139
7360	H	4.100030	0.053895	-2.086024
7361	O	-1.877340	-0.403417	1.808413
7362	H	-0.952902	-0.443318	2.116136
7363	H	-1.994397	0.479243	1.397818
7364	O	4.963463	-1.351198	-1.263377
7365	H	5.631776	-1.871956	-1.718884
7366	H	4.326481	-1.988372	-0.821897
7367	O	5.056541	0.193996	1.074346
7368	H	5.247462	-0.294229	0.251841
7369	H	4.739917	1.071343	0.790507
7370	O	3.435224	-1.315260	2.449709
7371	H	3.805864	-1.544165	3.307455
7372	H	4.076173	-0.689969	1.999857
7373	O	-4.705951	-0.053061	-1.909982
7374	H	-3.810822	0.186969	-2.203811
7375	H	-4.972468	0.606898	-1.245058
7376	O	-1.901408	0.306396	-1.880533
7377	H	-0.987479	0.482997	-2.177303
7378	H	-1.876288	-0.580347	-1.456831
7379	O	-0.639687	3.779912	0.844604
7380	H	-1.404104	3.196229	0.650420
7381	H	-0.764292	4.590164	0.342603
7382	O	-2.461266	1.840112	0.290489
7383	H	-3.433217	1.905175	0.363141
7384	H	-2.267394	1.380382	-0.560876
7385	O	-4.756785	-2.349753	-0.623455
7386	H	-5.382439	-3.003931	-0.948574
7387	H	-4.813867	-1.541751	-1.204401
7388	O	3.282739	-2.834135	0.055598
7389	H	3.314736	-2.529984	0.980368
7390	H	2.359555	-2.702333	-0.234076
7391	O	0.730154	-1.889212	-0.450222
7392	H	-0.157586	-2.272378	-0.559529
7393	H	0.709723	-1.394265	0.402138
7394	O	0.916574	-0.357350	1.792974
7395	H	1.113181	0.529956	1.418176
7396	H	1.738498	-0.667773	2.221535
7397	O	-2.022748	-2.004498	-0.397867
7398	H	-2.895807	-2.419364	-0.515277
7399	H	-2.038408	-1.533933	0.465566
7400	O	-4.670979	-0.819435	1.736085
7401	H	-3.748814	-0.823201	2.044991
7402	H	-4.757960	-1.527732	1.072210

7403

7404 Cartesian coordinates of : W19_ 3

7405

7406	O	1.336582	1.069522	2.066576
7407	O	1.295364	2.784850	-0.076384
7408	O	1.641918	-1.501240	-1.328338
7409	O	1.815253	-1.531111	1.366966
7410	O	-1.444995	0.711090	2.160158
7411	O	-1.452908	2.342545	-0.007855
7412	O	-1.109887	-1.741774	-1.458157
7413	O	-0.947649	-1.776791	1.247974
7414	H	1.244087	1.703747	1.324187
7415	H	-0.643510	2.877030	0.034070
7416	H	1.637192	-1.559561	-0.342483
7417	H	-1.066899	-0.860574	1.598671
7418	H	0.465519	1.032837	2.498531
7419	H	-1.340267	1.797990	-0.822374
7420	H	0.788966	-1.859382	-1.631507
7421	H	-0.048014	-2.048059	1.494213

7422	H	2.726876	-1.792000	1.590601
7423	H	-2.354365	0.641023	2.505968
7424	H	1.969179	3.472384	-0.078556
7425	H	-1.982693	-2.084758	-1.725738
7426	H	1.707825	-0.589538	1.629520
7427	H	-1.506581	1.301914	1.372484
7428	H	1.494246	2.172181	-0.836444
7429	H	-1.108142	-1.759594	-0.471421
7430	H	2.811973	1.248072	-2.127637
7431	O	1.855924	1.093924	-2.040100
7432	H	1.771145	0.149290	-1.760030
7433	H	-0.140198	1.077951	-2.606310
7434	O	-1.003217	0.842547	-2.234482
7435	H	-0.963313	-0.110073	-1.978844
7436	O	-3.870644	0.618126	-2.132603
7437	H	-3.926279	-0.349675	-2.037468
7438	H	-2.984953	0.812646	-2.474660
7439	H	-4.472414	-2.799344	-1.893285
7440	O	-3.847573	-2.151985	-1.553058
7441	H	-3.902170	-2.168745	-0.554773
7442	O	-3.731994	-2.130697	1.061946
7443	H	-3.997734	-1.300694	1.505064
7444	H	-2.803631	-2.279566	1.308015
7445	O	-4.207556	0.367623	2.230145
7446	H	-4.304586	1.004750	1.453317
7447	H	-4.932255	0.536347	2.839959
7448	H	-4.237718	1.493475	-0.648473
7449	O	-4.232303	1.973264	0.211275
7450	H	-3.389598	2.455728	0.204464
7451	O	4.138400	1.015786	1.433349
7452	H	3.294254	1.155174	1.890643
7453	H	4.410666	0.098736	1.623183
7454	H	5.262660	-2.330882	1.742990
7455	O	4.584325	-1.745666	1.393135
7456	H	4.620476	-1.776682	0.395737
7457	O	4.437734	-1.546924	-1.217325
7458	H	3.526854	-1.746021	-1.497262
7459	H	4.575437	-0.600916	-1.402077
7460	O	4.509978	1.294439	-1.193426
7461	H	4.346417	1.289796	-0.213844
7462	H	5.317530	1.794777	-1.346796

7463

7464 Cartesian coordinates of : W19_ 4

7465

7466	O	4.010317	-1.584261	-1.880925
7467	H	3.052868	-1.501071	-2.040159
7468	H	4.114541	-2.140192	-1.087358
7469	O	4.285828	-2.592171	0.740477
7470	H	4.600266	-1.703079	1.069181
7471	H	4.849097	-3.273373	1.119538
7472	O	-4.564797	-0.313117	1.891068
7473	H	-4.319766	-1.246928	1.633113
7474	H	-5.189424	-0.359017	2.621147
7475	O	-4.955583	0.318591	-0.866564
7476	H	-4.861275	-0.567955	-1.253720
7477	H	-5.055835	0.191124	0.092042
7478	O	-1.100114	-1.802151	0.938336
7479	H	-1.283114	-0.906505	1.295128
7480	H	-0.164930	-2.009266	1.123353
7481	O	4.841083	-0.117433	1.397373
7482	H	4.051903	0.305636	1.778367
7483	H	5.027523	0.350664	0.562783
7484	O	-2.011758	0.730146	1.498567
7485	H	-2.904482	0.529155	1.842135
7486	H	-2.154930	1.030039	0.561219
7487	O	-3.753413	-2.623969	0.969466
7488	H	-2.781966	-2.611681	1.047065
7489	H	-3.944524	-2.678448	0.016126
7490	O	1.647729	-1.765446	0.989708
7491	H	1.861063	-0.894612	1.396800
7492	H	2.465021	-2.295655	1.023313
7493	O	4.947221	0.772822	-1.270263
7494	H	4.681683	-0.132898	-1.602671
7495	H	5.669930	1.097995	-1.815291
7496	O	1.294309	-0.947491	-1.614889

7497	H	1.307813	-1.317184	-0.704763
7498	H	0.382856	-1.053610	-1.943138
7499	O	-0.046136	2.302721	2.436860
7500	H	-0.841933	1.761853	2.212718
7501	H	-0.268662	2.848058	3.197827
7502	O	2.299465	1.506753	-0.873770
7503	H	3.241812	1.482779	-1.127015
7504	H	1.880911	0.722530	-1.290161
7505	O	-1.678787	3.829982	-1.502178
7506	H	-1.550477	4.317633	-2.319934
7507	H	-0.821274	3.833896	-1.011622
7508	O	2.203722	0.785903	1.743842
7509	H	1.523653	1.288107	2.227534
7510	H	2.213084	1.148797	0.828219
7511	O	-2.481309	1.321375	-1.062639
7512	H	-3.451197	1.150505	-1.109781
7513	H	-2.278123	2.243544	-1.347297
7514	O	-1.533411	-1.150155	-1.699380
7515	H	-1.777835	-0.200261	-1.617315
7516	H	-1.374788	-1.447822	-0.775543
7517	O	-4.000167	-2.202328	-1.816402
7518	H	-4.252389	-2.761074	-2.557707
7519	H	-3.075216	-1.886368	-1.967336
7520	O	0.574152	3.587306	-0.073241
7521	H	1.218661	2.969714	-0.461281
7522	H	0.382643	3.258349	0.820907

7523

7524 Cartesian coordinates of : W19_ 5

7525

7526	O	1.723749	0.829174	2.118974
7527	H	1.130444	0.108702	2.397811
7528	H	2.638624	0.485773	2.150694
7529	O	3.973822	-1.193048	-2.182289
7530	H	4.531931	-1.662299	-2.809266
7531	H	3.910685	-1.740679	-1.343483
7532	O	-1.532117	0.905812	0.770149
7533	H	-1.385803	0.644511	-0.167969
7534	H	-2.458921	1.206372	0.813912
7535	O	-1.615950	-3.512398	-0.146139
7536	H	-2.066755	-3.121379	-0.915139
7537	H	-0.682984	-3.222339	-0.185543
7538	O	-2.465102	2.727728	-1.674835
7539	H	-1.724225	3.224839	-1.281332
7540	H	-2.068204	1.914329	-2.035574
7541	O	-0.129489	2.971997	1.972487
7542	H	0.686814	2.598396	2.338109
7543	H	-0.630433	2.193184	1.658676
7544	O	4.401606	1.117835	-0.655782
7545	H	3.548410	1.583609	-0.716962
7546	H	4.388825	0.426898	-1.344159
7547	O	-4.329458	-1.031505	0.205220
7548	H	-3.834300	-1.372763	0.974305
7549	H	-4.351849	-0.059325	0.247045
7550	O	-0.170213	3.937159	-0.471890
7551	H	0.050477	4.857697	-0.645453
7552	H	-0.147525	3.792958	0.510215
7553	O	0.861194	-2.251870	0.083486
7554	H	0.506876	-1.788125	0.871978
7555	H	0.936906	-1.583215	-0.630380
7556	O	1.318568	-0.412882	-1.939684
7557	H	2.162292	-0.714956	-2.322976
7558	H	1.507549	0.431277	-1.470363
7559	O	3.640509	-2.372588	0.114020
7560	H	3.912874	-1.744363	0.805980
7561	H	2.677513	-2.505706	0.224567
7562	O	-2.717528	-2.500396	1.997937
7563	H	-3.205637	-3.160020	2.501101
7564	H	-2.311739	-2.969228	1.210264
7565	O	-1.355824	0.159165	-1.885903
7566	H	-1.960770	-0.595446	-2.042228
7567	H	-0.464037	-0.115813	-2.171041
7568	O	1.698139	1.805926	-0.459097
7569	H	1.117120	2.574581	-0.605673
7570	H	1.572708	1.502145	0.467033
7571	O	-4.079157	1.787252	0.171157

7572	H	-4.713977	2.411692	0.534702
7573	H	-3.590272	2.235458	-0.576156
7574	O	-3.136674	-1.933246	-1.912791
7575	H	-3.728690	-2.208134	-2.619388
7576	H	-3.693466	-1.600234	-1.147487
7577	O	4.303474	-0.086738	1.660744
7578	H	4.446968	0.417702	0.807715
7579	H	5.073485	0.052158	2.220640
7580	O	-0.369779	-1.009953	2.231233
7581	H	-0.919706	-0.344365	1.759013
7582	H	-1.019374	-1.653273	2.560850

7583

7584 Cartesian coordinates of : W19_ 6

7585

7586	O	1.587043	-1.972763	-1.279243
7587	H	1.031484	-2.642022	-1.720070
7588	H	1.100385	-1.126659	-1.353119
7589	O	1.669479	2.339060	-1.927040
7590	H	1.314934	3.170505	-1.570552
7591	H	2.598769	2.238820	-1.650512
7592	O	2.123945	0.924695	1.121241
7593	H	1.539215	1.633476	1.468586
7594	H	2.780226	1.363411	0.552205
7595	O	-2.733102	-1.831453	0.748876
7596	H	-2.629688	-1.619204	-0.204284
7597	H	-3.478167	-1.303809	1.085675
7598	O	-0.485326	-0.436830	1.475613
7599	H	-1.251737	-1.015932	1.276591
7600	H	0.252999	-1.041533	1.683300
7601	O	4.073063	1.544275	-0.818288
7602	H	4.181764	0.551397	-0.862177
7603	H	4.950386	1.937058	-0.841878
7604	O	0.139923	0.401791	-1.096934
7605	H	0.786912	1.103977	-1.401997
7606	H	0.219741	0.307041	-0.123559
7607	O	0.487889	3.035418	1.770956
7608	H	0.353647	3.594733	0.986752
7609	H	-0.397426	2.837900	2.111910
7610	O	4.175915	-1.067534	-0.660652
7611	H	3.396353	-1.499040	-1.054025
7612	H	4.125696	-1.237085	0.296865
7613	O	-0.048590	4.256783	-0.752131
7614	H	-0.221507	5.173143	-0.988726
7615	H	-0.865017	3.739185	-0.931221
7616	O	-4.381243	0.335258	1.391934
7617	H	-3.642237	0.911679	1.710620
7618	H	-5.151197	0.505425	1.943092
7619	O	-4.031790	0.777887	-1.424110
7620	H	-4.357088	0.559322	-0.534203
7621	H	-3.607473	-0.020965	-1.776026
7622	O	-2.119873	1.727272	1.846069
7623	H	-2.042140	2.015276	0.910652
7624	H	-1.472463	0.997931	1.931128
7625	O	3.562400	-1.058410	2.117709
7626	H	3.014904	-0.250301	1.942326
7627	H	4.142716	-0.873261	2.861861
7628	O	-1.870706	2.294649	-0.858431
7629	H	-2.730326	1.937591	-1.182418
7630	H	-1.215106	1.596088	-1.064851
7631	O	-0.563870	-3.626005	-1.947973
7632	H	-0.717709	-3.859720	-0.987605
7633	H	-0.658161	-4.431192	-2.466146
7634	O	1.332113	-2.528616	1.411053
7635	H	1.531845	-2.361472	0.464738
7636	H	2.154764	-2.345500	1.894063
7637	O	-2.021807	-1.238684	-1.820954
7638	H	-1.254200	-0.647427	-1.700897
7639	H	-1.651381	-2.090017	-2.121340
7640	O	-0.932887	-3.969390	0.626848
7641	H	-1.680847	-3.409395	0.897303
7642	H	-0.153475	-3.658639	1.121582

7643

7644 Cartesian coordinates of : W19_ 7

7645

7646	O	-2.428693	1.886990	-0.475888
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7647	H	-2.413085	1.510454	0.432715
7648	H	-3.315578	2.272508	-0.595886
7649	O	-5.206699	-0.371830	-1.695060
7650	H	-4.313007	-0.502541	-2.054924
7651	H	-5.279836	0.574845	-1.473925
7652	O	-2.400763	-0.471039	-1.853153
7653	H	-2.337333	0.432100	-1.468558
7654	H	-1.534668	-0.670854	-2.246633
7655	O	0.046201	-2.025611	0.577665
7656	H	0.163581	-1.228275	1.139163
7657	H	-0.878001	-2.309390	0.684551
7658	O	2.799318	-2.252152	0.392619
7659	H	2.755616	-1.834404	-0.491310
7660	H	1.904216	-2.578869	0.581367
7661	O	0.371083	-0.803077	-1.865929
7662	H	0.293160	-1.357168	-1.057520
7663	H	1.255782	-0.964784	-2.235397
7664	O	-5.069316	0.805554	1.778648
7665	H	-4.161384	0.799442	2.126000
7666	H	-5.289885	-0.118369	1.558556
7667	O	-5.489460	-1.694955	0.554283
7668	H	-5.487084	-1.267915	-0.347693
7669	H	-6.233094	-2.303408	0.598971
7670	O	3.304803	0.079123	1.690584
7671	H	4.257904	0.180794	1.860816
7672	H	3.178218	-0.829946	1.331456
7673	O	6.062992	0.391540	1.243014
7674	H	6.035675	1.175708	0.641257
7675	H	6.836600	0.487856	1.806904
7676	O	3.181335	-0.785112	-1.955071
7677	H	3.184473	0.125091	-1.596399
7678	H	4.095984	-1.103998	-1.836853
7679	O	-2.713002	-1.812199	0.517264
7680	H	-3.643571	-2.065849	0.655435
7681	H	-2.661153	-1.441326	-0.392286
7682	O	5.665055	2.415223	-0.467942
7683	H	6.081657	2.417851	-1.335077
7684	H	4.698554	2.335245	-0.612812
7685	O	0.518434	0.387307	1.828400
7686	H	1.433369	0.412425	2.155996
7687	H	0.496684	0.943423	1.019113
7688	O	3.071796	1.619684	-0.539675
7689	H	2.175678	1.987910	-0.636830
7690	H	3.083589	1.132362	0.317855
7691	O	-5.194747	2.162709	-0.462797
7692	H	-5.231621	1.732515	0.437393
7693	H	-5.844577	2.871568	-0.483614
7694	O	-2.273727	0.502133	1.886255
7695	H	-2.360718	-0.397452	1.496883
7696	H	-1.381273	0.558720	2.266503
7697	O	0.322804	1.645721	-0.619247
7698	H	-0.548597	2.070914	-0.701410
7699	H	0.298229	0.835618	-1.175953
7700	O	5.433257	-1.737381	-0.579394
7701	H	4.889352	-2.338589	-0.051233
7702	H	5.790768	-1.085227	0.046751

7703

7704 Cartesian coordinates of : W19_ 8

7705

7706	O	1.498155	-1.665669	-1.190206
7707	O	1.829929	-1.267929	1.459307
7708	O	1.037026	2.718569	-0.264683
7709	O	1.599427	0.861348	-2.233326
7710	O	-1.255788	-1.881013	-1.140600
7711	O	-0.927531	-1.638322	1.535507
7712	O	-1.703138	2.307888	-0.114007
7713	O	-1.235966	0.606079	-2.194097
7714	H	1.532679	-1.552355	-0.209541
7715	H	-0.004799	-1.869374	1.733825
7716	H	1.138318	2.099819	-1.016680
7717	H	-1.152811	-0.309077	-1.833698
7718	H	0.624123	-2.040295	-1.398682
7719	H	-0.993047	-0.684154	1.778501
7720	H	0.093516	2.945612	-0.219515
7721	H	-0.387255	0.829403	-2.606737

7722	H	2.538983	1.081565	-2.329241
7723	H	-2.139165	-2.245480	-1.335089
7724	H	2.743166	-1.541146	1.648336
7725	H	-2.650703	2.527420	-0.055573
7726	H	1.583089	-0.047488	-1.857712
7727	H	-1.206683	-1.794695	-0.157876
7728	H	1.797685	-0.289272	1.612207
7729	H	-1.608752	1.688159	-0.872618
7730	H	2.795153	1.568690	1.944384
7731	O	1.846222	1.396132	1.852347
7732	H	1.558984	1.920972	1.053121
7733	H	-0.093964	1.272702	2.457153
7734	O	-0.974976	1.010114	2.147772
7735	H	-1.157928	1.520546	1.324169
7736	O	-3.808985	0.514169	2.249172
7737	H	-4.091506	1.114308	1.536235
7738	H	-2.921962	0.796911	2.519789
7739	H	-5.243438	2.604694	-0.148327
7740	O	-4.455749	2.064966	-0.034830
7741	H	-4.412140	1.419488	-0.795281
7742	O	-4.062462	0.369447	-1.996293
7743	H	-4.109688	-0.572415	-1.736955
7744	H	-3.178772	0.510690	-2.373367
7745	O	-3.997173	-2.272316	-1.099894
7746	H	-3.968864	-2.232926	-0.090911
7747	H	-4.641796	-2.939607	-1.353413
7748	H	-3.859943	-1.170003	1.776550
7749	O	-3.707806	-2.088312	1.453083
7750	H	-2.780242	-2.267518	1.678064
7751	O	4.254150	-1.732100	-1.290097
7752	H	3.315738	-1.939776	-1.460584
7753	H	4.393860	-0.827815	-1.620832
7754	H	5.069274	1.625711	-2.018306
7755	O	4.394858	1.082894	-1.597417
7756	H	4.436081	1.271747	-0.637702
7757	O	4.637661	-1.568745	1.264042
7758	H	5.271606	-2.200236	1.618090
7759	H	4.549872	-1.730067	0.274192
7760	O	4.654831	1.145383	1.218339
7761	H	4.763250	0.176993	1.362706
7762	H	5.416604	1.577614	1.618363

7763

7764 Cartesian coordinates of : W19_9

7765

7766	O	3.951779	0.067103	2.115785
7767	O	4.039680	2.375683	0.460378
7768	O	4.038154	-1.488363	-1.946655
7769	O	3.988539	-2.154652	0.540406
7770	O	1.115592	0.169763	2.348346
7771	O	1.274138	2.236698	0.590055
7772	O	1.276288	-1.482061	-1.678597
7773	O	1.188777	-2.160919	0.934061
7774	H	4.062303	0.900564	1.624640
7775	H	2.184129	2.576113	0.678301
7776	H	4.105338	-1.777643	-0.981442
7777	H	1.203218	-1.326375	1.457984
7778	H	3.073105	0.106529	2.524737
7779	H	1.217944	1.856289	-0.319787
7780	H	4.708457	-1.964011	-2.446450
7781	H	0.310276	-2.540859	1.107826
7782	H	3.116203	-2.518439	0.762668
7783	H	0.259334	0.196167	2.804717
7784	H	4.736784	3.037732	0.490304
7785	H	2.167422	-1.652269	-2.036429
7786	H	4.088283	-1.368518	1.126644
7787	H	1.119498	0.929289	1.720468
7788	H	4.036110	1.979549	-0.457456
7789	H	1.311481	-1.739503	-0.725121
7790	H	2.852223	1.409696	-2.184080
7791	O	3.776798	1.293316	-1.909993
7792	H	3.964061	0.335472	-1.973655
7793	H	0.056414	1.392175	-2.167996
7794	O	0.955524	1.176318	-1.872430
7795	H	1.005733	0.189885	-1.807755
7796	O	-1.836251	1.135889	-1.682912

7797	H	-1.747105	0.152168	-1.599692
7798	H	-2.763296	1.313766	-1.916737
7799	H	-0.633040	-1.731480	-1.812413
7800	O	-1.497179	-1.496416	-1.432498
7801	H	-1.466270	-1.745943	-0.476054
7802	O	-1.593005	-2.157982	1.189886
7803	H	-1.663262	-1.346214	1.729707
7804	H	-2.470973	-2.594545	1.249476
7805	O	-1.690461	0.267124	2.601572
7806	H	-1.709246	0.991075	1.930324
7807	H	-2.442283	0.399423	3.188143
7808	H	-1.547678	1.808073	-0.170987
7809	O	-1.481013	2.208961	0.735230
7810	H	-0.572105	2.553691	0.813652
7811	O	-4.622911	1.350553	-1.460228
7812	H	-5.358392	1.668377	-1.992991
7813	H	-4.584887	1.904133	-0.648397
7814	H	-3.421562	-1.618698	-1.633176
7815	O	-4.324098	-1.512294	-1.290750
7816	H	-4.509986	-0.558528	-1.286538
7817	H	-4.389310	-2.400847	0.199894
7818	O	-4.197626	-2.882256	1.037260
7819	H	-4.644212	-3.732011	0.990390
7820	H	-3.146304	2.853208	0.857641
7821	O	-4.121474	2.844986	0.772284
7822	H	-4.438413	3.730909	0.970051

7823

7824

7825 Cartesian coordinates of the water Eicosamer

7826

7827 Cartesian coordinates of : W20_1

7828

7829	O	-0.580747	2.972975	-2.394811
7830	H	-1.479235	2.589612	-2.388686
7831	H	0.025213	2.228636	-2.566636
7832	O	-0.257099	-0.047190	-0.013671
7833	H	0.139304	-0.737883	0.561011
7834	H	-0.418872	0.756162	0.526718
7835	O	-0.412264	-3.995441	-0.181891
7836	H	-1.363599	-3.653266	-0.194999
7837	H	-0.446446	-4.956067	-0.141996
7838	O	-1.166615	-1.002741	3.167461
7839	H	-0.431181	-1.474935	2.732715
7840	H	-0.812383	-0.146235	3.470594
7841	O	4.009600	-0.249748	-0.562196
7842	H	3.592728	-0.607016	-1.369963
7843	H	3.772065	0.688434	-0.491159
7844	O	1.159382	0.856347	-2.127263
7845	H	1.706556	0.224143	-2.625303
7846	H	0.665276	0.345477	-1.446117
7847	O	-3.019990	1.598673	-2.286858
7848	H	-3.220597	1.526698	-1.305071
7849	H	-3.807645	1.937379	-2.723001
7850	O	-1.858214	-0.933722	-2.015525
7851	H	-2.335766	-0.193451	-2.428880
7852	H	-1.424397	-0.544728	-1.224092
7853	O	2.124454	0.895243	2.283177
7854	H	2.209616	1.333952	1.409063
7855	H	2.593196	0.044616	2.235137
7856	O	2.455402	2.162952	-0.139528
7857	H	2.085330	3.058792	-0.070192
7858	H	1.983189	1.767830	-0.905961
7859	O	0.074014	1.446461	3.718680
7860	H	0.274619	1.814780	4.583873
7861	H	0.938465	1.236121	3.252989
7862	O	-3.265026	-1.065219	1.645031
7863	H	-4.027181	-1.209975	2.215510
7864	H	-2.462212	-1.009275	2.247478
7865	O	0.727201	-2.132850	1.472554
7866	H	1.701186	-2.117462	1.538702
7867	H	0.451148	-2.926229	0.970606
7868	O	-0.895346	2.291549	1.302104
7869	H	-0.419845	3.045275	0.897050
7870	H	-0.652110	2.231822	2.245228
7871	O	0.417733	4.120787	-0.278981

7872	H	0.323071	5.077903	-0.295859
7873	H	-0.003780	3.762326	-1.116304
7874	O	0.414460	-2.525547	-2.434514
7875	H	-0.376610	-1.962556	-2.533796
7876	H	0.226826	-3.127163	-1.689952
7877	O	-3.314608	1.391035	0.276655
7878	H	-3.361959	0.502437	0.678832
7879	H	-2.552727	1.829385	0.701402
7880	O	-2.748696	-2.933585	-0.341834
7881	H	-2.661996	-2.315838	-1.093689
7882	H	-2.982232	-2.362653	0.417618
7883	O	3.401341	-1.523711	1.622058
7884	H	4.168030	-1.924981	2.041441
7885	H	3.700897	-1.104586	0.764287
7886	O	2.694097	-1.335399	-2.792059
7887	H	3.141371	-1.668238	-3.575626
7888	H	1.870058	-1.886181	-2.651674

7889

7890 Cartesian coordinates of : W20_2

7891

7892	O	5.661441	0.214716	-1.993603
7893	H	5.684633	-0.608985	-1.429364
7894	H	6.356778	0.145900	-2.654663
7895	O	-2.878575	1.914864	0.207958
7896	H	-2.851131	1.403908	-0.632303
7897	H	-3.789358	2.251415	0.289436
7898	O	-5.477260	-0.326515	1.801010
7899	H	-5.625727	0.569441	1.446173
7900	H	-4.572954	-0.334032	2.158663
7901	O	-2.878543	-1.914833	-0.207983
7902	H	-3.789309	-2.251427	-0.289469
7903	H	-2.851134	-1.403877	0.632281
7904	O	2.878551	-0.207850	1.914840
7905	H	3.789333	-0.289344	2.251397
7906	H	2.851169	0.632359	1.403785
7907	O	5.477344	1.800938	0.326327
7908	H	5.625751	1.446061	-0.569623
7909	H	4.573051	2.158628	0.333809
7910	O	-0.101273	-1.916093	-0.319266
7911	H	-0.071590	-1.197320	-0.989063
7912	H	-0.998637	-2.289795	-0.355051
7913	O	-5.661403	-1.993646	-0.214952
7914	H	-5.684453	-1.429544	0.608866
7915	H	-6.356842	-2.654598	-0.146021
7916	O	5.477124	-1.801074	-0.326268
7917	H	5.625584	-1.446189	0.569676
7918	H	4.572780	-2.158655	-0.333778
7919	O	2.675982	-1.920493	-0.198150
7920	H	2.679669	-1.397924	0.635824
7921	H	1.792328	-2.318977	-0.271994
7922	O	-2.676004	0.198268	-1.920566
7923	H	-1.792340	0.272064	-2.319026
7924	H	-2.679718	-0.635715	-1.398009
7925	O	-5.477237	0.326425	-1.801003
7926	H	-5.625674	-0.569536	-1.446168
7927	H	-4.572939	0.333969	-2.158673
7928	O	-5.661425	1.993549	0.214961
7929	H	-6.356887	2.654475	0.146007
7930	H	-5.684439	1.429443	-0.608857
7931	O	0.101323	-0.319144	1.916110
7932	H	0.998688	-0.354996	2.289805
7933	H	0.071707	-0.988818	1.197232
7934	O	5.661364	-0.214954	1.993544
7935	H	6.356836	-0.145966	2.654460
7936	H	5.684465	0.608792	1.429335
7937	O	-0.101318	1.916219	0.319225
7938	H	-0.071683	1.197402	0.988968
7939	H	-0.998691	2.289898	0.355040
7940	O	0.101331	0.319262	-1.916137
7941	H	0.071699	0.988941	-1.197260
7942	H	0.998701	0.355110	-2.289819
7943	O	-2.676022	-0.198250	1.920561
7944	H	-1.792361	-0.272059	2.319030
7945	H	-2.679730	0.635732	1.398007
7946	O	2.878555	0.207967	-1.914794

7947	H	2.851073	-0.632305	-1.403826
7948	H	3.789351	0.289266	-2.251353
7949	O	2.676031	1.920647	0.198215
7950	H	2.679724	1.398088	-0.635764
7951	H	1.792388	2.319142	0.272045
7952				
7953	Cartesian coordinates of : W20_ 3			
7954				
7955	O	1.199161	4.035064	1.515263
7956	H	0.209514	3.902588	1.552540
7957	H	1.408791	4.795518	2.066037
7958	O	-1.480663	3.967725	-1.462169
7959	H	-0.483836	3.915488	-1.502804
7960	H	-1.747335	4.744626	-1.963274
7961	O	-4.003792	-0.921336	-1.330858
7962	H	-3.552330	-0.083219	-1.538451
7963	H	-4.269317	-0.871652	-0.394936
7964	O	2.481391	1.392891	-1.371206
7965	H	3.167730	0.755947	-1.642855
7966	H	2.513188	1.424098	-0.388527
7967	O	1.136392	3.866241	-1.306656
7968	H	1.664071	3.099324	-1.589482
7969	H	1.349766	4.018226	-0.368018
7970	O	2.921589	-3.018071	1.567443
7971	H	3.456009	-3.582713	2.134298
7972	H	3.343696	-2.112041	1.563463
7973	O	4.043204	-0.664897	1.288770
7974	H	4.280854	-0.601599	0.345942
7975	H	3.545656	0.144425	1.503978
7976	O	-2.598415	-3.118718	1.256806
7977	H	-2.597640	-3.343203	0.308187
7978	H	-1.665103	-3.084924	1.531233
7979	O	0.071821	0.118886	-1.291171
7980	H	0.070849	0.116421	-0.303472
7981	H	0.907223	0.573168	-1.535729
7982	O	-4.207590	-1.066119	1.488793
7983	H	-4.976735	-1.288592	2.022177
7984	H	-3.591816	-1.853213	1.503217
7985	O	0.029406	-2.591454	-1.396394
7986	H	0.019658	-1.617784	-1.534225
7987	H	-0.856599	-2.916235	-1.645003
7988	O	4.201225	-0.794877	-1.531820
7989	H	3.656411	-1.632421	-1.529390
7990	H	4.983658	-0.962819	-2.065994
7991	O	-0.050103	0.015558	1.413998
7992	H	-0.957966	0.358114	1.570698
7993	H	-0.032055	-0.955993	1.565260
7994	O	-2.345281	1.330726	-1.393737
7995	H	-2.242690	2.277892	-1.602212
7996	H	-1.455304	0.934398	-1.530977
7997	O	2.798699	-2.996156	-1.257705
7998	H	1.854784	-3.008485	-1.497563
7999	H	2.847235	-3.216245	-0.309841
8000	O	0.171696	-2.680358	1.331433
8001	H	1.068932	-2.927451	1.624127
8002	H	0.180842	-2.733019	0.348080
8003	O	-1.396333	3.706402	1.349192
8004	H	-1.846859	2.881066	1.599639
8005	H	-1.620825	3.870736	0.415053
8006	O	2.237646	1.470011	1.355374
8007	H	2.049864	2.396347	1.597465
8008	H	1.403811	0.977091	1.517861
8009	O	-2.687028	-3.174491	-1.565622
8010	H	-3.188448	-2.309269	-1.574896
8011	H	-3.162117	-3.788835	-2.133494
8012	O	-2.518150	1.125330	1.332468
8013	H	-3.216449	0.496293	1.593186
8014	H	-2.558096	1.189092	0.351081
8015				
8016	Cartesian coordinates of : W20_ 4			
8017				
8018	O	2.879288	1.313760	1.421188
8019	H	2.851000	0.334377	1.506880
8020	H	3.791427	1.582315	1.634166
8021	O	-2.884504	-1.320790	1.415979

8022	H	-2.870735	-0.340084	1.495334
8023	H	-3.793010	-1.599074	1.630802
8024	O	-5.658304	1.488690	-1.352995
8025	H	-6.358506	2.060943	-1.680705
8026	H	-5.669945	1.521055	-0.355379
8027	O	-2.884778	1.319810	-1.415512
8028	H	-3.793513	1.597319	-1.630455
8029	H	-2.870033	0.339161	-1.495323
8030	O	-2.675994	-1.398672	-1.310682
8031	H	-2.675133	-1.501788	-0.331808
8032	H	-1.791977	-1.660573	-1.619383
8033	O	-0.101858	-1.329079	1.397413
8034	H	-0.084941	-0.352115	1.509904
8035	H	-0.995100	-1.619075	1.651166
8036	O	5.651079	1.485946	1.352069
8037	H	6.346712	2.061848	1.683176
8038	H	5.665380	1.520652	0.354396
8039	O	-5.478524	1.321220	1.263229
8040	H	-4.571220	1.527735	1.545510
8041	H	-5.640767	0.390827	1.503838
8042	O	-2.677008	1.397521	1.310595
8043	H	-2.675766	1.500535	0.331657
8044	H	-1.793610	1.660818	1.619812
8045	O	-5.658046	-1.490160	1.352444
8046	H	-5.669338	-1.522539	0.354849
8047	H	-6.358602	-2.062136	1.679886
8048	O	5.478928	1.324456	-1.264341
8049	H	5.640035	0.393920	-1.505039
8050	H	4.573034	1.533245	-1.549485
8051	O	0.107723	1.412568	1.335711
8052	H	0.097472	1.502525	0.356450
8053	H	1.000332	1.667194	1.626131
8054	O	-0.102052	1.333821	-1.397270
8055	H	-0.995872	1.621991	-1.651097
8056	H	-0.083588	0.356980	-1.510215
8057	O	2.679308	-1.414181	1.306525
8058	H	2.690420	-1.501857	0.326561
8059	H	1.791232	-1.679054	1.600676
8060	O	2.880870	-1.315743	-1.421160
8061	H	3.793439	-1.583626	-1.632893
8062	H	2.851965	-0.336486	-1.507127
8063	O	-5.477525	-1.322497	-1.263789
8064	H	-4.570324	-1.529031	-1.546341
8065	H	-5.639931	-0.392151	-1.504463
8066	O	5.478887	-1.324296	1.264709
8067	H	4.573363	-1.534217	1.550076
8068	H	5.638648	-0.393460	1.505303
8069	O	0.108608	-1.408209	-1.335953
8070	H	0.098740	-1.497271	-0.356627
8071	H	1.000358	-1.665027	-1.626946
8072	O	2.679959	1.411754	-1.306004
8073	H	2.689803	1.499794	-0.326041
8074	H	1.793573	1.679846	-1.602111
8075	O	5.653645	-1.486128	-1.351943
8076	H	6.350369	-2.061017	-1.682473
8077	H	5.666972	-1.520822	-0.354375

8078

8079 Cartesian coordinates of : W20_ 5

8080

8081	O	1.551870	1.301125	1.887991
8082	H	2.476017	1.508306	2.108021
8083	H	1.504426	0.316379	1.862964
8084	O	-1.294371	-1.305066	1.922324
8085	H	-0.409653	-1.569222	2.222950
8086	H	-1.292977	-0.318973	1.936624
8087	O	4.373290	1.378161	1.727057
8088	H	4.294060	1.653120	0.759807
8089	H	5.035882	1.946713	2.132368
8090	O	-1.582083	-2.152234	-0.644359
8091	H	-1.526105	-1.850683	0.293472
8092	H	-2.498625	-2.459821	-0.776008
8093	O	4.332474	-1.337020	1.852036
8094	H	4.451969	-0.358665	1.868775
8095	H	5.031072	-1.724956	2.388292
8096	O	1.507661	-1.417484	1.782133

8097	H	2.418715	-1.639730	2.035096
8098	H	1.402869	-1.694874	0.840682
8099	O	3.972185	-2.152895	-0.844192
8100	H	4.165104	-1.925773	0.083081
8101	H	3.050497	-2.464954	-0.868771
8102	O	4.029524	2.060320	-0.741599
8103	H	3.120587	2.381947	-0.874489
8104	H	4.179977	1.353337	-1.399476
8105	O	-4.312136	2.302001	-0.651012
8106	H	-4.367489	1.485747	-1.225345
8107	H	-5.011853	2.902039	-0.925948
8108	O	-4.351785	-2.237300	-0.653151
8109	H	-4.345768	-1.968858	0.320717
8110	H	-5.045904	-2.892046	-0.775626
8111	O	1.181671	-2.146077	-0.806223
8112	H	0.284179	-2.513356	-0.890916
8113	H	1.206383	-1.335497	-1.369300
8114	O	1.404171	0.083449	-2.319878
8115	H	1.365835	0.868932	-1.725752
8116	H	2.306385	0.054472	-2.683963
8117	O	1.239346	2.220670	-0.646918
8118	H	1.284406	1.898205	0.283848
8119	H	0.352167	2.603633	-0.762726
8120	O	-4.118701	-1.490935	1.799189
8121	H	-3.218228	-1.681742	2.108103
8122	H	-4.214317	-0.514181	1.894405
8123	O	-1.237621	1.419146	1.906128
8124	H	-0.354652	1.672505	2.219513
8125	H	-1.301807	1.724699	0.970665
8126	O	-4.196514	0.139645	-2.122851
8127	H	-4.345558	-0.704083	-1.651921
8128	H	-3.297623	0.091149	-2.488496
8129	O	4.187790	-0.115999	-2.478093
8130	H	4.188248	-0.923352	-1.889063
8131	H	4.842964	-0.251123	-3.169606
8132	O	-4.073146	1.224062	1.965432
8133	H	-4.237322	1.668845	1.114699
8134	H	-3.172661	1.469496	2.229725
8135	O	-1.536069	2.219120	-0.669313
8136	H	-2.450663	2.554500	-0.715543
8137	H	-1.515141	1.423680	-1.251379
8138	O	-1.382329	0.006868	-2.249069
8139	H	-1.401628	-0.791377	-1.667753
8140	H	-0.515585	0.009101	-2.686789

8141

8142 Cartesian coordinates of : W20_ 6

8143

8144	O	0.437896	4.172569	-1.227280
8145	H	0.474870	4.147890	-0.225430
8146	H	0.549807	5.085968	-1.507985
8147	O	2.454479	-1.523305	1.193705
8148	H	2.483218	-1.455005	0.214467
8149	H	3.270216	-1.100937	1.510541
8150	O	2.366524	-1.526959	-1.561183
8151	H	2.042134	-2.453086	-1.662044
8152	H	1.582829	-0.973303	-1.724208
8153	O	4.402042	0.338971	-1.253855
8154	H	3.910743	-0.454315	-1.535521
8155	H	3.823719	1.078315	-1.504224
8156	O	2.051648	1.929686	-1.478514
8157	H	1.638989	2.809990	-1.574923
8158	H	1.369188	1.287339	-1.736975
8159	O	1.054741	-3.888455	-1.444897
8160	H	1.092650	-4.109067	-0.498546
8161	H	0.142174	-3.611106	-1.628789
8162	O	1.345148	-3.914739	1.413119
8163	H	1.903505	-3.097621	1.469071
8164	H	1.743409	-4.592704	1.966679
8165	O	-4.133296	0.999128	-1.126266
8166	H	-4.271984	1.147159	-0.173186
8167	H	-3.394269	1.570226	-1.396535
8168	O	4.687484	0.208681	1.365853
8169	H	4.732533	0.263744	0.373364
8170	H	5.583562	0.248935	1.711990
8171	O	-1.348832	-2.335690	-1.407127

8172	H	-2.298490	-2.242908	-1.607528
8173	H	-1.281005	-2.400849	-0.427169
8174	O	-4.042835	-1.619657	-1.403761
8175	H	-4.077338	-0.623466	-1.405424
8176	H	-4.803844	-1.936107	-1.900166
8177	O	2.338938	1.708273	1.293984
8178	H	2.356268	1.744478	0.315704
8179	H	3.206418	1.364228	1.570127
8180	O	-1.745504	2.198396	1.383940
8181	H	-2.612083	1.877839	1.699187
8182	H	-1.819240	2.286996	0.409159
8183	O	-0.018882	0.019116	-1.434812
8184	H	-0.554936	-0.784466	-1.636528
8185	H	0.021003	0.041583	-0.441345
8186	O	-0.937574	-2.343886	1.293463
8187	H	-0.304495	-3.043881	1.534482
8188	H	-0.474105	-1.487372	1.430097
8189	O	0.521931	3.824123	1.359336
8190	H	1.235146	3.192107	1.567654
8191	H	-0.310174	3.409087	1.646227
8192	O	-4.165938	0.906688	1.693939
8193	H	-3.960024	-0.072786	1.680081
8194	H	-4.906218	1.041171	2.293396
8195	O	0.039370	0.168767	1.233435
8196	H	0.947129	0.448219	1.466571
8197	H	-0.574980	0.906412	1.449160
8198	O	-1.624007	2.282353	-1.369140
8199	H	-1.067996	3.063578	-1.545612
8200	H	-1.069312	1.496717	-1.555393
8201	O	-3.647577	-1.636182	1.396014
8202	H	-3.866115	-1.835738	0.468031
8203	H	-2.748961	-1.980281	1.551922

8204

8205 Cartesian coordinates of : W20_ 7

8206

8207	O	-1.267090	-1.776030	0.086826
8208	H	-0.318074	-2.015242	0.074181
8209	H	-1.374790	-1.076707	0.762647
8210	O	4.775014	-1.163174	1.676403
8211	H	3.942321	-0.861408	2.079560
8212	H	4.556930	-1.953008	1.148281
8213	O	-0.246365	1.235760	-2.882140
8214	H	-1.032401	0.667100	-2.828605
8215	H	-0.448757	2.043611	-2.378270
8216	O	1.467712	-1.861007	0.122607
8217	H	1.711419	-1.289928	0.884890
8218	H	2.209968	-2.480620	-0.008622
8219	O	5.599443	0.650751	-0.040128
8220	H	5.391110	-0.013779	0.674883
8221	H	6.495741	0.970874	0.097743
8222	O	3.968996	-2.976644	-0.313593
8223	H	4.207873	-2.321335	-1.033983
8224	H	4.298823	-3.842886	-0.570226
8225	O	-2.050646	0.311108	1.776250
8226	H	-2.357153	0.907382	1.047103
8227	H	-2.858179	-0.076675	2.168146
8228	O	-0.859407	3.415852	-1.129738
8229	H	-0.903384	4.326091	-1.438671
8230	H	-0.185746	3.383819	-0.389377
8231	O	-5.376507	0.552172	0.039103
8232	H	-5.232150	0.154039	0.916228
8233	H	-4.672103	1.214655	-0.076071
8234	O	3.010837	1.657109	0.013807
8235	H	3.982149	1.600306	-0.040632
8236	H	2.647411	1.148389	-0.754642
8237	O	-2.377826	-0.403861	-2.006390
8238	H	-3.246725	-0.804389	-2.192035
8239	H	-1.921217	-0.997480	-1.370572
8240	O	1.935920	0.065147	-1.848789
8241	H	1.599449	-0.645623	-1.267870
8242	H	1.161504	0.467682	-2.314646
8243	O	4.474700	-1.048054	-1.992666
8244	H	3.626408	-0.622124	-2.219081
8245	H	4.995808	-0.384194	-1.506568
8246	O	2.237375	-0.019632	1.992992

8247	H	2.516039	0.669492	1.344406
8248	H	1.536723	0.383787	2.534714
8249	O	-2.867954	1.701023	-0.369347
8250	H	-2.306090	2.467588	-0.599992
8251	H	-2.685844	1.009450	-1.048050
8252	O	0.052404	1.482591	2.931193
8253	H	-0.776781	1.042594	2.617781
8254	H	-0.124905	1.844149	3.805188
8255	O	-4.460138	-0.964228	2.234564
8256	H	-4.911532	-1.304952	3.012582
8257	H	-4.266730	-1.734074	1.619689
8258	O	0.875152	3.233516	0.814471
8259	H	0.580516	2.715821	1.584347
8260	H	1.728758	2.853200	0.533136
8261	O	-4.978550	-1.359800	-1.721693
8262	H	-5.243811	-0.611465	-1.116882
8263	H	-5.718904	-1.555092	-2.303830
8264	O	-3.843592	-2.747149	0.446937
8265	H	-2.882808	-2.673145	0.294873
8266	H	-4.276705	-2.489502	-0.387104

8267

8268 Cartesian coordinates of : W20_ 8

8269

8270	O	-1.281966	-0.823000	3.263739
8271	H	-0.677929	-1.413924	2.776387
8272	H	-0.765549	-0.025703	3.487006
8273	O	-0.258936	2.924017	-2.466902
8274	H	0.270251	2.129188	-2.663403
8275	H	-1.190450	2.634555	-2.424151
8276	O	2.783907	1.838106	-0.217232
8277	H	2.309488	1.466398	-0.992625
8278	H	2.476508	2.759688	-0.179134
8279	O	-0.205198	-0.039408	-0.125500
8280	H	-0.997839	-0.207218	-0.692945
8281	H	-0.340118	0.803081	0.364454
8282	O	-0.582046	2.337739	1.210721
8283	H	-0.025602	3.030305	0.799479
8284	H	-0.310255	2.222041	2.142454
8285	O	-3.426996	-0.572687	1.806413
8286	H	-2.617440	-0.636036	2.395013
8287	H	-4.195492	-0.650688	2.381086
8288	O	2.479185	0.805253	2.326304
8289	H	2.725447	-0.135417	2.282286
8290	H	2.532480	1.163600	1.414240
8291	O	-0.870716	-3.937390	-0.292891
8292	H	-0.873366	-4.891890	-0.411855
8293	H	-0.495293	-3.526480	-1.126313
8294	O	3.982914	-0.791635	-0.538901
8295	H	3.710278	-1.223130	0.292354
8296	H	3.933841	0.165810	-0.392808
8297	O	0.355467	-2.160745	1.416063
8298	H	-0.028296	-2.937752	0.961252
8299	H	0.169826	-1.391029	0.819357
8300	O	-1.962577	-0.727467	-2.005318
8301	H	-2.419932	0.059755	-2.350510
8302	H	-2.607595	-1.301652	-1.520447
8303	O	-3.242934	-2.359125	-0.351792
8304	H	-2.553848	-3.028459	-0.199423
8305	H	-3.339634	-1.844751	0.470966
8306	O	-2.866792	1.876945	-2.243979
8307	H	-3.057588	1.863563	-1.258523
8308	H	-3.604985	2.313035	-2.680462
8309	O	0.927746	3.974235	-0.398190
8310	H	0.449983	3.652569	-1.220152
8311	H	0.955573	4.934909	-0.439370
8312	O	0.006493	-2.651632	-2.374705
8313	H	-0.585656	-1.888445	-2.508504
8314	H	0.930520	-2.353257	-2.447525
8315	O	0.351142	1.434712	3.611272
8316	H	0.546754	1.854952	4.453987
8317	H	1.224689	1.178762	3.177700
8318	O	2.660238	-1.692659	-2.643261
8319	H	3.243771	-2.087884	-3.297819
8320	H	3.214767	-1.418884	-1.864223
8321	O	2.937997	-1.903116	1.804898

8322	H	1.978975	-2.142099	1.674524
8323	H	3.345961	-2.568547	2.366688
8324	O	-3.144872	1.795279	0.330144
8325	H	-2.319936	2.132636	0.728382
8326	H	-3.340827	0.957311	0.791708
8327	O	1.326118	0.686308	-2.225572
8328	H	1.792555	-0.033980	-2.682892
8329	H	0.790564	0.275209	-1.508745

8330

8331 Cartesian coordinates of : W20_9

8332

8333	O	-1.542878	-1.778147	1.010103
8334	H	-0.602758	-2.029968	1.108812
8335	H	-1.624400	-0.863298	1.349034
8336	O	4.600688	-0.901693	1.782613
8337	H	3.805350	-0.441914	2.103322
8338	H	4.323544	-1.806310	1.549950
8339	O	1.619026	1.319973	-2.380286
8340	H	0.880915	1.951374	-2.405254
8341	H	1.249291	0.424382	-2.242566
8342	O	1.174696	-1.882166	0.852493
8343	H	1.517822	-1.049277	1.257734
8344	H	1.900020	-2.533443	0.883190
8345	O	5.239065	0.234483	-0.512570
8346	H	5.122104	-0.183294	0.384116
8347	H	6.181767	0.337253	-0.673511
8348	O	3.588399	-3.186082	0.513654
8349	H	3.665329	-2.761732	-0.389223
8350	H	3.899465	-4.093823	0.451415
8351	O	-2.116510	0.879728	1.587719
8352	H	-2.158339	1.143139	0.634532
8353	H	-3.042355	0.793331	1.888333
8354	O	-0.368131	3.235467	-1.748390
8355	H	-0.569211	4.058616	-2.204080
8356	H	0.123115	3.464701	-0.905845
8357	O	-4.939585	0.769937	-0.878826
8358	H	-5.052780	0.748869	0.087881
8359	H	-4.074493	1.190807	-1.039332
8360	O	3.026259	1.879870	-0.244524
8361	H	3.947781	1.593798	-0.375492
8362	H	2.543517	1.662193	-1.091222
8363	O	-1.911617	-1.304263	-1.660179
8364	H	-1.823275	-1.576627	-0.718863
8365	H	-2.798622	-1.594669	-1.937836
8366	O	0.891284	-1.270633	-1.823567
8367	H	0.931113	-1.478913	-0.864321
8368	H	-0.018898	-1.467956	-2.102521
8369	O	3.682445	-1.816814	-1.706696
8370	H	2.796906	-1.595282	-2.040212
8371	H	4.168035	-0.991107	-1.529707
8372	O	2.125513	0.441905	1.825286
8373	H	2.420089	0.984782	1.049176
8374	H	1.467282	0.974057	2.304980
8375	O	-2.224949	1.351253	-1.055975
8376	H	-1.620778	2.045111	-1.394249
8377	H	-1.976728	0.481591	-1.438586
8378	O	0.010401	2.147491	2.635595
8379	H	-0.832580	1.714059	2.357016
8380	H	-0.147966	2.568115	3.486523
8381	O	-4.781450	0.176299	1.880791
8382	H	-4.656085	-0.791799	1.652355
8383	H	-5.430047	0.235290	2.588707
8384	O	1.009809	3.653163	0.432265
8385	H	0.645504	3.234609	1.232374
8386	H	1.889658	3.257607	0.289340
8387	O	-4.681604	-1.718672	-1.672940
8388	H	-4.878789	-0.763144	-1.460111
8389	H	-5.355236	-2.036542	-2.281525
8390	O	-4.277749	-2.248430	1.061566
8391	H	-3.315749	-2.379173	1.141106
8392	H	-4.484428	-2.286765	0.109507

8393

8394 Cartesian coordinates of : W20_10

8395

8396	O	-0.993821	-1.310978	-1.394795
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8397	H	-0.970373	-1.345179	-0.411691
8398	H	-1.763202	-1.850595	-1.659607
8399	O	-5.157603	-0.718438	-1.237162
8400	H	-5.398582	-0.739493	-0.292427
8401	H	-4.852318	0.188631	-1.422176
8402	O	1.778848	-1.290350	-1.311519
8403	H	0.869719	-1.450273	-1.625003
8404	H	1.739738	-1.331510	-0.329620
8405	O	-3.244170	-2.569924	1.282773
8406	H	-2.359961	-2.207515	1.477057
8407	H	-3.240650	-2.815952	0.340358
8408	O	2.651042	1.438268	1.266238
8409	H	1.998252	2.111351	1.533397
8410	H	2.699062	1.469245	0.283204
8411	O	-4.112635	1.888665	-1.416457
8412	H	-3.139164	1.789748	-1.557161
8413	H	-4.426893	2.565312	-2.024048
8414	O	0.495624	3.196297	1.450297
8415	H	0.349424	3.991643	1.971387
8416	H	-0.309712	2.624578	1.535380
8417	O	-5.221918	-0.886235	1.553876
8418	H	-4.468827	-1.545779	1.548841
8419	H	-5.896820	-1.213600	2.156127
8420	O	-1.510015	1.455197	1.267817
8421	H	-2.457804	1.589435	1.521365
8422	H	-1.533041	1.434142	0.282031
8423	O	5.249389	0.393903	1.346197
8424	H	5.489124	0.546191	0.413612
8425	H	4.464716	0.943293	1.520581
8426	O	1.949822	-1.189882	1.424047
8427	H	2.747049	-1.696452	1.666521
8428	H	2.188801	-0.239221	1.515545
8429	O	2.848299	1.221127	-1.437963
8430	H	3.795594	1.121681	-1.646287
8431	H	2.444885	0.331294	-1.550976
8432	O	4.566611	-2.123516	1.560509
8433	H	4.919931	-1.188469	1.569518
8434	H	5.082185	-2.646961	2.181279
8435	O	-4.166999	1.715837	1.448147
8436	H	-4.599185	0.858673	1.617720
8437	H	-4.348865	1.931377	0.518162
8438	O	5.487129	0.337896	-1.460097
8439	H	5.189095	-0.616521	-1.469443
8440	H	6.244848	0.424327	-2.046188
8441	O	-3.418132	-2.639111	-1.543532
8442	H	-4.106189	-1.911866	-1.523067
8443	H	-3.744383	-3.338144	-2.118177
8444	O	4.466285	-2.060880	-1.257450
8445	H	3.517859	-2.010355	-1.473921
8446	H	4.520249	-2.320465	-0.319608
8447	O	-1.496291	1.378476	-1.461210
8448	H	-0.698455	1.946989	-1.607462
8449	H	-1.264321	0.440462	-1.633966
8450	O	0.651314	2.958194	-1.415795
8451	H	0.685948	3.238384	-0.485307
8452	H	1.495851	2.511477	-1.601546
8453	O	-0.817249	-1.194645	1.341610
8454	H	-1.020272	-0.247221	1.503652
8455	H	0.112441	-1.341872	1.597701

8456

8457 Cartesian coordinates of : W20_11

8458

8459	O	1.015962	-1.323435	1.341502
8460	H	1.874443	-1.639462	1.714523
8461	H	1.062859	-1.438158	0.370682
8462	O	-0.689218	3.352324	-1.284581
8463	H	-0.718044	4.272219	-1.564613
8464	H	-0.709532	3.331735	-0.278662
8465	O	1.525514	1.339370	1.395534
8466	H	2.419763	1.405338	1.788052
8467	H	1.265468	0.390870	1.488675
8468	O	-2.670496	1.376618	-1.252842
8469	H	-2.676905	1.396585	-0.267204
8470	H	-2.088952	2.105258	-1.532820
8471	O	-0.697233	3.002098	1.282041

8472	H	0.097512	2.487406	1.522486
8473	H	-1.467161	2.470493	1.554486
8474	O	-5.418559	0.259030	1.564423
8475	H	-5.115801	-0.694643	1.557094
8476	H	-6.156558	0.336949	2.176241
8477	O	3.822923	1.052742	-2.295069
8478	H	2.927876	1.361093	-2.010105
8479	H	4.106725	1.605404	-3.029923
8480	O	3.518758	-1.737301	2.219358
8481	H	4.097016	-2.027817	1.491864
8482	H	3.805956	-0.836939	2.446624
8483	O	-1.950584	-1.252176	-1.458550
8484	H	-2.187633	-0.302003	-1.544033
8485	H	-2.759945	-1.753783	-1.669905
8486	O	-4.573308	-2.179916	-1.505437
8487	H	-5.104809	-2.700643	-2.114669
8488	H	-4.933116	-1.246930	-1.493301
8489	O	-4.399835	-2.134716	1.310337
8490	H	-4.480328	-2.388451	0.372926
8491	H	-3.444617	-2.080285	1.496649
8492	O	-5.263903	0.329089	-1.244358
8493	H	-5.478378	0.472542	-0.304079
8494	H	-4.480848	0.877026	-1.431989
8495	O	4.135406	1.064671	2.245260
8496	H	4.652821	1.592036	2.861022
8497	H	4.663107	0.967241	1.401587
8498	O	5.388205	0.561935	0.013179
8499	H	4.916971	0.823017	-0.798454
8500	H	5.490822	-0.406707	-0.033607
8501	O	-2.777721	1.142439	1.453976
8502	H	-3.716573	1.045314	1.698376
8503	H	-2.374523	0.248257	1.544621
8504	O	1.399764	1.526266	-1.280891
8505	H	0.733193	2.209876	-1.491333
8506	H	1.499950	1.537600	-0.295065
8507	O	-1.726069	-1.361718	1.283769
8508	H	-0.806597	-1.500384	1.583027
8509	H	-1.698394	-1.399286	0.302611
8510	O	3.454416	-1.759216	-2.115754
8511	H	3.633810	-0.842815	-2.389297
8512	H	2.493032	-1.790878	-1.955299
8513	O	0.818175	-1.184394	-1.426167
8514	H	-0.103800	-1.411645	-1.648154
8515	H	0.887246	-0.210139	-1.498775
8516	O	5.059983	-2.217941	-0.104957
8517	H	5.663131	-2.949748	-0.265675
8518	H	4.433377	-2.161708	-0.880766

8519

8520 Cartesian coordinates of : W20_12

8521

8522	O	5.160240	-0.392678	0.729729
8523	H	4.581179	-0.512318	1.507779
8524	H	5.021908	-1.175828	0.166100
8525	O	-2.149505	-2.869416	-0.831367
8526	H	-1.286845	-2.483718	-0.509294
8527	H	-1.981163	-3.778643	-1.097594
8528	O	2.228186	-2.691783	0.847043
8529	H	2.906098	-2.675154	0.145833
8530	H	2.602307	-2.198738	1.600351
8531	O	-3.242168	-0.852256	-2.458165
8532	H	-2.854627	-1.626829	-2.009791
8533	H	-4.055217	-0.620352	-1.968529
8534	O	1.988986	2.157888	-0.075215
8535	H	1.549252	1.521759	-0.685917
8536	H	2.936204	2.159274	-0.317538
8537	O	0.828089	0.311341	-1.713173
8538	H	0.519337	-0.430011	-1.140718
8539	H	0.040756	0.623227	-2.201144
8540	O	-5.361878	-0.182295	-0.790501
8541	H	-5.029073	0.568276	-0.212422
8542	H	-6.261436	0.024243	-1.061186
8543	O	3.264439	-0.876000	2.719208
8544	H	2.579034	-0.139843	2.672049
8545	H	3.501301	-0.999420	3.643256
8546	O	4.610626	1.642632	-0.789632

8547	H	5.363214	2.230093	-0.905654
8548	H	4.880420	0.915672	-0.151606
8549	O	-3.522064	-0.369157	2.666732
8550	H	-3.800243	-1.115638	2.057786
8551	H	-3.791557	-0.596019	3.561672
8552	O	0.112146	4.107854	0.258536
8553	H	0.202101	4.556330	1.104699
8554	H	0.908340	3.546448	0.144545
8555	O	1.540164	1.025666	2.420515
8556	H	0.602460	0.766620	2.341615
8557	H	1.752938	1.474542	1.576414
8558	O	-1.815985	2.230824	-0.113613
8559	H	-1.753270	1.967195	-1.053534
8560	H	-1.218937	3.001648	0.017021
8561	O	4.214476	-2.290906	-1.097932
8562	H	4.644115	-2.969615	-1.626796
8563	H	3.897903	-1.568758	-1.717669
8564	O	-0.016965	-1.600435	0.021256
8565	H	-0.357319	-0.995706	0.720335
8566	H	0.808281	-2.047220	0.363972
8567	O	-1.629159	1.152444	-2.670711
8568	H	-2.262779	0.369894	-2.635145
8569	H	-1.785727	1.616277	-3.499058
8570	O	-1.038975	0.302055	1.654874
8571	H	-1.840416	0.056236	2.157747
8572	H	-1.312080	0.993235	1.007587
8573	O	-4.246175	-2.125082	0.887734
8574	H	-3.515169	-2.497506	0.359601
8575	H	-4.804826	-1.621591	0.267891
8576	O	3.422624	-0.253269	-2.513234
8577	H	3.884602	0.514929	-2.132639
8578	H	2.467694	-0.079171	-2.399895
8579	O	-4.357146	1.591080	0.820803
8580	H	-4.135608	1.093262	1.627870
8581	H	-3.522795	1.984865	0.498917

8582

8583 Cartesian coordinates of : W20_13

8584

8585	O	0.944665	4.109440	1.365569
8586	H	0.941768	4.116681	0.367831
8587	H	1.092526	5.012377	1.663219
8588	O	-4.094349	-1.312909	-1.206200
8589	H	-4.267107	-1.267576	-0.247626
8590	H	-4.053411	-0.390253	-1.513792
8591	O	-4.039167	-1.275442	1.607191
8592	H	-3.287932	-1.933234	1.620018
8593	H	-4.722481	-1.619698	2.190938
8594	O	-3.919391	1.478761	1.175482
8595	H	-3.878991	0.554037	1.484308
8596	H	-3.108455	1.923542	1.477792
8597	O	-1.293496	2.420010	1.436796
8598	H	-0.662245	3.135163	1.637356
8599	H	-0.805992	1.581795	1.581046
8600	O	-2.178805	-3.107535	1.375911
8601	H	-2.173624	-3.352178	0.433021
8602	H	-1.247112	-2.991005	1.632470
8603	O	-2.337112	-3.242267	-1.456859
8604	H	-2.983663	-2.482150	-1.474810
8605	H	-2.723056	-3.954659	-1.975740
8606	O	4.388032	-0.288247	1.228722
8607	H	4.592721	-0.206038	0.279743
8608	H	3.877824	0.503269	1.474380
8609	O	-4.140064	1.515790	-1.426429
8610	H	-4.148739	1.561374	-0.426584
8611	H	-4.943667	1.938511	-1.744933
8612	O	0.554270	-2.518452	1.373067
8613	H	1.475010	-2.708567	1.630708
8614	H	0.532651	-2.543860	0.390109
8615	O	3.334370	-2.678828	1.506053
8616	H	3.727079	-1.760656	1.503204
8617	H	3.923581	-3.240538	2.018995
8618	O	-1.515100	2.419275	-1.321276
8619	H	-1.545315	2.462105	-0.340227
8620	H	-2.428743	2.243339	-1.613393
8621	O	2.625783	1.673580	-1.359924

8622	H	3.350265	1.089638	-1.652382
8623	H	2.692460	1.728414	-0.380727
8624	O	0.249845	0.191709	1.276211
8625	H	0.301670	-0.747656	1.551199
8626	H	0.208388	0.171716	0.291208
8627	O	0.287777	-2.349522	-1.350704
8628	H	-0.571773	-2.757486	-1.570176
8629	H	0.195377	-1.390704	-1.535174
8630	O	0.882750	3.879822	-1.261735
8631	H	0.021821	3.519292	-1.538322
8632	H	1.565341	3.258564	-1.568404
8633	O	4.458244	-0.396127	-1.597430
8634	H	3.923645	-1.240360	-1.589915
8635	H	5.221445	-0.542537	-2.164528
8636	O	0.252565	0.365900	-1.435669
8637	H	-0.446450	1.042271	-1.573875
8638	H	1.120672	0.812744	-1.558473
8639	O	2.465622	1.746514	1.381078
8640	H	2.157931	2.640529	1.613797
8641	H	1.682938	1.158326	1.486571
8642	O	3.084417	-2.610371	-1.306983
8643	H	3.172513	-2.841273	-0.364452
8644	H	2.134280	-2.652075	-1.517331

8645

8646 Cartesian coordinates of : W20_14

8647

8648	O	0.504885	-1.208899	-1.562246
8649	H	-0.316917	-0.867889	-1.972710
8650	H	1.111441	-0.437593	-1.577068
8651	O	-3.855513	-1.448858	-1.975283
8652	H	-3.111989	-0.975289	-2.385815
8653	H	-3.476747	-2.106272	-1.363052
8654	O	0.034138	1.327422	3.445561
8655	H	0.727840	0.653888	3.362375
8656	H	0.329996	2.106716	2.943541
8657	O	-0.535376	-1.870934	0.839934
8658	H	-0.150069	-1.641928	-0.037622
8659	H	-1.278952	-2.481985	0.674790
8660	O	-5.217160	0.241475	-0.492443
8661	H	-4.801841	-0.400623	-1.133662
8662	H	-6.100614	0.453923	-0.807032
8663	O	-3.010313	-2.999900	0.246585
8664	H	-3.549114	-2.406147	0.850368
8665	H	-3.311669	-3.903575	0.383907
8666	O	2.206122	0.953549	-1.725883
8667	H	2.345691	1.175310	-0.769848
8668	H	3.038477	0.565558	-2.057309
8669	O	0.824169	3.383019	1.633410
8670	H	0.999987	4.284548	1.919776
8671	H	0.184896	3.433052	0.862875
8672	O	4.924596	-0.015331	0.563992
8673	H	4.962679	-0.104515	-0.405162
8674	H	4.274963	0.685534	0.752151
8675	O	-2.741844	1.487822	-0.166540
8676	H	-3.701146	1.341777	-0.253558
8677	H	-2.461229	1.049579	0.678231
8678	O	1.563325	-0.805354	2.275593
8679	H	2.339948	-1.394576	2.228072
8680	H	0.815101	-1.321279	1.918365
8681	O	-1.937771	0.177326	2.001581
8682	H	-1.389071	-0.531659	1.599886
8683	H	-1.342827	0.651162	2.629323
8684	O	-4.287043	-1.249997	1.698927
8685	H	-3.586052	-0.687829	2.079497
8686	H	-4.797229	-0.681108	1.094622
8687	O	-1.672744	0.275681	-2.362475
8688	H	-2.013122	0.707743	-1.543452
8689	H	-1.199552	0.975328	-2.842765
8690	O	2.507841	1.357426	0.888621
8691	H	2.059374	2.174904	1.187704
8692	H	2.078035	0.604432	1.355513
8693	O	0.208993	2.358978	-2.845923
8694	H	1.033007	1.904446	-2.551543
8695	H	0.443428	2.941658	-3.574955
8696	O	4.422678	-0.641276	-2.128940

8697	H	5.002994	-0.869697	-2.861120
8698	H	3.909051	-1.458163	-1.865525
8699	O	-0.805306	3.446403	-0.408108
8700	H	-0.435999	3.178311	-1.268000
8701	H	-1.620130	2.920112	-0.294566
8702	O	3.814022	-2.212305	1.466652
8703	H	4.341094	-1.412472	1.182213
8704	H	4.404893	-2.803401	1.943360
8705	O	2.945489	-2.588810	-1.203431
8706	H	2.001668	-2.414368	-1.356419
8707	H	3.094206	-2.647098	-0.242061

8708

8709 Cartesian coordinates of : W20_15

8710

8711	O	-3.851938	0.872490	2.033177
8712	H	-4.042242	1.184037	1.103142
8713	H	-4.611110	1.096612	2.580393
8714	O	-0.070215	-3.508169	-1.590322
8715	H	0.766705	-2.981737	-1.644654
8716	H	0.142755	-4.422094	-1.803997
8717	O	1.296118	-3.869100	2.307719
8718	H	0.413169	-3.590893	1.987496
8719	H	1.205673	-4.099388	3.236610
8720	O	2.077133	1.915355	-1.581931
8721	H	1.773927	2.840200	-1.507834
8722	H	1.284619	1.393251	-1.806173
8723	O	-4.137684	-1.115647	-1.330015
8724	H	-4.975005	-1.509775	-1.594016
8725	H	-3.930421	-1.432669	-0.398299
8726	O	-3.488791	-1.768480	1.090951
8727	H	-2.599526	-2.167091	1.166666
8728	H	-3.513203	-0.953558	1.624028
8729	O	2.500146	-1.705500	1.128614
8730	H	3.428448	-1.454217	1.269514
8731	H	2.281991	-2.505291	1.647340
8732	O	0.753996	4.257248	-0.805900
8733	H	0.932022	5.189473	-0.963767
8734	H	0.868290	4.082208	0.176307
8735	O	1.009321	3.542779	1.689038
8736	H	1.663591	2.815866	1.692039
8737	H	0.178063	3.148359	2.004215
8738	O	-0.160560	0.273318	-1.574204
8739	H	-0.165535	0.064672	-0.609041
8740	H	-0.791773	-0.358094	-2.030712
8741	O	0.121019	-0.177783	1.072014
8742	H	-0.349696	0.590929	1.468430
8743	H	1.075617	-0.075775	1.257496
8744	O	-0.839804	-2.707565	1.021085
8745	H	-0.666248	-3.046520	0.121854
8746	H	-0.447878	-1.804863	1.061214
8747	O	4.182411	-0.004093	-1.699916
8748	H	3.674581	0.810870	-1.851569
8749	H	3.548056	-0.725669	-1.859096
8750	O	4.844521	-0.256841	0.854771
8751	H	5.781873	-0.236859	1.067381
8752	H	4.745941	-0.163326	-0.129164
8753	O	-1.496980	2.615753	-0.939024
8754	H	-0.896301	3.374911	-1.057893
8755	H	-1.038187	1.844182	-1.331030
8756	O	1.899060	-1.701477	-1.470185
8757	H	1.294179	-0.950106	-1.613230
8758	H	2.107279	-1.715589	-0.499365
8759	O	-4.080185	1.558009	-0.486213
8760	H	-3.324018	2.072807	-0.816421
8761	H	-4.117772	0.723795	-0.990248
8762	O	2.526047	1.325555	1.104896
8763	H	2.473033	1.480408	0.139765
8764	H	3.400187	0.936887	1.275109
8765	O	-1.330398	2.002755	1.749888
8766	H	-1.508172	2.279250	0.824468
8767	H	-2.185377	1.715883	2.120513
8768	O	-1.738011	-1.501524	-2.650692
8769	H	-1.357810	-2.367507	-2.426924
8770	H	-2.641381	-1.460242	-2.280542

8771

8772 Cartesian coordinates of : W20_16

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8773
8774  O      0.499006   -1.000995   1.104115
8775  H     -0.362321   -0.652620   1.447162
8776  H      0.584659   -0.743561   0.157125
8777  O     -2.507140   -2.581022   -2.059470
8778  H     -2.488339   -3.324215   -2.670541
8779  H     -1.963395   -2.835568   -1.266602
8780  O      0.961644    3.212112   1.604038
8781  H      1.626547    2.531713   1.795919
8782  H      1.068880    3.464123   0.670706
8783  O     -1.929671   -0.201666   1.928799
8784  H     -2.428940    0.066136   1.118757
8785  H     -2.407108   -0.978676   2.270119
8786  O     -4.566715   -1.837209   -0.241903
8787  H     -4.363824   -0.883620   -0.280308
8788  H     -4.078251   -2.212869   -0.995175
8789  O     -1.250983   -3.165172    0.206753
8790  H     -0.532436   -2.589256    0.514252
8791  H     -1.919517   -3.152495    0.917656
8792  O      1.063307   -0.526685   -1.510172
8793  H      1.688793    0.237792   -1.466795
8794  H      1.600495   -1.311369   -1.734887
8795  O      1.156486    3.681922   -1.218377
8796  H      1.329590    4.552593   -1.589787
8797  H      0.272055    3.380898   -1.570879
8798  O      4.753965   -0.487908   -1.057421
8799  H      4.249224   -1.232789   -1.430085
8800  H      4.253925    0.318450   -1.274202
8801  O     -2.978689    3.262816    0.099040
8802  H     -3.566241    4.011135    0.238689
8803  H     -2.465162    3.092988    0.955426
8804  O      2.537599    0.851277    1.639743
8805  H      3.367752    0.392233    1.865670
8806  H      1.829109    0.177131    1.639249
8807  O     -1.624522    2.643349    2.186341
8808  H     -1.699724    1.697315    2.392074
8809  H     -0.669059    2.843625    2.053625
8810  O     -3.367133   -2.623764    1.950809
8811  H     -3.884986   -3.154483    2.563287
8812  H     -3.947355   -2.381696    1.174219
8813  O     -3.233674    0.582842   -0.295324
8814  H     -3.398902    1.543658   -0.223598
8815  H     -2.581420    0.449879   -1.020835
8816  O      2.771099    1.476420   -1.016632
8817  H      2.364272    2.338829   -1.233160
8818  H      2.722504    1.376133   -0.039965
8819  O     -1.499226    0.030975   -2.309942
8820  H     -0.567628   -0.177546   -2.085693
8821  H     -1.903274   -0.826620   -2.535984
8822  O      2.915482   -2.579055   -1.531520
8823  H      2.984177   -3.425529   -1.983348
8824  H      2.845957   -2.752594   -0.549326
8825  O     -1.214819    2.902521   -2.028738
8826  H     -1.383940    2.006839   -2.361731
8827  H     -1.877932    3.092116   -1.336072
8828  O      4.752761   -0.813728    1.546355
8829  H      4.878340   -0.673165    0.565235
8830  H      5.619684   -0.851969    1.961171
8831  O      2.736811   -2.700823    1.076012
8832  H      1.919627   -2.239439    1.331177
8833  H      3.479464   -2.183164    1.437393
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8834
8835 Cartesian coordinates of : W20_17

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8836
8837  O     -2.550425    0.933934   -1.736213
8838  H     -3.461957    0.776326   -2.041529
8839  H     -2.627502    1.266927   -0.814408
8840  O     -2.495256    1.644305    0.908568
8841  H     -2.178357    0.803796    1.302804
8842  H     -1.789251    2.304121    1.038137
8843  O     -1.627170   -1.531951   -1.010272
8844  H     -0.678415   -1.724000   -1.140654
8845  H     -1.828101   -0.661515   -1.419824
8846  O      0.865989   -1.190467    1.826915
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8847	H	-0.083775	-1.258518	2.046856
8848	H	0.919845	-1.373729	0.855771
8849	O	-0.008194	2.115501	-1.774035
8850	H	-0.149064	2.218601	-0.812848
8851	H	-0.864253	1.826395	-2.132527
8852	O	1.661509	1.231054	2.445082
8853	H	1.826565	1.295086	3.390920
8854	H	1.362826	0.298413	2.245207
8855	O	3.398973	-3.289331	-0.946025
8856	H	3.670227	-4.127577	-1.331466
8857	H	3.886782	-2.551485	-1.408995
8858	O	3.389184	1.870640	0.390954
8859	H	2.868713	1.709852	1.203305
8860	H	4.213693	1.363492	0.507535
8861	O	4.479656	-1.108563	-1.910023
8862	H	3.769416	-0.496263	-2.168782
8863	H	4.916918	-0.699149	-1.141491
8864	O	-5.158057	0.802341	0.896421
8865	H	-5.321470	0.708382	-0.059806
8866	H	-4.363318	1.356668	0.989949
8867	O	-4.601968	-1.584531	1.821184
8868	H	-4.897579	-0.666842	1.556237
8869	H	-5.201484	-1.908423	2.500092
8870	O	5.231308	-0.192796	0.657803
8871	H	6.101562	-0.252594	1.064129
8872	H	4.646775	-0.866891	1.097838
8873	O	-1.892109	-0.965519	1.625424
8874	H	-1.838988	-1.251461	0.682028
8875	H	-2.744991	-1.303738	1.955328
8876	O	3.604659	-2.073561	1.576288
8877	H	2.716197	-1.891593	1.921272
8878	H	3.497275	-2.689920	0.828676
8879	O	-5.183467	0.028165	-1.814178
8880	H	-5.903750	-0.022301	-2.449606
8881	H	-4.928263	-0.901899	-1.555456
8882	O	1.114958	-1.726850	-0.800737
8883	H	1.736321	-2.463904	-0.946532
8884	H	1.552604	-0.912421	-1.162098
8885	O	-0.027567	2.889517	0.954708
8886	H	0.572931	3.558625	0.566923
8887	H	0.514193	2.371997	1.578355
8888	O	1.875510	4.062055	-0.656330
8889	H	2.630763	3.486888	-0.451427
8890	H	1.483243	3.721752	-1.473103
8891	O	-4.315668	-2.275245	-0.900215
8892	H	-4.462099	-2.270448	0.062973
8893	H	-3.351143	-2.298324	-1.030944
8894	O	2.208426	0.539993	-1.679233
8895	H	1.423282	1.067699	-1.941167
8896	H	2.601287	1.028447	-0.920368

8897

8898 Cartesian coordinates of : W20_18

8899

8900	O	-1.214042	-1.489762	1.008556
8901	H	-0.419095	-1.839875	1.514811
8902	H	-1.501719	-0.659553	1.435322
8903	O	4.276328	-1.106356	1.438403
8904	H	3.681680	-0.644646	2.050098
8905	H	3.802474	-1.904315	1.127874
8906	O	0.971703	1.155176	-2.230600
8907	H	0.308648	0.450123	-2.114521
8908	H	0.499226	2.007232	-2.258613
8909	O	0.909969	-2.217146	2.294671
8910	H	1.347468	-1.345746	2.375677
8911	H	1.507370	-2.765348	1.754554
8912	O	4.927319	0.407894	-0.588517
8913	H	4.778948	-0.206813	0.186584
8914	H	5.853675	0.666678	-0.592325
8915	O	2.740283	-3.197160	0.443509
8916	H	2.316153	-2.877821	-0.408787
8917	H	3.073454	-4.085657	0.285283
8918	O	-2.358936	0.957924	1.720807
8919	H	-2.339861	1.314945	0.804658
8920	H	-3.274670	0.649996	1.865250
8921	O	-0.379144	3.523299	-1.547668

8922	H	-0.482048	4.380913	-1.971274
8923	H	0.065717	3.662669	-0.656718
8924	O	-4.688761	0.440947	-1.297960
8925	H	-4.960538	0.294899	-0.373895
8926	H	-3.964157	1.090542	-1.256585
8927	O	2.527718	1.610346	-0.030343
8928	H	3.460898	1.410435	-0.238177
8929	H	1.994829	1.342021	-0.809924
8930	O	-0.904485	-0.843001	-1.517743
8931	H	-1.676150	-1.258447	-1.951470
8932	H	-0.958613	-1.118994	-0.556975
8933	O	3.303704	-0.371992	-2.795572
8934	H	3.977706	-0.114200	-2.142386
8935	H	2.690166	0.373115	-2.882147
8936	O	1.682907	-2.285830	-1.744808
8937	H	0.792301	-1.901926	-1.751652
8938	H	2.283828	-1.641429	-2.185683
8939	O	1.948691	0.348159	2.324188
8940	H	2.088067	0.757284	1.442277
8941	H	1.309456	0.921855	2.777613
8942	O	-2.202408	1.599893	-0.923777
8943	H	-1.687360	2.387944	-1.194067
8944	H	-1.707420	0.812522	-1.225966
8945	O	-0.232113	2.158292	2.920765
8946	H	-1.072532	1.735351	2.634412
8947	H	-0.412091	2.606474	3.753564
8948	O	-4.829156	-0.298554	1.425575
8949	H	-5.588074	-0.436806	2.000500
8950	H	-4.480393	-1.199480	1.151279
8951	O	0.851703	3.641503	0.730140
8952	H	0.413650	3.248856	1.506299
8953	H	1.638290	3.087737	0.560504
8954	O	-3.480363	-1.719806	-2.181068
8955	H	-4.011733	-0.907047	-1.948128
8956	H	-3.843593	-2.091501	-2.990900
8957	O	-3.724670	-2.483279	0.541708
8958	H	-2.786255	-2.364847	0.792718
8959	H	-3.727675	-2.481525	-0.431213

8960

8961 Cartesian coordinates of : W20_19

8962

8963	O	0.902659	-2.894626	1.121762
8964	H	0.807949	-3.297337	0.239107
8965	H	0.018373	-2.808812	1.523666
8966	O	2.661959	2.425627	-1.629112
8967	H	1.934663	1.958396	-2.084665
8968	H	2.242917	2.896656	-0.884554
8969	O	-1.570392	-1.796663	1.739772
8970	H	-1.590727	-1.671681	0.763953
8971	H	-2.500135	-1.736897	2.020267
8972	O	-1.397620	2.436344	0.561803
8973	H	-1.057539	1.805725	1.240022
8974	H	-0.664987	3.067537	0.439828
8975	O	-4.133506	1.701979	0.802365
8976	H	-4.082730	0.877458	1.319933
8977	H	-3.272966	2.151452	0.862501
8978	O	-4.256992	-0.982077	1.740665
8979	H	-5.045146	-1.251861	2.222599
8980	H	-4.359960	-1.294886	0.797805
8981	O	3.664435	0.168922	1.314030
8982	H	3.765903	-0.723811	1.703553
8983	H	4.231934	0.232677	0.522664
8984	O	2.070146	2.147713	2.516225
8985	H	2.758690	1.521883	2.223836
8986	H	1.310846	1.608539	2.795508
8987	O	-4.629377	1.000986	-1.668451
8988	H	-4.559589	1.351291	-0.735943
8989	H	-5.346655	1.459975	-2.115346
8990	O	-0.238501	0.612457	2.172813
8991	H	0.301777	0.310841	1.405414
8992	H	-0.792915	-0.168078	2.358208
8993	O	-1.463104	-1.603246	-0.985063
8994	H	-0.686421	-2.049264	-1.372766
8995	H	-1.489940	-0.671040	-1.298431
8996	O	-4.268333	-1.641249	-0.802136

8997	H	-3.348659	-1.857817	-1.037342
8998	H	-4.495804	-0.832074	-1.295559
8999	O	2.667434	-1.414703	-2.642888
9000	H	2.064084	-0.714694	-2.948994
9001	H	3.338390	-0.944780	-2.114676
9002	O	1.262573	-0.309458	0.125008
9003	H	1.157201	-1.252642	0.367969
9004	H	2.160232	-0.061842	0.448245
9005	O	0.869051	-3.046393	-1.632236
9006	H	0.811817	-3.775787	-2.258213
9007	H	1.618323	-2.464592	-1.951986
9008	O	-1.843739	0.988667	-1.712376
9009	H	-2.783050	1.081600	-1.953316
9010	H	-1.696681	1.553359	-0.917896
9011	O	3.408448	-2.403262	2.192455
9012	H	3.603458	-2.808729	3.041710
9013	H	2.521669	-2.706388	1.918369
9014	O	0.776280	0.588546	-2.421651
9015	H	0.833256	0.246497	-1.503051
9016	H	-0.153516	0.843497	-2.546878
9017	O	1.210788	3.604516	0.509799
9018	H	1.384321	4.537336	0.675030
9019	H	1.559909	3.103791	1.302328
9020	O	4.372953	0.482197	-1.301882
9021	H	5.194509	0.666480	-1.768351
9022	H	3.785901	1.287822	-1.411753

9023

9024 Cartesian coordinates of : W20_20

9025

9026	O	3.019614	-1.420663	1.242716
9027	H	2.927430	-1.503571	0.263894
9028	H	3.771031	-1.969098	1.513889
9029	O	-2.809592	-1.541777	-1.217468
9030	H	-2.759705	-1.551593	-0.234674
9031	H	-3.714781	-1.816533	-1.449695
9032	O	-5.636577	1.257732	1.478460
9033	H	-6.339443	1.586343	2.046880
9034	H	-5.590287	0.265922	1.579870
9035	O	-2.880427	1.459824	1.209720
9036	H	-3.791199	1.644051	1.501954
9037	H	-2.895691	1.475053	0.226245
9038	O	-2.730811	1.181386	-1.502540
9039	H	-2.683560	0.199174	-1.536236
9040	H	-1.870418	1.513730	-1.810311
9041	O	-0.036901	-1.397067	-1.314267
9042	H	0.014478	-1.426223	-0.331538
9043	H	-0.925652	-1.711343	-1.554165
9044	O	5.837514	-1.691257	1.528309
9045	H	6.588402	-2.014908	2.034789
9046	H	5.719911	-0.737105	1.722566
9047	O	-5.313932	-1.350763	1.480903
9048	H	-4.388887	-1.572669	1.682245
9049	H	-5.484254	-1.652536	0.569936
9050	O	-2.508109	-1.239102	1.477214
9051	H	-2.563879	-0.257235	1.508952
9052	H	-1.595583	-1.471772	1.721783
9053	O	-5.584208	-1.616511	-1.311566
9054	H	-5.644733	-0.625433	-1.413451
9055	H	-6.282266	-2.016348	-1.838758
9056	O	4.722920	0.800548	1.464383
9057	H	5.032378	1.140173	0.603860
9058	H	3.979332	0.193571	1.279096
9059	O	0.272691	-1.120258	1.399872
9060	H	0.238919	-0.138644	1.431459
9061	H	1.184378	-1.376236	1.629400
9062	O	-0.105715	1.580365	1.143517
9063	H	-1.009505	1.793434	1.434344
9064	H	-0.117491	1.614922	0.160825
9065	O	2.727468	-1.215183	-1.415802
9066	H	2.699012	-0.227654	-1.440407
9067	H	1.846792	-1.526335	-1.687136
9068	O	2.816910	1.495160	-1.364743
9069	H	3.742130	1.676923	-1.604019
9070	H	2.690198	1.909026	-0.473154
9071	O	-5.522282	1.010895	-1.325465

9072	H	-4.635183	1.317864	-1.579005
9073	H	-5.665906	1.297444	-0.405078
9074	O	5.526683	-1.322709	-1.284281
9075	H	4.606205	-1.549179	-1.503227
9076	H	5.701470	-1.652909	-0.386086
9077	O	0.049385	1.327350	-1.602019
9078	H	0.078112	0.344675	-1.620772
9079	H	0.933628	1.629536	-1.869897
9080	O	2.487456	2.561377	1.075371
9081	H	3.163770	2.177437	1.652777
9082	H	1.607078	2.337604	1.423955
9083	O	5.588485	1.315344	-1.208645
9084	H	6.382675	1.747368	-1.536546
9085	H	5.686510	0.335559	-1.343923

9086

9087 Cartesian coordinates of : W20_21

9088

9089	O	-0.442715	-1.662850	2.199111
9090	H	0.458352	-1.308278	2.321135
9091	H	-0.446466	-2.092246	1.316315
9092	O	3.727202	-2.011298	1.435043
9093	H	3.147064	-2.559772	0.874318
9094	H	3.156793	-1.528438	2.056834
9095	O	-1.145232	-0.502935	-1.864663
9096	H	-1.949577	-0.793487	-2.332603
9097	H	-1.428965	0.244026	-1.284965
9098	O	-0.448695	-2.662767	-0.332404
9099	H	-0.586539	-1.886266	-0.916778
9100	H	0.447428	-3.007949	-0.506730
9101	O	4.841523	-0.301770	-0.190217
9102	H	4.536061	-0.974535	0.485253
9103	H	5.778362	-0.134104	-0.052947
9104	O	2.275277	-3.260460	-0.650115
9105	H	2.643775	-2.607881	-1.314856
9106	H	2.557890	-4.137032	-0.931027
9107	O	-1.845246	0.493218	2.214252
9108	H	-2.780667	0.228880	2.281116
9109	H	-1.337823	-0.382529	2.191167
9110	O	-0.417948	3.881620	-0.622732
9111	H	-0.829430	4.743326	-0.502047
9112	H	0.226997	3.735627	0.138410
9113	O	-4.504639	0.658912	-0.767061
9114	H	-4.660477	0.245544	0.101197
9115	H	-3.688495	1.181425	-0.648880
9116	O	2.469045	1.102420	0.078335
9117	H	3.400074	0.835101	-0.044843
9118	H	1.996305	0.869782	-0.753880
9119	O	0.829540	3.154010	-3.000021
9120	H	0.387093	3.505627	-2.201728
9121	H	1.488825	3.800681	-3.267025
9122	O	1.336968	0.540929	-2.348951
9123	H	0.450017	0.125728	-2.352587
9124	H	1.225261	1.433977	-2.736805
9125	O	3.293008	-1.441611	-2.235026
9126	H	2.655332	-0.743634	-2.477419
9127	H	3.994205	-1.006629	-1.718138
9128	O	1.876736	-0.154784	2.441578
9129	H	2.000076	0.290340	1.574878
9130	H	1.480309	0.508219	3.030599
9131	O	-1.913820	1.545069	-0.280647
9132	H	-1.462523	2.401331	-0.410863
9133	H	-1.790736	1.254922	0.653650
9134	O	0.105527	1.874591	3.414792
9135	H	-0.733797	1.447124	3.116102
9136	H	-0.048449	2.234985	4.293521
9137	O	-4.251885	-0.814989	1.626598
9138	H	-4.915181	-1.217564	2.195661
9139	H	-3.838830	-1.553241	1.100502
9140	O	1.250859	3.290605	1.248559
9141	H	0.857721	2.899199	2.050083
9142	H	1.828426	2.605928	0.855657
9143	O	-3.776195	-1.254901	-2.396698
9144	H	-4.340881	-1.412783	-3.158791
9145	H	-4.165319	-0.502194	-1.866562
9146	O	-3.251391	-2.653535	0.000295

9147	H	-2.316135	-2.918761	-0.006084
9148	H	-3.459426	-2.380247	-0.911076
9149				
9150	Cartesian coordinates of : W20_22			
9151				
9152	O	-1.129690	-2.375286	-1.505996
9153	H	-0.689449	-1.547404	-1.765912
9154	H	-2.081519	-2.248821	-1.691343
9155	O	-3.800655	-1.702464	1.168073
9156	H	-2.913110	-2.005718	1.436355
9157	H	-3.906286	-0.783556	1.475605
9158	O	-1.648926	2.256297	1.216260
9159	H	-2.524478	1.986882	1.553259
9160	H	-1.730171	2.237908	0.231972
9161	O	1.108224	-3.848846	1.758182
9162	H	1.100115	-4.548001	2.418894
9163	H	0.213497	-3.428063	1.741637
9164	O	2.295429	1.822702	-1.457946
9165	H	2.277253	1.901086	-0.468662
9166	H	3.163432	1.439422	-1.671759
9167	O	0.394021	3.920918	-1.433261
9168	H	1.186337	3.418806	-1.685569
9169	H	0.495227	4.125393	-0.488094
9170	O	-1.643365	2.132895	-1.503102
9171	H	-1.031974	2.891937	-1.650121
9172	H	-1.092876	1.343055	-1.665005
9173	O	0.272643	0.068236	-1.446128
9174	H	0.990266	0.730800	-1.614678
9175	H	0.178296	0.046344	-0.462088
9176	O	2.436754	-1.321513	1.424917
9177	H	2.497575	-1.467688	0.460138
9178	H	2.155661	-2.178456	1.786437
9179	O	-1.081495	-2.414779	1.269658
9180	H	-0.707472	-1.517312	1.429765
9181	H	-1.098267	-2.479646	0.289617
9182	O	2.499848	-1.688710	-1.359575
9183	H	2.195550	-2.628161	-1.379329
9184	H	1.708081	-1.165593	-1.579523
9185	O	2.095200	1.914550	1.193798
9186	H	2.996781	1.660443	1.499088
9187	H	1.817153	2.769667	1.557010
9188	O	4.534474	0.093832	-1.367968
9189	H	5.318917	-0.061485	-1.903168
9190	H	3.954756	-0.693605	-1.459989
9191	O	1.207116	-4.023696	-1.091816
9192	H	1.203819	-4.174554	-0.130310
9193	H	0.305071	-3.760896	-1.336690
9194	O	-3.837603	-1.730655	-1.438340
9195	H	-4.549918	-2.265068	-1.804044
9196	H	-3.899544	-1.784944	-0.438106
9197	O	-4.171282	1.085430	1.439681
9198	H	-4.982631	1.421537	1.833619
9199	H	-4.277683	1.127053	0.443846
9200	O	-0.035712	0.048494	1.261668
9201	H	0.892803	0.169375	1.531856
9202	H	-0.520104	0.884175	1.427989
9203	O	-4.195869	1.067697	-1.170160
9204	H	-4.097479	0.147855	-1.476819
9205	H	-3.425022	1.563426	-1.500553
9206	O	4.410801	0.629774	1.503928
9207	H	4.695057	0.512758	0.582869
9208	H	3.922781	-0.187650	1.713341
9209	O	0.353670	4.078832	1.449230
9210	H	0.209607	4.903068	1.923998
9211	H	-0.458724	3.535964	1.545632
9212				
9213				
9214	Cartesian coordinates of the water 21-mer			
9215				
9216	Cartesian coordinates of : W21_1			
9217				
9218	O	-3.045755	1.578608	-2.148127
9219	H	-3.766504	2.118487	-2.485896
9220	H	-2.353519	2.202421	-1.787760
9221	O	-1.270795	3.155986	-1.059886

9222	H	-0.345635	3.290528	-1.336286
9223	H	-1.341469	3.332023	-0.103069
9224	O	-2.876529	-0.095916	-0.003526
9225	H	-3.144152	0.409860	-0.797133
9226	H	-3.164517	-1.025819	-0.090542
9227	O	-1.613082	-0.456057	-3.514878
9228	H	-2.249238	0.199717	-3.183840
9229	H	-0.746279	-0.026025	-3.394501
9230	O	-2.612878	1.217315	2.415442
9231	H	-2.858294	0.737859	1.600048
9232	H	-2.061218	0.602550	2.936474
9233	O	-1.476057	3.421620	1.719431
9234	H	-1.970357	2.606771	2.047218
9235	H	-1.840174	4.194058	2.161340
9236	O	-3.015650	-2.809656	0.044975
9237	H	-3.714616	-3.465521	0.124482
9238	H	-2.432136	-2.871690	0.862525
9239	O	-1.297502	-2.782377	-2.200073
9240	H	-1.486535	-1.946513	-2.692576
9241	H	-1.915925	-2.840300	-1.450005
9242	O	1.375047	3.313194	-1.985521
9243	H	2.066396	3.056342	-1.303300
9244	H	1.699086	4.079710	-2.467286
9245	O	0.716767	0.677710	-2.507702
9246	H	0.379383	0.543655	-1.593150
9247	H	0.953617	1.620791	-2.575842
9248	O	-0.136869	0.037441	0.019791
9249	H	-1.115586	-0.063069	0.018686
9250	H	0.251500	-0.830900	0.262910
9251	O	-1.035370	-0.673039	3.765541
9252	H	-1.217711	-0.792363	4.703284
9253	H	-0.063537	-0.437122	3.686594
9254	O	0.878714	1.999096	1.597045
9255	H	0.210149	2.685322	1.780045
9256	H	0.429034	1.332715	1.024503
9257	O	-1.368049	-2.848120	2.030866
9258	H	-0.469311	-2.830135	1.647910
9259	H	-1.381963	-2.119937	2.680640
9260	O	2.967003	2.508901	-0.106354
9261	H	3.378296	1.632176	-0.214291
9262	H	2.321541	2.415320	0.624328
9263	O	1.141861	-3.359557	-1.769759
9264	H	1.320511	-4.237181	-2.120931
9265	H	0.167958	-3.141861	-1.976868
9266	O	1.024993	-2.374705	0.743780
9267	H	1.199409	-2.868553	-0.085840
9268	H	1.874647	-2.198209	1.187799
9269	O	2.737180	-1.122002	-2.248063
9270	H	2.053675	-0.459532	-2.494042
9271	H	2.262959	-1.970768	-2.151095
9272	O	1.434139	0.107640	3.494754
9273	H	2.115480	-0.434865	3.063467
9274	H	1.332104	0.903856	2.932417
9275	O	4.060931	-0.121448	-0.324366
9276	H	4.980254	-0.074256	-0.608098
9277	H	3.542124	-0.565322	-1.084336
9278	O	3.329944	-1.377969	1.930369
9279	H	3.699021	-0.889311	1.152372
9280	H	4.057184	-1.848233	2.349741

9281

9282 Cartesian coordinates of : W21_ 2

9283

9284	O	0.334664	1.976105	-0.636692
9285	O	0.496201	0.815885	1.856302
9286	O	3.096903	1.729318	-0.804550
9287	O	3.089396	-0.831714	-1.777384
9288	O	2.878191	-1.790473	0.780348
9289	O	3.268171	0.742452	1.744660
9290	O	0.104254	-1.661230	0.724351
9291	O	0.332725	-0.531108	-1.774410
9292	O	5.862114	-0.882460	-1.963839
9293	O	5.884051	1.465313	-0.782787
9294	O	6.023500	0.403994	1.824472
9295	O	5.673431	-1.919972	0.649239
9296	H	3.034764	0.863921	-1.268034

9297	H	2.235442	2.166631	-0.916049
9298	H	1.408867	0.912855	2.178738
9299	H	0.399394	-0.118838	1.567081
9300	H	2.956291	-0.925108	1.241584
9301	H	1.970091	-2.104468	0.930597
9302	H	0.380725	0.408122	-1.488473
9303	H	1.206092	-0.753546	-2.140595
9304	H	0.353750	1.681840	0.300994
9305	H	-0.541386	2.372968	-0.783594
9306	H	3.257858	1.207888	0.878240
9307	H	3.044240	-1.294324	-0.910669
9308	H	0.135158	-1.371628	-0.214260
9309	H	-0.814037	-1.936192	0.896245
9310	H	4.747874	-2.199683	0.753188
9311	H	5.815028	-1.770345	-0.303378
9312	H	5.967486	-0.524990	1.463026
9313	H	6.041831	1.296701	0.164041
9314	H	5.003502	1.872505	-0.850495
9315	H	5.953606	0.045334	-1.607496
9316	H	3.988185	-0.982483	-2.122217
9317	H	4.190727	0.765037	2.057651
9318	H	6.533544	-1.013556	-2.640141
9319	H	6.733861	0.431418	2.472417
9320	H	-2.551104	-0.578753	1.330272
9321	O	-2.654392	-1.448383	0.883608
9322	H	-3.541214	-1.775919	1.123955
9323	H	-2.257869	1.559332	0.976995
9324	O	-2.264771	1.091939	1.842794
9325	H	-1.367068	1.170593	2.207794
9326	H	-2.530953	-0.964826	-0.825747
9327	O	-2.443144	-0.480616	-1.676870
9328	H	-1.558118	-0.681435	-2.027374
9329	H	-2.462898	1.203422	-1.159290
9330	O	-2.436422	2.075284	-0.703460
9331	H	-3.340292	2.432839	-0.767218
9332	H	-5.895440	2.864581	-0.566654
9333	O	-5.208081	2.192133	-0.537121
9334	H	-5.229548	1.775370	0.370120
9335	H	-4.227903	-0.301276	-2.267743
9336	O	-5.177776	-0.111988	-2.174766
9337	H	-5.242705	0.738069	-1.701950
9338	H	-4.153207	1.106274	2.133714
9339	O	-5.063744	1.010921	1.806511
9340	H	-5.256666	0.054959	1.790252
9341	H	-5.839905	-1.942547	0.659940
9342	O	-5.358979	-1.780071	1.519081
9343	H	-5.730142	-2.371706	2.180634
9344	H	-7.293160	-2.144582	-1.154019
9345	O	-6.381425	-2.046051	-0.867372
9346	H	-5.963635	-1.328669	-1.419005

9347

9348 Cartesian coordinates of : W21_ 3

9349

9350	O	-0.349779	1.363783	1.480604
9351	O	-0.557708	1.614179	-1.248773
9352	O	-3.107433	1.069848	1.561681
9353	O	-3.109926	-1.637267	1.133167
9354	O	-2.960255	-1.193381	-1.566259
9355	O	-3.328972	1.487496	-1.137389
9356	O	-0.185071	-1.100057	-1.523472
9357	O	-0.348250	-1.375887	1.215856
9358	O	-5.876201	-1.756119	1.337845
9359	O	-5.895146	0.867830	1.471210
9360	O	-6.091844	1.243939	-1.314954
9361	O	-5.752880	-1.358354	-1.448614
9362	H	-3.048251	0.088461	1.530750
9363	H	-2.238410	1.390926	1.857421
9364	H	-1.473689	1.861373	-1.464468
9365	H	-0.466901	0.661383	-1.473548
9366	H	-3.032810	-0.212880	-1.534675
9367	H	-2.062226	-1.394246	-1.880316
9368	H	-0.390605	-0.417645	1.431485
9369	H	-1.220060	-1.745976	1.438668
9370	H	-0.389352	1.582662	0.522670
9371	H	0.528180	1.643003	1.792677

9372	H	-3.301212	1.459071	-0.154818
9373	H	-3.090179	-1.608941	0.150297
9374	H	-0.191638	-1.323180	-0.566629
9375	H	0.724285	-1.254842	-1.833880
9376	H	-4.834084	-1.555372	-1.699171
9377	H	-5.877470	-1.703274	-0.545659
9378	H	-6.043557	0.257878	-1.463125
9379	H	-6.073176	1.192390	0.569663
9380	H	-5.006807	1.183284	1.709778
9381	H	-5.960885	-0.772115	1.484928
9382	H	-4.004105	-1.934668	1.381549
9383	H	-4.255921	1.664461	-1.380396
9384	H	-6.537405	-2.198502	1.878483
9385	H	-6.812155	1.593421	-1.848032
9386	H	2.484516	0.156951	-1.549034
9387	O	2.569079	-0.822477	-1.580658
9388	H	3.483855	-1.008469	-1.861674
9389	H	2.215511	1.828169	-0.157489
9390	O	2.212369	1.858205	-1.140230
9391	H	1.311701	2.108577	-1.407231
9392	H	2.438171	-1.235921	0.132698
9393	O	2.420984	-1.267441	1.116707
9394	H	1.550095	-1.621826	1.366892
9395	H	2.458397	0.460057	1.526825
9396	O	2.422110	1.441793	1.561463
9397	H	3.316385	1.739845	1.807900
9398	H	5.849036	2.326626	1.932872
9399	O	5.182498	1.760764	1.531515
9400	H	5.190633	1.923942	0.543779
9401	H	4.279975	-1.303659	1.452532
9402	O	5.184385	-1.016322	1.233684
9403	H	5.271461	-0.092059	1.537266
9404	H	4.104198	2.145515	-1.344889
9405	O	5.019448	1.961392	-1.073569
9406	H	5.252506	1.091706	-1.449799
9407	H	5.253341	-0.895414	-0.550770
9408	O	5.328380	-0.779035	-1.523297
9409	H	6.108636	-1.309312	-1.741705
9410	H	7.837061	-3.006215	0.088187
9411	O	7.219637	-2.324218	-0.188492
9412	H	6.689553	-2.074557	0.585796

9413

9414 Cartesian coordinates of : W21_4

9415

9416	O	0.298276	3.760151	0.666941
9417	H	1.066682	3.531047	1.221253
9418	H	-0.481182	3.277367	0.994530
9419	O	4.170854	-2.434116	-1.031342
9420	H	3.295717	-2.859183	-1.271049
9421	H	4.868721	-2.934987	-1.464374
9422	O	0.222152	0.348851	0.901406
9423	H	-0.540445	0.949591	1.065909
9424	H	0.473830	0.499097	-0.040018
9425	O	-0.361462	-1.794622	-1.883064
9426	H	0.119776	-0.946254	-1.936510
9427	H	-0.555928	-1.943371	-0.932661
9428	O	-3.052238	1.686471	-1.431247
9429	H	-3.017974	2.329447	-2.146112
9430	H	-2.917565	0.774273	-1.838112
9431	O	1.066363	0.608663	-1.668197
9432	H	0.948153	1.532512	-1.958061
9433	H	2.031310	0.471191	-1.525517
9434	O	-3.842590	0.619007	2.384557
9435	H	-4.132386	0.638460	3.301608
9436	H	-3.624538	-0.334758	2.148946
9437	O	-5.317078	0.853669	0.005211
9438	H	-4.995338	0.913253	0.923016
9439	H	-4.668669	1.341929	-0.533914
9440	O	3.478710	-2.318191	1.702861
9441	H	3.930564	-2.338274	0.839984
9442	H	3.337342	-1.382516	1.932369
9443	O	-2.887822	-0.708189	-2.392572
9444	H	-2.042640	-1.196439	-2.335802
9445	H	-3.575188	-1.234672	-1.945603
9446	O	3.621395	0.256914	-0.849164

9447	H	3.981683	-0.624936	-1.064922
9448	H	3.419830	0.253319	0.112995
9449	O	1.835662	-3.534316	-1.407863
9450	H	1.094913	-3.014481	-1.773385
9451	H	1.558012	-3.831186	-0.522828
9452	O	1.390623	-3.861495	1.368237
9453	H	1.434316	-4.647363	1.921336
9454	H	2.176110	-3.286160	1.594105
9455	O	3.627816	3.042080	-0.807028
9456	H	3.886907	2.125966	-1.008955
9457	H	2.827323	3.224897	-1.332326
9458	O	-4.955394	-1.639446	-0.741909
9459	H	-5.228133	-0.714197	-0.486165
9460	H	-5.746920	-2.125127	-0.992807
9461	O	-1.884462	2.041076	1.049130
9462	H	-2.560349	1.689438	1.662718
9463	H	-2.273680	1.977559	0.151130
9464	O	2.870299	3.190211	1.707180
9465	H	3.310995	3.888059	2.202432
9466	H	3.240912	3.199394	0.779739
9467	O	1.021973	3.378656	-1.809130
9468	H	0.740148	4.081628	-2.402005
9469	H	0.664270	3.578540	-0.895197
9470	O	2.789282	0.411537	1.769185
9471	H	1.816929	0.413278	1.627176
9472	H	3.000193	1.324099	2.037416
9473	O	-3.368744	-1.797678	1.575268
9474	H	-2.445901	-2.035049	1.353090
9475	H	-3.908305	-1.960095	0.780663
9476	O	-0.732502	-2.168951	0.837666
9477	H	-0.099172	-2.840307	1.158018
9478	H	-0.339213	-1.287247	1.028887

9479

9480 Cartesian coordinates of : W21_ 5

9481

9482	O	-0.309760	3.607866	1.878269
9483	H	-0.024651	2.877818	2.503617
9484	H	-0.406350	4.411631	2.398689
9485	O	2.916762	1.382511	-0.072676
9486	H	2.485899	0.890007	0.664446
9487	H	2.508680	2.284806	-0.090428
9488	O	-0.294854	-0.866012	-1.726114
9489	H	-0.862460	-0.064560	-1.683128
9490	H	0.566408	-0.533745	-2.062505
9491	O	0.269961	1.541382	3.360341
9492	H	-0.468537	0.910151	3.328897
9493	H	1.023405	1.024311	3.014739
9494	O	2.502874	-3.260229	0.027351
9495	H	2.572069	-4.189088	-0.216405
9496	H	2.869512	-2.730946	-0.734576
9497	O	-1.528981	-0.366362	2.304241
9498	H	-2.390234	-0.807310	2.446079
9499	H	-0.958831	-1.020056	1.860636
9500	O	3.620316	-1.747859	-1.817931
9501	H	4.310793	-1.205640	-1.394825
9502	H	3.086290	-1.126735	-2.340650
9503	O	-4.248969	0.075301	-2.160574
9504	H	-4.502772	0.201362	-1.199896
9505	H	-5.035613	0.220582	-2.694975
9506	O	-2.535925	-3.135988	0.424410
9507	H	-2.678107	-2.920133	-0.528368
9508	H	-1.593104	-2.964838	0.586958
9509	O	-2.697753	-2.312606	-2.151202
9510	H	-3.294861	-1.552247	-2.264579
9511	H	-1.800423	-1.975997	-2.307381
9512	O	-4.646984	0.507134	0.378943
9513	H	-4.522097	-0.265176	0.965307
9514	H	-3.997723	1.172869	0.662694
9515	O	-2.197610	1.853901	0.839471
9516	H	-1.712282	2.628816	1.182730
9517	H	-1.860031	1.073920	1.334192
9518	O	1.902212	-0.157098	1.912133
9519	H	2.708942	-0.709265	2.064828
9520	H	1.248838	-0.759386	1.508769
9521	O	4.086264	-1.714013	1.831521

9522	H	4.670019	-1.234390	1.219826
9523	H	3.711927	-2.455689	1.327255
9524	O	5.170548	-0.032375	-0.211749
9525	H	4.496683	0.685695	-0.156714
9526	H	6.035009	0.374900	-0.322062
9527	O	-3.938616	-1.659620	1.984020
9528	H	-3.467497	-2.314068	1.374269
9529	H	-4.525250	-2.153719	2.564730
9530	O	0.273593	2.700757	-2.788968
9531	H	0.094243	3.322259	-3.501567
9532	H	-0.584738	2.288520	-2.538511
9533	O	1.470222	3.606026	-0.330523
9534	H	0.823140	3.695716	0.392800
9535	H	0.979684	3.441459	-1.153353
9536	O	0.110275	-1.981944	0.642733
9537	H	0.863510	-2.593936	0.508681
9538	H	-0.042000	-1.554597	-0.244245
9539	O	-1.853961	1.379796	-1.769056
9540	H	-2.716602	1.074621	-2.113329
9541	H	-1.997576	1.622172	-0.819945
9542	O	1.989758	0.445185	-2.439788
9543	H	1.589607	1.210919	-2.884427
9544	H	2.322089	0.792983	-1.577088
9545				
9546	Cartesian coordinates of : W21_ 6			
9547				
9548	O	-5.321914	-1.255301	-1.232066
9549	H	-5.634643	-1.094263	-0.322295
9550	H	-4.611020	-1.918657	-1.166364
9551	O	0.328762	3.495172	0.931631
9552	H	0.377804	4.382773	1.299786
9553	H	1.147570	3.013695	1.196172
9554	O	5.271477	1.013935	-1.055100
9555	H	4.340078	1.178324	-1.293591
9556	H	5.322265	1.121180	-0.088426
9557	O	2.379589	1.800932	1.270783
9558	H	2.490044	1.567336	0.310251
9559	H	3.280418	1.794439	1.644669
9560	O	-4.660705	1.855694	0.598257
9561	H	-3.727271	1.983019	0.849814
9562	H	-4.681756	1.815874	-0.374610
9563	O	1.407062	-0.714690	1.854503
9564	H	0.458540	-0.808517	2.070954
9565	H	1.609879	0.241982	1.799871
9566	O	-3.601476	-2.166244	1.968157
9567	H	-3.568726	-2.668349	1.137930
9568	H	-4.384358	-1.589759	1.907146
9569	O	-5.721456	-0.398189	1.395556
9570	H	-5.340262	0.502179	1.185215
9571	H	-6.520334	-0.267097	1.914880
9572	O	1.708793	-1.482066	-0.753224
9573	H	1.623209	-1.289018	0.208975
9574	H	2.472989	-2.082296	-0.843769
9575	O	5.932319	-1.397340	-1.843930
9576	H	5.746353	-0.455256	-1.570713
9577	H	6.096827	-1.395351	-2.791066
9578	O	-1.889229	1.790150	0.939288
9579	H	-1.168678	2.426272	1.103937
9580	H	-1.653173	0.930404	1.358485
9581	O	-1.320452	-0.768083	1.631943
9582	H	-1.215465	-1.069324	0.704749
9583	H	-2.117913	-1.250960	1.955757
9584	O	-1.855742	1.059885	-1.684567
9585	H	-2.758874	1.101628	-2.054203
9586	H	-1.934630	1.359292	-0.749381
9587	O	2.498943	1.116311	-1.298644
9588	H	1.776034	1.680292	-1.669084
9589	H	2.189569	0.187272	-1.297132
9590	O	0.417685	2.707819	-1.863451
9591	H	0.287368	3.163641	-1.015740
9592	H	-0.403082	2.212012	-2.033259
9593	O	-3.174834	-3.019821	-0.753430
9594	H	-3.125454	-3.897788	-1.143957
9595	H	-2.330164	-2.554635	-0.958385
9596	O	4.995570	1.021512	1.767944

9597	H	4.735905	0.062057	1.873250
9598	H	5.704859	1.204089	2.391719
9599	O	4.149796	-2.804953	-0.569852
9600	H	4.375725	-3.739973	-0.545024
9601	H	4.843223	-2.342943	-1.123219
9602	O	-4.589572	1.082662	-2.124936
9603	H	-4.894705	0.160898	-1.879841
9604	H	-5.117851	1.383532	-2.870378
9605	O	-1.019404	-1.441608	-1.059729
9606	H	-1.254939	-0.570643	-1.455164
9607	H	-0.059264	-1.589125	-1.173070
9608	O	4.100608	-1.438357	1.917765
9609	H	3.148427	-1.389935	2.112977
9610	H	4.188906	-1.957669	1.096951

9611

9612 Cartesian coordinates of : W21_ 7

9613

9614	O	-0.964529	-3.764071	0.924703
9615	H	-1.712414	-3.278828	1.339850
9616	H	-0.942607	-4.645690	1.310132
9617	O	-4.375793	-1.028572	-0.295279
9618	H	-3.819737	-1.443393	0.384731
9619	H	-3.939773	-1.160020	-1.167503
9620	O	0.823636	1.235549	-2.168246
9621	H	0.887841	0.261912	-2.038851
9622	H	-0.064184	1.430076	-2.497411
9623	O	-2.877932	-2.106658	1.934965
9624	H	-3.541644	-2.360017	2.585260
9625	H	-2.401413	-1.308520	2.291945
9626	O	-1.296274	3.760879	-0.173486
9627	H	-1.314112	4.644528	-0.553216
9628	H	-1.578013	3.115045	-0.866067
9629	O	1.184609	0.277218	2.250721
9630	H	2.106832	0.354156	2.562538
9631	H	1.071261	0.995092	1.583098
9632	O	-2.111354	1.645866	-1.638601
9633	H	-1.721522	0.957002	-1.032026
9634	H	-3.050253	1.710024	-1.375509
9635	O	4.220377	-1.309331	-1.817386
9636	H	4.286069	-1.488935	-0.835059
9637	H	4.939483	-1.776006	-2.253328
9638	O	3.747421	2.385720	0.600208
9639	H	3.896857	2.090855	-0.326064
9640	H	2.799043	2.607691	0.614224
9641	O	3.700106	1.468730	-1.977217
9642	H	3.937548	0.526832	-2.038843
9643	H	2.784556	1.547005	-2.286441
9644	O	4.106435	-1.773765	0.752214
9645	H	3.214497	-2.125589	0.918499
9646	H	4.192171	-0.997799	1.340821
9647	O	1.328001	-2.073834	0.907430
9648	H	0.591559	-2.693221	1.047052
9649	H	1.152672	-1.251828	1.422707
9650	O	-1.534452	0.056907	2.505002
9651	H	-1.950412	0.947822	2.351965
9652	H	-0.611405	0.174138	2.795292
9653	O	-2.738003	2.301035	1.796544
9654	H	-2.214230	2.966483	1.320934
9655	H	-3.475174	2.083878	1.193848
9656	O	-4.522965	1.541879	-0.209639
9657	H	-5.420926	1.859515	-0.345239
9658	H	-4.553341	0.535592	-0.185786
9659	O	3.970674	0.515528	2.343487
9660	H	4.601847	0.738316	3.034478
9661	H	3.970553	1.272672	1.670657
9662	O	-0.967671	-2.619127	-1.651013
9663	H	-0.962593	-3.312623	-0.971374
9664	H	-0.041912	-2.447419	-1.911811
9665	O	-3.042704	-1.037496	-2.673278
9666	H	-2.313024	-1.669741	-2.552825
9667	H	-2.643290	-0.155913	-2.708969
9668	O	0.968519	2.243552	0.395874
9669	H	0.270432	2.921609	0.393509
9670	H	0.906329	1.822487	-0.491646
9671	O	1.453386	-1.388854	-1.738143

9672	H	2.384694	-1.490890	-2.011229
9673	H	1.445575	-1.533187	-0.763813
9674	O	-0.941071	-0.216926	-0.209064
9675	H	-1.057708	-1.116206	-0.570282
9676	H	-1.153460	-0.220744	0.743403
9677				
9678	Cartesian coordinates of : W21_ 8			
9679				
9680	O	5.502311	-2.217044	-0.687635
9681	H	5.647452	-1.979201	0.242224
9682	H	5.778167	-1.445274	-1.211724
9683	O	2.903295	1.677340	0.514918
9684	H	2.911703	1.342242	-0.411695
9685	H	2.218888	2.373378	0.540362
9686	O	-0.222382	-0.768064	1.898961
9687	H	-1.071927	-1.151040	2.174543
9688	H	-0.126700	-0.995404	0.946409
9689	O	-3.005561	-1.153744	1.664529
9690	H	-3.918031	-1.456058	1.815723
9691	H	-3.093645	-0.195896	1.465477
9692	O	-5.308826	0.651835	-2.057713
9693	H	-5.613088	1.072952	-1.238467
9694	H	-4.385521	0.923495	-2.188012
9695	O	-3.224645	1.458918	0.812263
9696	H	-2.961783	1.352047	-0.130375
9697	H	-4.182398	1.633618	0.834771
9698	O	3.020903	0.515533	-1.949828
9699	H	2.943333	-0.399754	-1.594345
9700	H	3.948997	0.591030	-2.237811
9701	O	-2.497225	0.786531	-1.727199
9702	H	-2.475452	-0.184444	-1.569376
9703	H	-1.612475	1.042331	-2.038928
9704	O	0.602969	3.142563	0.218601
9705	H	0.441892	4.089774	0.171708
9706	H	0.026406	2.756405	0.954994
9707	O	2.823679	-1.869178	-0.631936
9708	H	3.732814	-2.225278	-0.755414
9709	H	2.784652	-1.561051	0.296446
9710	O	-0.799284	1.974103	2.015908
9711	H	-1.737382	1.946108	1.749884
9712	H	-0.519500	1.037373	2.062224
9713	O	5.641572	1.211593	0.626706
9714	H	5.660779	0.442230	1.222009
9715	H	4.759554	1.610294	0.741249
9716	O	-5.265873	-1.965206	-1.252853
9717	H	-4.336346	-2.225277	-1.370342
9718	H	-5.346428	-1.090461	-1.695157
9719	O	-5.773805	-1.445132	1.203765
9720	H	-5.608120	-1.731939	0.243241
9721	H	-6.466132	-2.010880	1.560296
9722	O	5.818114	0.378211	-1.865810
9723	H	6.563122	0.727971	-2.363859
9724	H	5.844115	0.778575	-0.954071
9725	O	0.165015	-1.284270	-0.770008
9726	H	1.027466	-1.717921	-0.908979
9727	H	0.234454	-0.381296	-1.149164
9728	O	-2.504111	-1.855901	-0.953793
9729	H	-2.633160	-1.723985	0.010834
9730	H	-1.552070	-2.024944	-1.065267
9731	O	2.581221	-0.654511	1.860674
9732	H	1.685978	-0.820508	2.205584
9733	H	2.586498	0.261901	1.498722
9734	O	-5.988835	1.216178	0.686638
9735	H	-6.049041	0.276940	0.979354
9736	H	-6.747604	1.687983	1.042891
9737	O	0.319361	1.277505	-1.822800
9738	H	0.392878	1.998551	-1.163196
9739	H	1.195667	1.201461	-2.239070
9740	O	5.231605	-1.222291	2.028544
9741	H	5.629281	-1.533167	2.847808
9742	H	4.266737	-1.132627	2.183038
9743				
9744	Cartesian coordinates of : W21_ 9			
9745				
9746	O	-3.168978	-1.509637	-2.342219

9747	H	-3.372531	-2.113401	-1.606115
9748	H	-2.198943	-1.405899	-2.355229
9749	O	-1.051214	1.515841	1.721975
9750	H	-1.422742	0.646397	2.040867
9751	H	-0.122259	1.541008	2.017754
9752	O	4.723773	2.157277	-0.177804
9753	H	3.800562	2.131421	-0.487708
9754	H	4.703519	1.845352	0.745336
9755	O	1.662282	0.951303	1.787702
9756	H	1.860241	1.211337	0.858402
9757	H	2.507620	1.055183	2.261063
9758	O	-5.007702	0.961747	0.502588
9759	H	-4.415385	1.684441	0.782814
9760	H	-4.939926	0.893330	-0.470807
9761	O	1.610757	-1.740129	1.153729
9762	H	0.776398	-2.238248	1.182345
9763	H	1.447327	-0.839890	1.507824
9764	O	-1.976270	-0.832471	2.441128
9765	H	-1.592184	-1.454857	1.790544
9766	H	-2.937599	-0.967697	2.391544
9767	O	-4.679802	-1.282895	1.705479
9768	H	-5.419860	-1.428830	2.303004
9769	H	-4.839632	-0.400373	1.238242
9770	O	2.275223	-1.208040	-1.457991
9771	H	2.076961	-1.501769	-0.541528
9772	H	3.187941	-1.493097	-1.646623
9773	O	6.173616	0.590656	-1.709859
9774	H	5.672066	1.232850	-1.133671
9775	H	6.334113	1.025905	-2.551857
9776	O	-3.176066	3.018109	1.117681
9777	H	-3.395075	3.743888	1.710143
9778	H	-2.342581	2.606208	1.449953
9779	O	-0.974447	-2.503003	0.477457
9780	H	-0.818388	-1.985280	-0.346695
9781	H	-1.769342	-3.037362	0.318336
9782	O	-2.815401	2.891326	-1.725882
9783	H	-3.466231	2.225350	-2.010668
9784	H	-3.081677	3.182226	-0.838973
9785	O	2.109907	1.464159	-0.861448
9786	H	1.209239	1.741553	-1.118276
9787	H	2.222210	0.551312	-1.207097
9788	O	-0.621961	1.523537	-1.008265
9789	H	-0.807616	1.496163	-0.043852
9790	H	-1.351681	2.061551	-1.401824
9791	O	-3.687140	-3.109409	-0.041199
9792	H	-4.132903	-2.518889	0.610690
9793	H	-4.222264	-3.904709	-0.125457
9794	O	4.401933	0.880883	2.323799
9795	H	4.481728	-0.066040	2.016638
9796	H	4.982519	0.992726	3.082582
9797	O	5.018272	-1.725461	-1.363351
9798	H	5.567305	-2.454944	-1.666632
9799	H	5.501548	-0.877169	-1.575329
9800	O	-4.536264	0.707230	-2.212848
9801	H	-4.004417	-0.137602	-2.304695
9802	H	-5.204102	0.701775	-2.905464
9803	O	-0.489082	-1.037758	-1.766159
9804	H	0.431332	-1.216137	-2.026409
9805	H	-0.536524	-0.075753	-1.532544
9806	O	4.392676	-1.574985	1.396674
9807	H	3.471894	-1.887869	1.428313
9808	H	4.686450	-1.670398	0.471549

9809

9810 Cartesian coordinates of : W21_10

9811

9812	O	-5.655742	2.146769	-0.395230
9813	H	-5.862781	1.500754	-1.095570
9814	H	-4.722195	2.392148	-0.514620
9815	O	-0.459155	-2.072364	0.428213
9816	H	-0.442772	-1.650599	-0.459463
9817	H	0.403078	-2.509797	0.540211
9818	O	5.114193	-0.212284	1.881009
9819	H	4.204599	-0.096887	2.202638
9820	H	5.178066	-1.131040	1.565149
9821	O	2.300481	-2.291709	0.554197

9822	H	2.344780	-1.497179	1.132625
9823	H	3.181889	-2.706229	0.593836
9824	O	-5.994455	-1.424935	0.352292
9825	H	-6.083171	-0.749243	1.049470
9826	H	-5.124444	-1.840478	0.480718
9827	O	2.250113	-0.965646	-1.849044
9828	H	1.359820	-0.955426	-2.239079
9829	H	2.201090	-1.542667	-1.054527
9830	O	-3.283268	-0.407546	-1.858763
9831	H	-4.194397	-0.371058	-2.202048
9832	H	-3.311495	-0.999016	-1.073274
9833	O	-6.056919	-0.168819	-1.949221
9834	H	-6.770919	-0.418556	-2.543367
9835	H	-6.135537	-0.716946	-1.118257
9836	O	2.648017	1.404527	-0.509568
9837	H	2.552033	0.623220	-1.097154
9838	H	3.597093	1.640680	-0.525107
9839	O	7.545880	3.137784	-0.286492
9840	H	7.698486	3.660284	0.507548
9841	H	8.411179	2.876540	-0.617486
9842	O	-3.215391	-1.758810	0.527182
9843	H	-2.373192	-2.237619	0.611465
9844	H	-3.146977	-0.965380	1.105034
9845	O	-0.506233	-0.571561	-1.881393
9846	H	-0.393457	0.310345	-1.461631
9847	H	-1.406141	-0.588706	-2.249739
9848	O	-3.208086	0.631226	1.843975
9849	H	-4.110851	0.771804	2.182104
9850	H	-3.117777	1.213432	1.055875
9851	O	2.319089	0.104779	1.874146
9852	H	1.439840	0.270948	2.253975
9853	H	2.394212	0.677609	1.076891
9854	O	-0.456659	0.254139	1.902776
9855	H	-0.506641	-0.635782	1.488395
9856	H	-1.342220	0.446322	2.256059
9857	O	-2.861221	1.944567	-0.538468
9858	H	-2.937166	1.152722	-1.117580
9859	H	-1.941474	2.252323	-0.609911
9860	O	5.048160	-2.632324	0.408659
9861	H	5.117273	-2.123293	-0.449466
9862	H	5.683311	-3.353882	0.379930
9863	O	5.383436	1.299388	-0.326568
9864	H	6.111791	1.941776	-0.343710
9865	H	5.394999	0.836617	0.546559
9866	O	-5.976705	0.924634	1.904474
9867	H	-5.937105	1.474786	1.072187
9868	H	-6.646798	1.302745	2.481698
9869	O	-0.097698	1.715974	-0.406189
9870	H	-0.168720	1.299746	0.480992
9871	H	0.833617	1.979863	-0.511473
9872	O	5.055723	-1.093221	-1.712928
9873	H	4.160538	-1.059766	-2.089925
9874	H	5.260064	-0.191654	-1.394448

9875

9876 Cartesian coordinates of : W21_11

9877

9878	O	5.171815	1.485283	-1.321881
9879	H	5.408105	1.551156	-0.378673
9880	H	4.239208	1.761192	-1.389480
9881	O	0.260363	-3.234012	1.166236
9882	H	-0.558229	-2.731925	1.402234
9883	H	0.177986	-4.117772	1.537517
9884	O	-4.748384	-1.825867	-1.069983
9885	H	-3.799049	-1.690265	-1.252122
9886	H	-4.825069	-1.904084	-0.102147
9887	O	-1.874466	-1.639634	1.417792
9888	H	-1.989378	-1.457546	0.449692
9889	H	-2.772515	-1.836471	1.745995
9890	O	5.328093	-1.493725	0.817878
9891	H	4.416416	-1.766612	1.030072
9892	H	5.413828	-1.559116	-0.150817
9893	O	-1.749522	1.119413	1.786768
9894	H	-0.926164	1.624818	1.994918
9895	H	-1.572782	0.162638	1.862381
9896	O	2.773696	1.044442	1.556380

9897	H	2.628161	0.073688	1.552380
9898	H	3.726060	1.179639	1.722252
9899	O	5.550348	1.029602	1.431337
9900	H	6.249731	1.251520	2.053140
9901	H	5.571418	0.041252	1.270880
9902	O	-2.083154	1.646347	-0.823969
9903	H	-2.010009	1.461434	0.147550
9904	H	-3.005543	1.931609	-0.973828
9905	O	-6.084224	0.203131	-2.035566
9906	H	-5.627943	-0.619642	-1.697504
9907	H	-6.212176	0.094406	-2.982114
9908	O	2.544791	-1.633254	1.008826
9909	H	1.819013	-2.233794	1.259185
9910	H	2.468554	-1.492955	0.037971
9911	O	0.469000	2.613221	1.886955
9912	H	0.448476	3.013506	1.002276
9913	H	1.315489	2.137207	1.955785
9914	O	2.530893	-1.033310	-1.654863
9915	H	3.441494	-1.181147	-1.972828
9916	H	2.400091	-0.060696	-1.625171
9917	O	-2.060413	-1.121819	-1.208523
9918	H	-1.244725	-1.575554	-1.535505
9919	H	-1.963105	-0.156192	-1.313214
9920	O	0.165030	-2.533491	-1.640037
9921	H	0.284241	-2.963380	-0.777076
9922	H	0.999615	-2.072488	-1.836478
9923	O	2.391981	1.639875	-1.077323
9924	H	2.461067	1.501186	-0.105435
9925	H	1.625933	2.225081	-1.220966
9926	O	-4.632629	-1.620593	1.749951
9927	H	-4.675917	-0.620732	1.792996
9928	H	-5.274151	-1.969422	2.376329
9929	O	-4.829482	2.131044	-0.825105
9930	H	-5.313162	2.961849	-0.865495
9931	H	-5.340248	1.459312	-1.363705
9932	O	5.293808	-1.040859	-1.961650
9933	H	5.342506	-0.052841	-1.809079
9934	H	5.902675	-1.269519	-2.670143
9935	O	0.089237	3.214530	-0.921859
9936	H	-0.754755	2.707440	-1.020695
9937	H	-0.044839	4.081983	-1.315851
9938	O	-4.520535	0.985919	1.756691
9939	H	-3.596091	1.218415	1.960899
9940	H	-4.724209	1.402899	0.899425

9941

9942 Cartesian coordinates of : W21_12

9943

9944	O	-0.432147	4.063950	-0.540648
9945	H	-1.132791	3.851039	-1.211662
9946	H	-0.171653	4.980703	-0.673480
9947	O	-1.792428	0.514336	0.225595
9948	H	-1.481991	0.543080	-0.704129
9949	H	-1.445487	1.303800	0.690007
9950	O	0.788879	-1.388515	2.016950
9951	H	0.981419	-0.425313	1.977648
9952	H	-0.062880	-1.470623	2.481451
9953	O	-2.185618	3.173847	-2.303836
9954	H	-2.464174	3.573558	-3.132425
9955	H	-1.921894	2.241642	-2.496234
9956	O	-2.013610	-3.354742	-1.017415
9957	H	-2.046852	-4.284444	-1.265432
9958	H	-2.610612	-3.235315	-0.220490
9959	O	1.187419	-0.184095	-2.235322
9960	H	2.097875	-0.363604	-2.539783
9961	H	0.942131	-0.930931	-1.634253
9962	O	-3.599130	-2.792344	0.973691
9963	H	-3.074207	-2.429042	1.712513
9964	H	-4.111480	-2.026179	0.658368
9965	O	4.279275	0.754987	1.930532
9966	H	4.370960	0.985746	0.962074
9967	H	5.055830	1.091689	2.387282
9968	O	3.290147	-2.711322	-0.780214
9969	H	3.494979	-2.507169	0.162875
9970	H	2.323180	-2.817582	-0.807948
9971	O	3.542569	-1.996645	1.827851

9972	H	3.883688	-1.093971	1.952794
9973	H	2.621001	-1.977634	2.135342
9974	O	4.239027	1.376376	-0.612337
9975	H	3.393430	1.831620	-0.765921
9976	H	4.254761	0.629187	-1.243143
9977	O	1.498321	2.018956	-0.727379
9978	H	0.862281	2.749670	-0.826568
9979	H	1.261289	1.273771	-1.329466
9980	O	-1.385200	0.642372	-2.495907
9981	H	-2.040305	-0.093154	-2.639145
9982	H	-0.496899	0.334306	-2.753434
9983	O	-3.206350	-1.260577	-2.479778
9984	H	-2.811822	-2.073615	-2.111980
9985	H	-3.850310	-0.955148	-1.818743
9986	O	-4.365410	-0.280496	-0.064790
9987	H	-5.073526	0.298906	0.233269
9988	H	-3.514511	0.172531	0.135632
9989	O	3.897110	-0.780837	-2.345070
9990	H	3.738654	-1.582971	-1.744935
9991	H	4.508937	-1.045088	-3.038639
9992	O	-2.947971	1.375184	3.162561
9993	H	-3.251455	1.781410	3.979456
9994	H	-2.264199	1.963628	2.790646
9995	O	-0.846936	2.580415	1.801763
9996	H	-0.717699	3.299519	1.156435
9997	H	0.039932	2.250878	2.051297
9998	O	0.517388	-2.205467	-0.583838
9999	H	-0.341902	-2.644544	-0.737045
10000	H	0.549675	-1.930573	0.361118
10001	O	1.546256	1.238069	1.842921
10002	H	2.472475	1.212900	2.148930
10003	H	1.589237	1.462583	0.882406
10004	O	-1.937049	-1.135203	2.440858
10005	H	-2.350268	-0.429890	2.971723
10006	H	-1.801155	-0.701363	1.574090
10007				
10008	Cartesian coordinates of : W21_13			
10009				
10010	O	-1.909043	1.824847	2.894869
10011	H	-1.472480	0.943300	2.943556
10012	H	-1.921864	2.188981	3.785887
10013	O	1.921549	1.542798	0.792360
10014	H	1.755034	0.641574	1.144408
10015	H	1.203378	2.148595	1.097351
10016	O	0.275278	-0.595969	-2.127611
10017	H	-0.307262	-0.351650	-1.376588
10018	H	0.832551	0.192368	-2.274359
10019	O	-0.765714	-0.595873	2.614651
10020	H	-1.297490	-1.418034	2.555285
10021	H	0.181320	-0.840832	2.540764
10022	O	4.164955	-1.955556	-0.810642
10023	H	4.455731	-1.796547	0.103121
10024	H	4.216929	-1.098103	-1.264204
10025	O	-1.366885	-0.041554	-0.029596
10026	H	-2.182622	-0.586603	-0.007457
10027	H	-1.009609	-0.102717	0.879557
10028	O	4.260373	0.726417	-1.988824
10029	H	4.814991	0.871373	-2.761744
10030	H	3.404791	1.175334	-2.156190
10031	O	-3.989328	-0.356733	-2.244868
10032	H	-4.168450	-0.721808	-1.350528
10033	H	-4.796366	-0.453248	-2.760658
10034	O	-1.116062	-3.445388	-0.234882
10035	H	-1.477332	-3.107098	-1.083991
10036	H	-0.150483	-3.323267	-0.282354
10037	O	-1.879000	-2.278101	-2.610728
10038	H	-2.619767	-1.651591	-2.643044
10039	H	-1.087108	-1.757191	-2.823542
10040	O	-3.914832	-1.034771	0.349597
10041	H	-3.681918	-1.729696	0.992153
10042	H	-4.122052	-0.197542	0.829299
10043	O	-4.152832	1.501353	1.211814
10044	H	-3.472626	1.693694	1.881396
10045	H	-3.851564	1.940036	0.399361
10046	O	1.740014	-1.039251	1.709667

10047	H	2.666014	-1.168616	1.991235
10048	H	1.615668	-1.597176	0.899060
10049	O	4.525826	-1.061816	1.877655
10050	H	4.686509	-0.131531	1.551742
10051	H	5.182956	-1.264911	2.549873
10052	O	4.666611	1.309957	0.779568
10053	H	3.756361	1.643977	0.898575
10054	H	4.763942	1.208184	-0.182405
10055	O	-2.344782	-2.726956	1.884139
10056	H	-1.844443	-3.052817	1.061754
10057	H	-2.559261	-3.503980	2.410327
10058	O	-0.502198	3.567074	-1.636824
10059	H	-1.354243	3.080981	-1.719454
10060	H	-0.643129	4.453432	-1.984605
10061	O	-0.109697	3.219669	1.200952
10062	H	-0.380370	3.446827	0.295827
10063	H	-0.870982	2.854487	1.682161
10064	O	1.489323	-2.451257	-0.567444
10065	H	2.451463	-2.525639	-0.747634
10066	H	1.149852	-1.815664	-1.237804
10067	O	-2.653624	1.992884	-1.244216
10068	H	-3.156970	1.422604	-1.851718
10069	H	-2.096249	1.354268	-0.743498
10070	O	1.723168	1.746138	-1.861563
10071	H	1.114053	2.484249	-2.032489
10072	H	1.768293	1.668702	-0.873018

10073

10074 Cartesian coordinates of : W21_14

10075

10076	O	0.410523	3.407782	1.920902
10077	H	0.562328	2.597068	2.491217
10078	H	0.376242	4.171758	2.505031
10079	O	3.601016	1.153635	-0.014099
10080	H	3.085796	0.669028	0.662330
10081	H	3.219966	2.065626	-0.051611
10082	O	-0.813172	-1.406061	-1.783985
10083	H	-0.899674	-0.430119	-1.823538
10084	H	0.042261	-1.655224	-2.183651
10085	O	0.625991	1.169363	3.239128
10086	H	-0.212747	0.676477	3.188031
10087	H	1.292519	0.572163	2.850377
10088	O	1.873538	-2.734079	0.213725
10089	H	2.767728	-2.959178	0.521027
10090	H	1.919554	-2.607909	-0.754801
10091	O	-1.619953	-0.212748	2.308558
10092	H	-2.564059	-0.373357	2.502696
10093	H	-1.300460	-1.005815	1.820804
10094	O	1.794623	-2.024634	-2.475886
10095	H	2.089363	-2.525637	-3.242376
10096	H	2.194565	-1.099211	-2.532471
10097	O	-4.143151	0.839538	-2.116010
10098	H	-4.347832	1.075396	-1.162559
10099	H	-4.829107	1.228545	-2.667008
10100	O	-3.674742	-2.716698	0.684248
10101	H	-3.753863	-2.497339	-0.273971
10102	H	-2.729407	-2.894027	0.826099
10103	O	-3.580114	-1.946242	-1.922564
10104	H	-3.891788	-1.037866	-2.078254
10105	H	-2.623943	-1.923519	-2.096040
10106	O	-4.408712	1.458779	0.395700
10107	H	-4.518485	0.711353	1.016422
10108	H	-3.564309	1.881007	0.633305
10109	O	-1.678586	1.992664	0.749144
10110	H	-1.068103	2.666402	1.104530
10111	H	-1.572444	1.188349	1.312606
10112	O	2.328444	-0.511792	1.800076
10113	H	3.088717	-1.030514	2.115065
10114	H	1.883992	-1.141329	1.196795
10115	O	4.396735	-2.387475	1.474566
10116	H	4.958268	-1.793826	0.919587
10117	H	4.990758	-2.908056	2.023833
10118	O	5.707841	-0.551191	0.008310
10119	H	5.113420	0.228678	-0.020565
10120	H	6.005937	-0.702362	-0.893800
10121	O	-4.340335	-0.718855	2.145203

10122	H	-4.162383	-1.542305	1.583343
10123	H	-5.020731	-0.939706	2.788359
10124	O	0.820205	2.458584	-2.681285
10125	H	0.725152	3.053694	-3.431504
10126	H	-0.073229	2.088532	-2.479862
10127	O	2.158324	3.386608	-0.297990
10128	H	1.546516	3.490983	0.453574
10129	H	1.621871	3.211511	-1.089061
10130	O	-0.864588	-2.337044	0.763741
10131	H	-0.000693	-2.770871	0.855340
10132	H	-0.857935	-1.982553	-0.157241
10133	O	-1.422631	1.280258	-1.814843
10134	H	-2.343287	1.236682	-2.142839
10135	H	-1.492079	1.568121	-0.868615
10136	O	2.724808	0.369049	-2.485407
10137	H	2.087124	1.071958	-2.706722
10138	H	3.085965	0.611873	-1.603742

10139

10140 Cartesian coordinates of : W21_15

10141

10142	O	5.027305	1.487179	-1.345933
10143	H	5.297091	1.521442	-0.409710
10144	H	4.188496	1.977602	-1.410149
10145	O	0.619388	-1.446935	1.459984
10146	H	0.746238	-0.487926	1.661067
10147	H	-0.284977	-1.681523	1.737235
10148	O	-4.925961	-1.906502	-1.018327
10149	H	-3.974315	-1.843261	-1.214262
10150	H	-5.005333	-1.907491	-0.046895
10151	O	-2.144195	-1.550257	1.533116
10152	H	-2.206909	-1.540211	0.550222
10153	H	-3.031657	-1.792994	1.853397
10154	O	5.210147	-1.472060	0.843216
10155	H	5.310471	-1.504850	-0.125942
10156	H	4.396081	-1.963095	1.053510
10157	O	-1.970335	1.174050	1.815904
10158	H	-1.055644	1.437712	2.027415
10159	H	-1.980247	0.191688	1.839817
10160	O	3.098947	2.592354	1.646654
10161	H	3.053177	2.934278	0.739199
10162	H	3.921871	2.074541	1.702039
10163	O	5.459951	1.076497	1.396621
10164	H	6.251294	1.229025	1.921858
10165	H	5.352668	0.088896	1.296383
10166	O	-2.340091	1.528280	-0.862820
10167	H	-2.248986	1.509908	0.117874
10168	H	-3.221100	1.900661	-1.053784
10169	O	-6.216601	0.120702	-2.080927
10170	H	-5.769602	-0.690499	-1.711031
10171	H	-6.344261	-0.023783	-3.022639
10172	O	2.822740	-2.964166	1.080603
10173	H	2.830144	-3.788221	1.577661
10174	H	2.011552	-2.471263	1.342486
10175	O	0.771348	1.241326	1.585839
10176	H	0.661420	1.387137	0.623315
10177	H	1.609887	1.708251	1.813738
10178	O	2.806032	-2.591557	-1.780224
10179	H	2.914826	-2.933671	-0.878119
10180	H	3.601533	-2.061497	-1.967484
10181	O	-2.220412	-1.202669	-1.173353
10182	H	-1.326342	-1.416989	-1.501677
10183	H	-2.294867	-0.223631	-1.200893
10184	O	0.524896	-1.245466	-1.330743
10185	H	0.573017	-1.393604	-0.363532
10186	H	1.312923	-1.717221	-1.692953
10187	O	2.629569	2.967985	-1.173582
10188	H	2.547406	3.787295	-1.671525
10189	H	1.789431	2.467730	-1.293661
10190	O	-4.908718	-1.518823	1.782431
10191	H	-4.933533	-0.521567	1.791500
10192	H	-5.598158	-1.833761	2.374950
10193	O	-5.053997	2.147237	-0.921317
10194	H	-5.544110	2.967899	-1.030290
10195	H	-5.533622	1.438817	-1.437414
10196	O	5.160091	-1.060998	-1.931918

10197	H	5.080944	-0.072252	-1.815455
10198	H	5.849911	-1.222833	-2.582750
10199	O	0.402150	1.441794	-1.181628
10200	H	0.499482	0.483196	-1.399083
10201	H	-0.538925	1.666914	-1.306574
10202	O	-4.764240	1.110409	1.698677
10203	H	-3.866851	1.387158	1.948990
10204	H	-4.944567	1.504943	0.824989
10205				
10206	Cartesian coordinates of : W21_16			
10207				
10208	O	-1.278698	3.763942	0.623942
10209	H	-0.698504	3.561409	1.382325
10210	H	-0.660523	3.796454	-0.132137
10211	O	1.997710	0.119141	-2.085510
10212	H	2.127239	0.757333	-1.355034
10213	H	1.303117	0.486335	-2.667273
10214	O	-1.290453	-1.909142	-0.422677
10215	H	-1.420876	-1.488277	0.454565
10216	H	-1.522258	-1.202383	-1.064163
10217	O	0.673073	2.725389	2.350337
10218	H	0.480584	1.897027	2.818628
10219	H	1.413295	2.537493	1.755222
10220	O	4.585716	-1.385162	1.697580
10221	H	5.010349	-0.611310	1.286179
10222	H	4.590663	-2.092669	1.031197
10223	O	-1.936534	-0.561011	1.894865
10224	H	-2.779730	-0.934397	2.214971
10225	H	-1.318345	-0.413126	2.635773
10226	O	3.894574	-3.116866	-0.474700
10227	H	4.075785	-4.041887	-0.667960
10228	H	2.921038	-2.984461	-0.521579
10229	O	-4.805187	-0.759287	-2.029963
10230	H	-5.054523	-0.231941	-1.211049
10231	H	-5.530926	-0.696968	-2.658319
10232	O	0.233397	0.071930	3.466820
10233	H	0.451549	-0.087053	4.390471
10234	H	0.948100	-0.331672	2.914059
10235	O	-3.948579	-2.846213	-0.343031
10236	H	-2.981624	-2.772083	-0.447559
10237	H	-4.327840	-2.309557	-1.063249
10238	O	-5.165066	0.525945	0.193399
10239	H	-5.096228	-0.103928	0.932439
10240	H	-4.389953	1.117886	0.275771
10241	O	-2.624341	1.575102	0.253620
10242	H	-2.167147	2.461926	0.392494
10243	H	-2.284979	0.963537	0.935820
10244	O	2.497513	1.565844	0.259704
10245	H	3.473919	1.603614	0.249628
10246	H	2.285562	0.771370	0.805076
10247	O	5.199573	0.856331	0.080690
10248	H	6.007353	1.368066	-0.026752
10249	H	5.080029	0.293603	-0.734520
10250	O	4.622959	-0.770036	-1.895387
10251	H	3.758760	-0.494970	-2.251506
10252	H	4.497636	-1.670861	-1.549150
10253	O	-4.473356	-1.623366	1.912951
10254	H	-5.019596	-2.120195	2.529465
10255	H	-4.329929	-2.188841	1.099765
10256	O	-0.174374	1.348096	-3.246955
10257	H	-0.353227	1.645485	-4.144148
10258	H	-0.999034	0.926841	-2.891720
10259	O	0.694183	3.293954	-1.291034
10260	H	1.338198	2.794772	-0.766613
10261	H	0.390182	2.705971	-2.001442
10262	O	2.028568	-0.713803	1.677950
10263	H	2.971454	-0.988959	1.837059
10264	H	1.716336	-1.292390	0.946636
10265	O	-2.195455	0.218860	-1.953505
10266	H	-3.076215	-0.084126	-2.247189
10267	H	-2.360028	0.815490	-1.166256
10268	O	1.408206	-2.099571	-0.606453
10269	H	0.434806	-2.244218	-0.582446
10270	H	1.548113	-1.358978	-1.238640
10271				

10272 Cartesian coordinates of : W21_17

10273
10274 O -4.123477 1.549112 -1.265625
10275 H -3.301964 1.966341 -1.606578
10276 H -4.862492 2.099760 -1.543225
10277 O 0.804247 3.618140 -1.641893
10278 H 1.561644 3.014996 -1.722227
10279 H 0.868017 4.003161 -0.751301
10280 O -1.857224 3.410968 0.861233
10281 H -2.399330 2.863692 1.446603
10282 H -1.812745 2.934973 0.005463
10283 O 0.594854 4.307352 1.154035
10284 H -0.366352 4.059459 1.168845
10285 H 0.684058 5.178482 1.551543
10286 O -4.050189 -1.607355 1.808350
10287 H -4.611193 -2.045073 2.455984
10288 H -3.175657 -2.054671 1.820421
10289 O 0.553612 -3.615260 -1.453465
10290 H 1.114525 -2.872110 -1.724430
10291 H -0.359080 -3.402958 -1.717781
10292 O 1.470808 1.723566 1.353280
10293 H 1.347578 2.671133 1.547508
10294 H 2.244911 1.354349 1.848840
10295 O -2.098184 -2.721084 -1.308197
10296 H -3.021754 -2.426761 -1.444515
10297 H -1.976665 -2.716522 -0.337900
10298 O -4.457772 -1.336607 -1.046706
10299 H -4.359317 -0.397199 -1.270870
10300 H -4.532444 -1.388938 -0.080486
10301 O -0.725961 0.173889 1.172182
10302 H -1.560097 0.664276 1.319238
10303 H 0.044159 0.767064 1.341518
10304 O 1.796442 -0.983064 -1.555795
10305 H 2.247929 -0.109196 -1.537641
10306 H 0.847336 -0.737935 -1.669104
10307 O 4.548214 -1.762019 -0.934893
10308 H 3.904285 -1.738995 -1.656131
10309 H 4.024062 -2.058004 -0.166815
10310 O -0.794569 -0.324782 -1.455146
10311 H -0.775328 -0.183930 -0.475759
10312 H -1.337173 -1.130228 -1.591231
10313 O 3.594230 0.374524 2.160612
10314 H 3.260910 -0.512223 1.928625
10315 H 4.316093 0.553244 1.534417
10316 O -3.321105 1.074825 1.377755
10317 H -3.728264 1.233697 0.504492
10318 H -3.706226 0.249897 1.722021
10319 O 2.502360 -1.912433 0.955629
10320 H 1.989160 -2.684429 1.251298
10321 H 2.037087 -1.547991 0.172740
10322 O 5.249346 0.702346 -0.165911
10323 H 6.176044 0.940245 -0.265297
10324 H 5.130950 -0.215790 -0.515471
10325 O -1.488190 -2.411522 1.420532
10326 H -0.807617 -3.093759 1.573568
10327 H -1.042286 -1.538084 1.468949
10328 O 2.728122 1.545676 -1.087072
10329 H 3.681061 1.521312 -0.888831
10330 H 2.275774 1.606959 -0.216072
10331 O 0.700203 -4.081583 1.140137
10332 H 0.907781 -4.987160 1.390547
10333 H 0.657173 -4.038440 0.146816
10334 O -1.568625 2.277276 -1.667317
10335 H -1.268025 1.348283 -1.752549
10336 H -0.773655 2.833354 -1.839032

10337

10338

10339 Cartesian coordinates of the water 22-mer

10340

10341 Cartesian coordinates of : W22_1

10342

10343 O 0.029530 0.027772 1.961550
10344 H -0.629195 -0.505928 1.462991
10345 H 0.719861 -0.618508 2.215403
10346 O 0.029506 -0.027742 -1.961549

10347	H	-0.629238	0.505956	-1.463016
10348	H	0.719848	0.618537	-2.215377
10349	O	-1.760655	1.652463	-0.819315
10350	H	-2.690250	1.562795	-1.114180
10351	H	-1.771307	1.745598	0.156591
10352	O	-1.760590	-1.652431	0.819272
10353	H	-1.771254	-1.745575	-0.156633
10354	H	-2.690183	-1.562774	1.114150
10355	O	1.587087	1.954552	0.871033
10356	H	0.990504	1.236744	1.187292
10357	H	1.179712	2.799827	1.135012
10358	O	1.587055	-1.954519	-0.871009
10359	H	0.990470	-1.236713	-1.187269
10360	H	1.179687	-2.799796	-1.134995
10361	O	1.920611	-1.973895	1.847285
10362	H	1.858381	-1.926317	0.867763
10363	H	2.858097	-1.802730	2.050758
10364	O	1.920613	1.973894	-1.847261
10365	H	2.858095	1.802723	-2.050746
10366	H	1.858396	1.926330	-0.867737
10367	O	-1.727614	-2.158960	-1.896191
10368	H	-1.122477	-1.503071	-2.287138
10369	H	-1.242611	-3.004985	-1.842801
10370	O	-1.727627	2.158962	1.896155
10371	H	-1.122485	1.503076	2.287100
10372	H	-1.242625	3.004989	1.842766
10373	O	-4.419087	-1.272951	1.367332
10374	H	-4.947244	-1.690439	2.054460
10375	H	-4.466850	-0.280064	1.492948
10376	O	-4.419170	1.272913	-1.367292
10377	H	-4.466900	0.280025	-1.492907
10378	H	-4.947391	1.690382	-2.054382
10379	O	-0.017202	4.221967	1.143110
10380	H	0.130556	5.125206	1.438842
10381	H	-0.062745	4.219993	0.141285
10382	O	-0.017191	-4.221960	-1.143122
10383	H	0.130592	-5.125192	-1.438861
10384	H	-0.062737	-4.219995	-0.141296
10385	O	4.596418	-1.143844	1.712291
10386	H	5.353381	-1.301450	2.284391
10387	H	4.522797	-0.155918	1.568901
10388	O	4.596414	1.143829	-1.712306
10389	H	5.353371	1.301429	-2.284416
10390	H	4.522786	0.155903	-1.568915
10391	O	4.302113	-1.378830	-1.093569
10392	H	3.365508	-1.648601	-1.155222
10393	H	4.546684	-1.489365	-0.157191
10394	O	4.302143	1.378821	1.093558
10395	H	4.546703	1.489353	0.157176
10396	H	3.365545	1.648613	1.155225
10397	O	-4.403821	1.327775	1.443719
10398	H	-3.563854	1.726075	1.733373
10399	H	-4.530697	1.559425	0.506614
10400	O	-4.403813	-1.327815	-1.443683
10401	H	-4.530663	-1.559475	-0.506578
10402	H	-3.563844	-1.726093	-1.733360
10403	O	-0.151577	3.841417	-1.432892
10404	H	-0.803675	3.114276	-1.419568
10405	H	0.659172	3.450018	-1.803121
10406	O	-0.151575	-3.841418	1.432883
10407	H	0.659177	-3.450037	1.803122
10408	H	-0.803651	-3.114258	1.419540

10409

10410 Cartesian coordinates of : W22_ 2

10411

10412	O	0.306688	-0.914751	-1.459367
10413	O	-1.872955	3.208241	-1.322180
10414	O	-1.604876	3.058518	1.574002
10415	O	0.133413	-1.141519	1.303164
10416	O	0.768814	1.528142	1.523722
10417	O	-2.432240	-1.283009	-1.344804
10418	O	-3.626777	1.150304	-1.408294
10419	O	-3.535863	1.167982	1.379866
10420	O	-2.626551	-1.375626	1.387134
10421	H	-2.420893	-1.393203	-0.366594

10422	H	-1.503210	-1.327859	-1.636466
10423	H	-0.770592	-1.390867	1.570550
10424	H	0.143635	-1.161741	0.322190
10425	H	-2.899222	1.862716	1.664630
10426	H	-3.578911	1.259020	0.405957
10427	H	-2.585230	2.546972	-1.474882
10428	H	-2.081623	3.985624	-1.849477
10429	H	0.387822	0.063685	-1.512380
10430	H	1.163342	-1.283203	-1.738432
10431	H	-2.939987	-0.451304	1.534410
10432	H	-3.382951	-1.957675	1.582773
10433	H	-3.169128	0.285493	-1.529207
10434	H	-4.574821	0.997349	-1.586695
10435	H	-0.730784	2.665627	1.740468
10436	H	-1.607618	3.337492	0.644323
10437	H	1.704418	1.600596	1.782352
10438	H	0.520568	0.581756	1.609835
10439	H	0.614440	1.800759	-0.205226
10440	O	0.552466	1.801344	-1.187866
10441	H	-0.220470	2.349836	-1.414395
10442	H	-4.121214	-2.123314	-1.595738
10443	O	-5.040862	-2.296788	-1.328805
10444	H	-5.543478	-1.487498	-1.531826
10445	H	-7.093674	0.552059	-1.641142
10446	O	-6.240542	0.255469	-1.309573
10447	H	-6.282910	0.234915	-0.307767
10448	H	-5.538234	-3.406141	1.594670
10449	O	-5.133413	-2.590582	1.284441
10450	H	-5.134756	-2.601633	0.286790
10451	H	-5.312422	0.585142	1.585947
10452	O	-6.079728	0.062548	1.288201
10453	H	-5.871500	-0.866903	1.493883
10454	H	4.455202	1.224424	1.669567
10455	O	3.520242	1.176949	1.399384
10456	H	3.501703	1.340493	0.429476
10457	H	3.140344	0.332711	-1.471579
10458	O	3.282926	1.295096	-1.324002
10459	H	2.440613	1.732096	-1.539971
10460	H	1.957791	-1.639188	1.577827
10461	O	2.881516	-1.481588	1.314124
10462	H	3.056634	-0.525569	1.465713
10463	H	2.996125	-1.578301	-0.440113
10464	O	3.032543	-1.427306	-1.411959
10465	H	3.895847	-1.766331	-1.710753
10466	H	6.244674	0.953384	-0.350490
10467	O	6.043581	0.808740	-1.293197
10468	H	5.194329	1.248584	-1.468321
10469	H	6.096886	-0.325032	1.482362
10470	O	6.248544	0.660979	1.513503
10471	H	6.992595	0.832049	2.098454
10472	H	5.752445	-2.065597	0.232719
10473	O	5.647784	-1.878370	1.183196
10474	H	4.710543	-2.028891	1.394159
10475	H	5.956813	-0.803391	-1.600927
10476	O	5.778348	-1.784908	-1.631280
10477	H	6.412396	-2.188066	-2.231943
10478				
10479	Cartesian coordinates of : W22_ 3			
10480				
10481	O	-0.849364	-0.362485	-0.120260
10482	H	-0.148002	-0.573009	-0.796811
10483	H	-1.316040	-1.192250	0.114828
10484	O	1.692239	2.531117	0.722668
10485	H	1.228200	1.885214	1.302755
10486	H	2.647064	2.444403	0.906775
10487	O	3.160156	-1.780369	-0.829378
10488	H	3.340362	-1.524822	0.112347
10489	H	2.856699	-2.704373	-0.829267
10490	O	1.003665	-0.687905	-1.943604
10491	H	1.813736	-1.069384	-1.516760
10492	H	1.204885	0.256455	-2.118400
10493	O	-2.326680	1.681047	-1.099765
10494	H	-2.594763	2.293742	-0.387553
10495	H	-1.770119	0.978442	-0.683476
10496	O	0.211120	0.691248	2.090962

10497	H	-0.099614	0.212745	1.283526
10498	H	0.658133	0.022377	2.646116
10499	O	1.653704	1.948426	-1.965568
10500	H	0.968845	2.498947	-2.383826
10501	H	1.619779	2.153275	-1.003622
10502	O	-2.219734	-2.572740	0.797237
10503	H	-2.626705	-2.952141	-0.002707
10504	H	-2.909203	-2.045085	1.248282
10505	O	-3.946759	-0.605444	1.662862
10506	H	-4.683418	-0.682290	2.277495
10507	H	-3.367114	0.148472	1.998443
10508	O	1.473098	-1.498062	3.212708
10509	H	1.534987	-1.817359	4.117981
10510	H	1.042247	-2.221809	2.666405
10511	O	-2.555157	3.597878	0.923432
10512	H	-3.156882	4.333349	1.072805
10513	H	-1.659733	3.980765	0.684679
10514	O	0.334503	-3.290631	1.722762
10515	H	-0.597173	-3.132641	1.485834
10516	H	0.783237	-3.578966	0.905036
10517	O	-2.446519	1.317406	2.522850
10518	H	-1.487837	1.121369	2.548473
10519	H	-2.531852	2.184182	2.084519
10520	O	-3.120082	-2.779336	-1.801175
10521	H	-3.526500	-1.877311	-1.656586
10522	H	-3.734982	-3.289954	-2.336782
10523	O	1.420474	-4.019577	-0.762371
10524	H	1.587709	-4.948824	-0.949175
10525	H	0.705506	-3.721526	-1.390147
10526	O	4.340453	1.715481	0.815907
10527	H	4.382831	1.381292	-0.122805
10528	H	5.175003	2.153527	1.008531
10529	O	-4.164059	-0.468541	-1.142778
10530	H	-3.659489	0.337285	-1.354180
10531	H	-4.239165	-0.468532	-0.169492
10532	O	-0.717694	3.328424	-2.495161
10533	H	-1.362201	2.685887	-2.104975
10534	H	-1.111913	3.697859	-3.291063
10535	O	-0.372958	-3.021825	-2.417472
10536	H	-0.011037	-2.130675	-2.567428
10537	H	-1.328950	-2.927920	-2.253417
10538	O	-0.238639	4.430447	0.076385
10539	H	0.532474	3.931913	0.408676
10540	H	-0.278901	4.268951	-0.881983
10541	O	3.698807	-0.913289	1.626889
10542	H	3.925883	0.030959	1.585689
10543	H	2.995637	-1.041067	2.288486
10544	O	4.190052	0.749168	-1.632648
10545	H	3.424160	1.181215	-2.047421
10546	H	4.009211	-0.206205	-1.615644

10547

10548 Cartesian coordinates of : W22_ 4

10549

10550	O	-0.973750	2.359436	-3.000781
10551	H	-1.185794	2.719937	-3.867454
10552	H	-1.845539	2.107741	-2.568045
10553	O	-3.203902	1.636850	-1.879766
10554	H	-3.265580	0.666710	-1.790272
10555	H	-3.477563	1.997509	-1.016217
10556	O	-0.791889	0.187570	0.015244
10557	H	-1.033634	1.107844	0.306764
10558	H	-0.202161	0.288066	-0.769017
10559	O	0.690480	0.332871	-2.217535
10560	H	0.223593	1.044447	-2.700128
10561	H	1.563597	0.653956	-1.892701
10562	O	3.521273	-1.831780	-1.894729
10563	H	3.501009	-0.859239	-1.851738
10564	H	2.648843	-2.119717	-2.212221
10565	O	0.354215	3.762432	-0.955170
10566	H	-0.053782	3.391974	-1.757947
10567	H	-0.233280	3.502231	-0.217570
10568	O	2.900696	2.496609	2.211856
10569	H	2.953122	2.935135	1.344436
10570	H	3.265691	1.607013	2.089851
10571	O	0.280586	-0.857742	2.161952

10572	H	-0.121340	-0.457888	1.338610
10573	H	-0.476832	-1.262037	2.628551
10574	O	2.887994	3.480906	-0.462406
10575	H	1.917602	3.624059	-0.675314
10576	H	3.356861	4.289499	-0.690012
10577	O	-1.514680	-3.812759	0.771220
10578	H	-0.542852	-3.833893	0.730648
10579	H	-1.813471	-3.764953	-0.153445
10580	O	0.649634	-2.395062	-2.010995
10581	H	0.813477	-2.510722	-1.048917
10582	H	0.558269	-1.434749	-2.179920
10583	O	-2.972427	-1.026319	-1.091120
10584	H	-2.783508	-1.861979	-1.551377
10585	H	-2.129895	-0.729022	-0.682486
10586	O	2.981623	-0.267991	1.521818
10587	H	2.122759	-0.484455	1.924084
10588	H	3.456353	-1.110303	1.392221
10589	O	-4.073152	-0.352375	1.351437
10590	H	-3.932876	-0.758852	0.475743
10591	H	-3.446475	-0.812218	1.937862
10592	O	-2.177109	-2.061165	2.641158
10593	H	-2.019123	-2.736088	1.926156
10594	H	-2.528082	-2.540644	3.398864
10595	O	-1.230140	2.613055	0.990984
10596	H	-2.183568	2.722689	1.158244
10597	H	-0.737656	2.477317	1.845789
10598	O	1.149131	-2.995023	0.632747
10599	H	0.933122	-2.272861	1.258975
10600	H	2.105488	-3.165784	0.715335
10601	O	-1.820980	-3.416759	-2.025404
10602	H	-2.037487	-4.078289	-2.689425
10603	H	-0.890917	-3.114447	-2.182004
10604	O	3.044822	0.810319	-1.031453
10605	H	3.218346	1.770360	-0.960165
10606	H	2.953312	0.481374	-0.111384
10607	O	3.903698	-2.716070	0.545025
10608	H	4.696058	-3.245511	0.675471
10609	H	3.866774	-2.436022	-0.412502
10610	O	-3.933210	2.213660	0.816274
10611	H	-4.749190	2.662884	1.056814
10612	H	-4.015926	1.265266	1.117801
10613	O	0.321987	1.965669	3.015474
10614	H	1.235738	2.266020	2.814899
10615	H	0.357298	0.996993	2.996498
10616				
10617	Cartesian coordinates of : W22_ 5			
10618				
10619	O	-1.045102	0.153705	0.269789
10620	H	-0.406073	0.003319	0.999592
10621	H	-1.058879	1.109475	0.052778
10622	O	-1.497757	2.656351	-0.768609
10623	H	-0.817510	3.014753	-1.369940
10624	H	-1.527397	3.259364	0.000891
10625	O	-0.282214	-0.683742	-2.149929
10626	H	-0.667419	-0.476341	-1.265525
10627	H	-1.025282	-0.783255	-2.774873
10628	O	2.659351	1.333656	0.393184
10629	H	2.301941	1.156764	-0.507366
10630	H	3.557732	0.956091	0.393173
10631	O	0.907303	0.348630	2.227956
10632	H	1.624402	0.672521	1.639492
10633	H	1.242189	-0.441690	2.690318
10634	O	1.743637	1.065826	-2.175193
10635	H	1.507076	1.989873	-2.378051
10636	H	0.927111	0.526561	-2.281992
10637	O	1.506290	-2.578545	-1.329166
10638	H	0.906877	-3.289599	-1.041036
10639	H	0.882916	-1.909123	-1.682929
10640	O	-3.595874	-0.675689	0.391433
10641	H	-2.646131	-0.418881	0.459714
10642	H	-3.880518	-0.720927	1.316052
10643	O	-0.829245	-3.810122	-0.321266
10644	H	-1.052610	-4.737739	-0.192021
10645	H	-1.606909	-3.406787	-0.803660
10646	O	-0.878678	-2.260233	2.050980

10647	H	-0.887929	-2.813634	1.247609
10648	H	0.002674	-2.352054	2.455632
10649	O	3.118133	-2.280392	0.908304
10650	H	3.824549	-1.635584	0.731110
10651	H	2.544047	-2.307374	0.114153
10652	O	1.717100	-2.153085	3.056987
10653	H	2.331822	-2.264639	2.268882
10654	H	2.112355	-2.579040	3.822514
10655	O	-2.739587	-0.770948	-3.394946
10656	H	-3.117538	-0.005611	-2.871163
10657	H	-3.094949	-0.732929	-4.287616
10658	O	0.790802	3.670097	-2.032616
10659	H	0.910010	4.461415	-2.566130
10660	H	1.125668	3.860246	-1.105690
10661	O	-2.739834	-0.627971	3.042434
10662	H	-2.061550	-1.269929	2.709945
10663	H	-2.997293	-0.932351	3.918288
10664	O	4.871583	-0.307057	-0.078393
10665	H	4.560558	-0.561351	-0.991153
10666	H	5.831679	-0.253909	-0.088538
10667	O	-2.968094	-2.726710	-1.374447
10668	H	-2.944526	-2.221587	-2.205849
10669	H	-3.354294	-2.122695	-0.710198
10670	O	-3.612245	1.075410	-1.776318
10671	H	-2.954763	1.734625	-1.485585
10672	H	-3.881276	0.590425	-0.974656
10673	O	-1.231699	1.775787	3.167755
10674	H	-0.378047	1.326253	3.006779
10675	H	-1.901231	1.070660	3.090250
10676	O	3.672054	-0.966868	-2.311514
10677	H	3.074056	-0.220810	-2.501927
10678	H	3.102634	-1.742729	-2.177189
10679	O	-1.078822	3.861274	1.657961
10680	H	-1.399875	4.649218	2.106874
10681	H	-1.223319	3.079794	2.276362
10682	O	1.489459	3.875356	0.457260
10683	H	0.694079	3.869238	1.021654
10684	H	2.008477	3.072125	0.647862

10685

10686 Cartesian coordinates of : W22_ 6

10687

10688	O	0.489738	0.092996	-1.373406
10689	H	0.074395	0.978555	-1.484624
10690	H	1.455182	0.143457	-1.552545
10691	O	-0.927655	2.230727	1.481613
10692	H	-1.835748	2.037673	1.813048
10693	H	-0.438619	1.388226	1.590366
10694	O	-0.868591	-2.540135	1.322159
10695	H	-0.172722	-3.195200	1.525947
10696	H	-0.946300	-2.512208	0.338833
10697	O	-0.888060	-2.232844	-1.381910
10698	H	-0.413156	-1.381844	-1.509865
10699	H	-1.772632	-2.106845	-1.781537
10700	O	-0.849218	2.428476	-1.228916
10701	H	-0.947239	2.437558	-0.245724
10702	H	-0.263869	3.175775	-1.455864
10703	O	3.170435	0.089619	1.375929
10704	H	2.202037	0.033932	1.536452
10705	H	3.439566	0.994433	1.624528
10706	O	0.475051	-0.120895	1.317441
10707	H	0.458436	-0.092081	0.330000
10708	H	0.017929	-0.953314	1.548536
10709	O	3.193200	-0.002308	-1.358772
10710	H	3.460904	-0.887395	-1.668849
10711	H	3.274533	-0.021234	-0.377537
10712	O	1.413792	-4.105293	1.452491
10713	H	1.613543	-4.878311	1.989697
10714	H	2.234004	-3.531164	1.443872
10715	O	3.543960	2.839265	1.552991
10716	H	2.642083	3.274558	1.589798
10717	H	4.133797	3.354846	2.111673
10718	O	3.613513	-2.743936	-1.641415
10719	H	4.198109	-3.243787	-2.219421
10720	H	2.724200	-3.200343	-1.645534
10721	O	-3.379736	-1.440974	-2.234578

10722	H	-3.883264	-1.834325	-2.954396
10723	H	-3.956594	-1.470523	-1.414957
10724	O	1.235868	4.243342	-1.421443
10725	H	2.065364	3.689828	-1.467516
10726	H	1.380135	5.029159	-1.957203
10727	O	-5.015327	1.441158	-0.102628
10728	H	-4.382998	1.526623	-0.875582
10729	H	-5.757489	2.033072	-0.256460
10730	O	1.207273	3.995390	1.400643
10731	H	0.398623	3.494664	1.621893
10732	H	1.111204	4.275130	0.473202
10733	O	3.583044	-2.667948	1.179582
10734	H	3.609766	-1.729772	1.440165
10735	H	3.804845	-2.698240	0.230968
10736	O	-3.233279	-1.618098	2.268307
10737	H	-3.568542	-2.072442	3.047601
10738	H	-2.373142	-2.036342	2.035172
10739	O	-4.815150	-1.325994	-0.060585
10740	H	-5.094579	-0.393032	0.005324
10741	H	-4.328649	-1.527865	0.758880
10742	O	-3.312075	1.410601	-2.071250
10743	H	-2.444952	1.824883	-1.900048
10744	H	-3.166331	0.472042	-2.283384
10745	O	1.301671	-3.952803	-1.375908
10746	H	1.252262	-4.208377	-0.437702
10747	H	0.480880	-3.461244	-1.566215
10748	O	3.418516	2.796051	-1.266332
10749	H	3.668928	2.803534	-0.323902
10750	H	3.460640	1.867239	-1.552882
10751	O	-3.370256	1.288901	2.180524
10752	H	-3.297969	0.327763	2.299366
10753	H	-4.010273	1.430547	1.460134

10754

10755 Cartesian coordinates of : W22_ 7

10756

10757	O	0.132107	0.364173	-1.383195
10758	H	0.864388	1.002652	-1.555122
10759	H	0.209699	0.170023	-0.407113
10760	O	0.491017	-0.158729	1.175316
10761	H	0.981972	-1.012727	1.234673
10762	H	-0.377469	-0.279118	1.644453
10763	O	1.637010	-2.573017	1.084967
10764	H	1.500498	-2.637284	0.112633
10765	H	2.599908	-2.519720	1.240984
10766	O	-3.404945	-1.439506	0.353284
10767	H	-3.375616	-2.408340	0.464234
10768	H	-2.983383	-1.249767	-0.513216
10769	O	2.063875	2.263406	-1.257376
10770	H	2.922589	1.950432	-1.598375
10771	H	2.128499	2.229539	-0.274908
10772	O	1.983850	2.051730	1.465893
10773	H	1.400151	1.261403	1.520846
10774	H	1.474889	2.794320	1.840413
10775	O	1.113779	-2.318520	-1.590069
10776	H	0.804280	-1.397802	-1.673553
10777	H	0.324079	-2.869812	-1.801209
10778	O	-2.186051	2.261549	1.588506
10779	H	-1.595155	2.926228	1.983108
10780	H	-1.992578	2.311101	0.627944
10781	O	-1.857622	-0.408550	2.331050
10782	H	-2.444321	-0.788362	1.637444
10783	H	-2.043776	0.551130	2.333692
10784	O	-1.712897	2.424437	-1.136475
10785	H	-2.537737	2.265551	-1.632660
10786	H	-1.112666	1.674939	-1.324857
10787	O	-2.344134	-0.797578	-2.097889
10788	H	-1.468823	-0.375054	-2.037608
10789	H	-2.980443	-0.112051	-2.373580
10790	O	-4.084851	1.397267	-2.092882
10791	H	-4.399179	1.318166	-1.149815
10792	H	-4.815658	1.717974	-2.629871
10793	O	4.424380	0.874237	-1.726511
10794	H	4.186336	-0.091311	-1.808818
10795	H	5.170318	1.037566	-2.311776
10796	O	4.318451	-1.925958	1.111473

10797	H	5.071017	-2.298216	1.581086
10798	H	4.360210	-0.932712	1.211622
10799	O	-2.478042	-4.024846	0.615289
10800	H	-1.827200	-3.758931	1.320635
10801	H	-2.841606	-4.881132	0.860887
10802	O	0.059253	4.043629	1.904706
10803	H	0.132907	4.268007	0.935834
10804	H	0.117534	4.870357	2.393979
10805	O	3.855999	-1.692131	-1.664585
10806	H	2.969572	-2.050308	-1.848139
10807	H	4.095186	-1.976492	-0.764500
10808	O	4.417633	0.694034	1.093901
10809	H	4.548588	0.931266	0.158241
10810	H	3.689691	1.248647	1.426587
10811	O	0.231374	4.356839	-0.713166
10812	H	0.992710	3.888300	-1.095844
10813	H	-0.549976	3.876462	-1.041915
10814	O	-0.781922	-3.101110	2.413880
10815	H	0.132281	-3.023468	2.083617
10816	H	-1.047294	-2.230703	2.748495
10817	O	-4.589711	1.089421	0.470858
10818	H	-4.017286	1.612022	1.056203
10819	H	-4.397771	0.150360	0.640777
10820	O	-1.323769	-3.463759	-1.933007
10821	H	-1.876605	-2.725393	-2.232163
10822	H	-1.711028	-3.773887	-1.095089

10823

10824 Cartesian coordinates of : W22_ 8

10825

10826	O	1.937972	-0.664420	3.395927
10827	H	2.111994	-0.774091	4.335416
10828	H	1.945315	-1.578376	2.963062
10829	O	1.825126	-2.889047	2.109871
10830	H	0.917645	-2.936923	1.751629
10831	H	2.381482	-2.868926	1.306032
10832	O	1.337515	-0.138001	-0.699191
10833	H	1.940280	0.250726	-1.370723
10834	H	1.596236	0.273718	0.149113
10835	O	-0.243978	0.156561	1.898735
10836	H	0.429132	-0.006253	2.587541
10837	H	-0.127873	1.069706	1.553436
10838	O	-2.955101	2.889668	1.520977
10839	H	-1.981011	2.933804	1.538959
10840	H	-3.194457	2.028817	1.904384
10841	O	2.883097	0.927352	1.377808
10842	H	2.743102	0.438233	2.212876
10843	H	3.610012	0.480878	0.869916
10844	O	1.966136	3.362897	-1.804172
10845	H	2.151116	3.564086	-0.869342
10846	H	0.999661	3.336160	-1.911650
10847	O	-0.992308	-0.006645	-1.989126
10848	H	-1.807042	0.040152	-1.442239
10849	H	-0.221820	-0.043186	-1.377443
10850	O	2.399938	3.481630	0.985889
10851	H	2.709961	2.565768	1.216143
10852	H	2.939157	4.115707	1.467821
10853	O	-3.841905	-2.374817	-1.272132
10854	H	-3.829290	-1.396849	-1.174661
10855	H	-4.639536	-2.605399	-1.758735
10856	O	-2.988622	0.095423	1.966407
10857	H	-2.021842	0.052248	2.120912
10858	H	-3.304057	-0.832636	2.042445
10859	O	-0.603211	-2.364378	0.821520
10860	H	-0.646624	-2.531998	-0.140057
10861	H	-0.442284	-1.408711	0.947645
10862	O	-0.813891	2.733302	-1.778123
10863	H	-0.862769	1.805013	-2.091455
10864	H	-1.737697	3.043191	-1.733405
10865	O	1.296687	-4.183261	-2.107905
10866	H	0.392760	-3.818072	-2.135129
10867	H	1.213227	-5.140785	-2.094519
10868	O	-1.107862	-2.766423	-1.921614
10869	H	-2.068699	-2.894156	-1.823620
10870	H	-1.014605	-1.842188	-2.231463
10871	O	4.554618	-0.282911	-0.314265

10872	H	4.221841	-1.190076	-0.439034
10873	H	4.344579	0.190217	-1.136537
10874	O	-3.364100	0.233843	-0.676300
10875	H	-3.235822	0.245645	0.308707
10876	H	-3.644338	1.129199	-0.942129
10877	O	-3.324054	-2.584984	1.579742
10878	H	-3.715331	-2.718528	0.702708
10879	H	-2.366352	-2.698666	1.433007
10880	O	-0.238794	2.673096	0.896782
10881	H	0.596030	3.151446	1.056229
10882	H	-0.387661	2.669964	-0.076412
10883	O	-3.513696	3.013440	-1.032785
10884	H	-4.209618	3.632320	-1.274355
10885	H	-3.379078	3.073203	-0.043867
10886	O	2.789841	-2.489652	-0.461364
10887	H	2.467460	-3.205789	-1.041406
10888	H	2.143111	-1.764878	-0.575766
10889	O	3.125832	1.082152	-2.394295
10890	H	2.755513	1.998484	-2.261058
10891	H	3.194260	0.929208	-3.342054

10892

10893 Cartesian coordinates of : W22_ 9

10894

10895	O	0.274207	1.507415	-1.897425
10896	H	1.051043	1.026754	-2.231942
10897	H	-0.213687	0.896486	-1.301951
10898	O	-2.829245	-2.451971	-2.152606
10899	H	-2.100162	-2.522410	-1.486773
10900	H	-2.562664	-2.947204	-2.933541
10901	O	-1.429599	0.249397	-0.216351
10902	H	-2.267917	0.322599	-0.726274
10903	H	-1.543927	0.813723	0.591612
10904	O	-3.620051	0.254441	-1.825200
10905	H	-4.415774	0.191133	-1.258113
10906	H	-3.457641	-0.634435	-2.189528
10907	O	-1.895393	3.966371	0.151352
10908	H	-2.363968	4.806624	0.168315
10909	H	-2.092814	3.540589	-0.725087
10910	O	0.872768	3.263476	0.128765
10911	H	0.655058	2.699613	-0.644869
10912	H	0.098916	3.840668	0.235228
10913	O	0.705480	1.879425	2.576936
10914	H	0.948227	2.335634	1.748682
10915	H	1.263261	1.085809	2.624525
10916	O	4.291674	-2.814382	-0.114639
10917	H	3.321787	-2.719396	-0.160648
10918	H	4.646462	-2.379903	-0.910695
10919	O	-3.054319	-2.777820	1.839512
10920	H	-3.209184	-3.419745	2.539639
10921	H	-3.758024	-2.906048	1.143788
10922	O	1.669461	-1.875437	-0.079545
10923	H	1.805931	-1.309912	0.712183
10924	H	0.755858	-2.219220	-0.061231
10925	O	5.195360	-0.961554	-2.045964
10926	H	5.509711	-0.355038	-1.315724
10927	H	5.882946	-1.003418	-2.717197
10928	O	-3.890748	-0.088455	2.157652
10929	H	-3.454650	-0.957830	2.212540
10930	H	-3.203637	0.603403	2.213989
10931	O	3.264231	1.804561	0.019477
10932	H	2.955661	1.299939	-0.764786
10933	H	2.727911	2.611467	0.083715
10934	O	-4.775502	-2.838522	-0.142925
10935	H	-4.267525	-2.860014	-0.972161
10936	H	-5.234203	-1.978362	-0.120889
10937	O	2.567020	-0.140972	1.839822
10938	H	2.884468	0.578775	1.252573
10939	H	3.372539	-0.573540	2.177207
10940	O	-2.224437	2.740295	-2.192293
10941	H	-1.340862	2.402069	-2.420274
10942	H	-2.822574	1.975582	-2.240662
10943	O	2.577661	-0.038062	-1.900746
10944	H	3.439841	-0.349842	-2.233194
10945	H	2.215312	-0.765405	-1.347896
10946	O	5.063589	-1.389000	1.944205

10947	H	5.605919	-1.847475	2.592749
10948	H	4.825511	-2.035242	1.219719
10949	O	-1.857522	1.790079	1.914471
10950	H	-0.960910	1.803147	2.338542
10951	H	-1.982251	2.660680	1.490922
10952	O	5.756000	0.546141	0.022044
10953	H	5.065242	1.228244	0.091728
10954	H	5.672620	-0.012942	0.816267
10955	O	-5.495725	-0.154395	0.134557
10956	H	-6.351718	0.243841	0.319139
10957	H	-4.916524	-0.047533	0.951030
10958	O	-1.090223	-2.351536	-0.088361
10959	H	-1.578779	-2.711576	0.675816
10960	H	-1.202333	-1.366249	-0.018379

10961

10962 Cartesian coordinates of : W22_10

10963

10964	O	5.101860	0.201319	0.896275
10965	H	4.430231	-0.202619	1.472744
10966	H	5.302424	-0.443635	0.193646
10967	H	4.835748	-0.542233	-2.039653
10968	O	5.126536	-1.308554	-1.460668
10969	H	5.775448	-1.829204	-1.942998
10970	H	3.194024	0.616726	-2.797479
10971	O	4.155415	0.758702	-2.701089
10972	H	4.252185	1.492112	-2.067320
10973	H	4.655475	1.599139	0.174879
10974	O	4.329559	2.366052	-0.375636
10975	H	4.896420	3.121403	-0.191309
10976	H	1.745915	-0.513999	-1.630830
10977	O	1.431010	0.224570	-2.192389
10978	H	1.385612	0.994611	-1.584980
10979	H	2.629808	-1.313246	0.355795
10980	O	2.550310	-1.719092	-0.533686
10981	H	3.459192	-1.804773	-0.881538
10982	H	2.311545	-1.538479	2.525638
10983	O	2.727567	-0.780077	2.072083
10984	H	2.153070	-0.011188	2.247943
10985	H	2.506980	2.446851	-0.281059
10986	O	1.551728	2.244053	-0.310901
10987	H	1.323829	1.795239	0.531963
10988	H	0.179858	1.794487	2.460151
10989	O	0.695379	1.093565	2.020340
10990	H	0.078760	0.335848	1.895669
10991	H	0.961886	-3.305605	1.869302
10992	O	1.057127	-2.902422	2.785798
10993	H	1.133166	-3.619781	3.422168
10994	H	-0.102364	-3.354651	-0.030165
10995	O	0.759146	-3.646776	0.319561
10996	H	1.432246	-3.123327	-0.157752
10997	O	-1.277332	-0.337722	-2.214201
10998	H	-1.603676	0.462123	-1.743050
10999	H	-0.336782	-0.167375	-2.430145
11000	H	-2.518432	-2.424187	-0.364262
11001	O	-1.567446	-2.215187	-0.356054
11002	H	-1.419104	-1.560553	-1.090677
11003	O	-2.426496	1.670709	-0.758542
11004	H	-3.341775	1.686419	-1.143216
11005	H	-2.531985	1.302124	0.138389
11006	O	-0.796679	3.712976	0.108457
11007	H	-1.422373	3.154634	-0.395536
11008	H	0.092712	3.424535	-0.168629
11009	H	-1.380264	3.758798	3.142228
11010	O	-1.249917	3.016303	2.544584
11011	H	-1.078465	3.386709	1.617716
11012	O	-0.902469	-1.091873	1.974008
11013	H	-1.125334	-1.523883	1.109789
11014	H	-0.385183	-1.736275	2.491626
11015	H	-2.443902	1.655072	2.315159
11016	O	-2.831362	0.837791	1.939524
11017	H	-2.230210	0.101902	2.172107
11018	H	-2.979969	-0.804630	-3.036993
11019	O	-3.939901	-0.944381	-2.975312
11020	H	-4.067740	-1.600831	-2.273843
11021	H	-4.734426	-1.565252	0.077792

11022	O	-4.383013	-2.307172	-0.458142
11023	H	-4.967968	-3.060389	-0.329873
11024	H	-4.708422	0.554117	-2.277133
11025	O	-4.905339	1.298372	-1.670012
11026	H	-5.301233	0.899006	-0.881542
11027	H	-4.392440	0.341736	1.390596
11028	O	-5.173561	-0.034977	0.922291
11029	H	-5.921464	0.033095	1.524359
11030				
11031	Cartesian coordinates of : W22_11			
11032				
11033	O	-1.511215	-1.991593	-2.994352
11034	H	-1.629474	-2.228637	-3.919120
11035	H	-0.913687	-2.692160	-2.570821
11036	O	0.063590	-3.650702	-1.860050
11037	H	0.994213	-3.328850	-1.842693
11038	H	-0.150448	-3.917871	-0.950424
11039	O	-0.264420	-0.311897	0.773025
11040	H	-1.036366	-0.900898	0.964060
11041	H	-0.297084	-0.163543	-0.203953
11042	O	-0.464593	0.246380	-1.866935
11043	H	-0.799605	-0.501141	-2.407955
11044	H	-1.140633	0.965067	-1.867509
11045	O	0.291559	3.828714	-2.000673
11046	H	-0.598246	3.452064	-2.111917
11047	H	0.924320	3.111689	-2.185493
11048	O	-3.561517	-1.395024	-1.175638
11049	H	-2.949376	-1.635516	-1.895334
11050	H	-3.161957	-1.734968	-0.351339
11051	O	-3.677957	1.387834	1.812332
11052	H	-4.009393	1.311635	0.898957
11053	H	-2.850037	1.892944	1.760892
11054	O	1.446929	0.802619	2.783006
11055	H	0.749485	0.271413	2.371170
11056	H	2.166760	0.190612	3.018163
11057	O	-4.411110	1.040483	-0.911218
11058	H	-4.115987	0.091793	-1.057996
11059	H	-5.334188	1.101650	-1.175420
11060	O	4.512342	0.466102	0.671540
11061	H	3.998171	1.293649	0.671148
11062	H	4.453998	0.111963	-0.235148
11063	O	1.935471	1.478793	-1.785953
11064	H	2.024799	1.708889	-0.831668
11065	H	1.119726	0.938388	-1.876720
11066	O	2.582072	-2.723727	-1.443148
11067	H	2.462353	-2.540012	-0.494914
11068	H	3.063964	-1.961339	-1.804252
11069	O	-1.127530	2.391646	1.071553
11070	H	-0.652052	1.542418	1.116471
11071	H	-0.480013	3.118695	1.134880
11072	O	1.679276	-2.246898	1.172045
11073	H	2.378033	-1.960988	1.794046
11074	H	1.091434	-1.477370	1.013734
11075	O	3.613841	-0.968737	2.646263
11076	H	4.051318	-0.459367	1.901457
11077	H	4.299496	-1.264418	3.252357
11078	O	-2.230534	-2.110684	1.164029
11079	H	-1.752550	-2.950145	1.280015
11080	H	-2.738642	-1.880782	1.978823
11081	O	2.389544	2.286437	0.773369
11082	H	2.018155	1.801081	1.551949
11083	H	2.050662	3.198155	0.818465
11084	O	3.924345	-0.256352	-2.001971
11085	H	4.552697	-0.094669	-2.712699
11086	H	3.210304	0.431674	-2.067088
11087	O	-2.068715	2.367451	-1.487560
11088	H	-3.006366	2.096504	-1.493519
11089	H	-1.827528	2.458235	-0.538516
11090	O	0.688403	4.452324	0.528390
11091	H	0.651075	5.388617	0.745051
11092	H	0.528602	4.349121	-0.450216
11093	O	-0.262949	-4.096105	0.974500
11094	H	-0.133147	-4.981885	1.327579
11095	H	0.531258	-3.562592	1.207452
11096	O	-3.520100	-0.926492	3.146224

11097	H	-3.617479	-0.040073	2.717658
11098	H	-4.340423	-1.113603	3.610147
11099				
11100	Cartesian coordinates of : W22_12			
11101				
11102	O	-2.529169	-0.862166	-2.913491
11103	H	-3.014142	-0.600446	-2.106528
11104	H	-2.566985	-1.829459	-2.900324
11105	O	-2.637054	-3.469209	-1.678898
11106	H	-2.664058	-4.395037	-1.940442
11107	H	-3.214529	-3.369030	-0.892244
11108	O	-0.386064	-2.275729	-0.470825
11109	H	-1.059103	-2.722447	-1.018268
11110	H	-0.321688	-1.352036	-0.813804
11111	O	-0.295136	0.107274	-1.738138
11112	H	-1.005223	-0.163164	-2.364819
11113	H	-0.593907	0.946874	-1.320367
11114	O	1.341869	3.407859	-2.102249
11115	H	0.416474	3.167665	-1.913713
11116	H	1.777864	2.601894	-2.426396
11117	O	-3.544869	-0.199384	-0.406629
11118	H	-2.794279	-0.021381	0.220397
11119	H	-3.990925	-0.984122	-0.046548
11120	O	-2.732586	2.897417	2.113606
11121	H	-3.237554	3.080708	1.306132
11122	H	-1.906378	3.404942	2.063735
11123	O	0.805121	0.667811	1.849197
11124	H	0.958740	-0.137858	2.396914
11125	H	1.579789	0.802998	1.263349
11126	O	-3.833484	2.509912	-0.506889
11127	H	-3.985938	1.540082	-0.508832
11128	H	-4.495891	2.909052	-1.079534
11129	O	4.517425	-0.814889	0.592005
11130	H	4.110079	0.068762	0.656141
11131	H	4.490007	-1.040562	-0.355390
11132	O	2.290947	0.729089	-2.242654
11133	H	2.878194	-0.037305	-2.386567
11134	H	1.376409	0.375603	-2.186346
11135	O	2.218982	-3.245145	-0.714031
11136	H	2.554900	-3.280533	0.200350
11137	H	1.284921	-2.965051	-0.649657
11138	O	0.017585	3.284702	1.583323
11139	H	0.351925	2.453144	1.973537
11140	H	0.805178	3.785019	1.297387
11141	O	3.279455	-2.760946	1.837683
11142	H	3.785018	-1.989479	1.450108
11143	H	3.907179	-3.283714	2.346337
11144	O	1.011986	-1.705758	3.129972
11145	H	1.756822	-2.200651	2.742023
11146	H	0.195653	-2.193539	2.944634
11147	O	-3.886629	-2.827857	0.684236
11148	H	-4.569827	-3.285558	1.184177
11149	H	-3.094352	-2.713633	1.282513
11150	O	2.906884	1.440244	0.292478
11151	H	2.688039	1.265062	-0.653627
11152	H	2.946817	2.406357	0.402712
11153	O	3.786455	-1.617367	-2.023932
11154	H	4.301988	-2.089317	-2.684966
11155	H	3.162469	-2.277571	-1.599610
11156	O	-1.024904	2.569358	-0.842799
11157	H	-1.994883	2.661053	-0.841848
11158	H	-0.707459	2.806906	0.058371
11159	O	2.287336	4.188196	0.224589
11160	H	2.773722	5.018010	0.223090
11161	H	1.969689	4.012954	-0.704253
11162	O	-1.636062	-2.267105	1.945268
11163	H	-1.099498	-2.282195	1.117678
11164	H	-1.788334	-1.313472	2.102759
11165	O	-1.824138	0.420611	1.496046
11166	H	-2.191405	1.260388	1.859616
11167	H	-0.847125	0.544732	1.439168
11168				
11169	Cartesian coordinates of : W22_13			
11170				
11171	O	-0.498006	-1.573813	-1.491711

11172	O	-0.665157	-1.731979	1.244390
11173	O	-3.250622	-1.200118	-1.561479
11174	O	-3.162751	1.509373	-1.208798
11175	O	-2.931883	1.148264	1.486413
11176	O	-3.425559	-1.528854	1.154397
11177	O	-0.148401	0.974543	1.424655
11178	O	-0.405143	1.179165	-1.342618
11179	O	-5.926625	1.739136	-1.344372
11180	O	-6.028995	-0.886693	-1.402484
11181	O	-6.167737	-1.161785	1.398006
11182	O	-5.721129	1.425996	1.447885
11183	H	-3.160129	-0.219986	-1.560497
11184	H	-2.399039	-1.556767	-1.866142
11185	H	-1.588190	-1.928276	1.481391
11186	H	-0.522520	-0.778457	1.431011
11187	H	-3.045652	0.171615	1.489377
11188	H	-2.009140	1.321773	1.742493
11189	H	-0.503197	0.212372	-1.487637
11190	H	-1.277155	1.567164	-1.529867
11191	H	-0.538772	-1.762017	-0.527645
11192	H	0.408071	-1.793010	-1.770218
11193	H	-3.416080	-1.534079	0.171035
11194	H	-3.113476	1.506870	-0.225957
11195	H	-0.061801	1.204998	0.475587
11196	H	0.697100	1.155224	1.866331
11197	H	-4.788377	1.594604	1.665269
11198	H	-5.860794	1.748365	0.538781
11199	H	-6.073765	-0.174722	1.515546
11200	H	-6.193951	-1.174554	-0.486111
11201	H	-5.158360	-1.240223	-1.652922
11202	H	-6.045738	0.755173	-1.463016
11203	H	-4.050143	1.837795	-1.440551
11204	H	-4.353404	-1.658605	1.422242
11205	H	-6.585547	2.189008	-1.881465
11206	H	-6.884184	-1.465526	1.963374
11207	H	2.324249	-0.365398	1.913478
11208	O	2.498880	0.518292	2.308741
11209	H	3.446506	0.497649	2.514379
11210	H	2.088775	-1.781355	0.197487
11211	O	2.094874	-1.942833	1.170833
11212	H	1.198698	-2.235862	1.407354
11213	H	2.550994	1.798479	-0.923106
11214	O	2.331938	1.264733	-1.731034
11215	H	1.400189	1.462906	-1.930138
11216	H	2.332321	-0.451029	-1.559023
11217	O	2.279005	-1.434166	-1.477002
11218	H	3.144385	-1.794367	-1.742675
11219	H	5.508175	-2.823654	-2.025101
11220	O	4.992023	-2.144923	-1.579877
11221	H	5.003009	-2.338281	-0.597661
11222	H	4.178761	0.859828	-1.842741
11223	O	5.010414	0.615847	-1.400941
11224	H	5.204149	-0.307711	-1.651107
11225	H	3.905327	-2.477113	1.272690
11226	O	4.843906	-2.407709	1.019156
11227	H	5.164007	-1.575304	1.407354
11228	H	4.910520	0.432538	0.509644
11229	O	5.183137	0.347024	1.445173
11230	H	5.835866	1.053176	1.550546
11231	H	6.444667	3.472804	-0.166468
11232	O	5.925188	2.704563	0.088711
11233	H	5.873999	2.105656	-0.679582
11234	H	2.898800	1.912721	1.167596
11235	O	3.060647	2.560253	0.456493
11236	H	4.006798	2.781049	0.470353
11237				
11238	Cartesian coordinates of : W22_14			
11239				
11240	O	-0.277112	1.317085	-1.515110
11241	H	-0.324606	0.344456	-1.656061
11242	H	0.631400	1.582349	-1.747039
11243	O	2.345166	1.973350	1.341497
11244	H	2.815679	1.249525	1.807005
11245	H	1.389730	1.879297	1.527215
11246	O	-6.033840	-1.407360	-1.315356

11247	H	-6.005332	-1.476085	-0.319572
11248	H	-6.750214	-1.964055	-1.634861
11249	O	-0.313438	1.300620	1.215400
11250	H	-0.358676	1.396250	0.235135
11251	H	-1.196600	1.536043	1.550503
11252	O	4.993190	2.632970	-1.373988
11253	H	4.764353	3.278804	-0.666566
11254	H	5.570654	3.071932	-2.005423
11255	O	4.398120	-3.987645	0.835077
11256	H	4.422654	-4.933353	0.666688
11257	H	4.727786	-3.525406	0.022635
11258	O	4.933241	-2.448680	-1.273270
11259	H	4.068207	-2.234595	-1.657169
11260	H	5.260148	-1.587508	-0.943785
11261	O	5.399006	0.045746	-0.175148
11262	H	4.956192	0.111717	0.686129
11263	H	5.373379	0.920945	-0.592585
11264	O	-3.264315	-1.270850	-1.520640
11265	H	-3.226479	-0.289834	-1.572611
11266	H	-4.190148	-1.518094	-1.697323
11267	O	-5.751741	-1.338350	1.295162
11268	H	-4.837373	-1.575145	1.527331
11269	H	-5.877679	-0.412026	1.570464
11270	O	-5.853916	1.473257	1.485083
11271	H	-5.922928	1.543221	0.491635
11272	H	-6.523669	2.043880	1.873798
11273	O	-0.487123	-1.407393	-1.533780
11274	H	-1.387533	-1.650360	-1.809100
11275	H	-0.441871	-1.553248	-0.562121
11276	O	2.483378	-2.134809	1.088758
11277	H	3.041033	-2.947121	1.121937
11278	H	2.462707	-1.870119	0.137523
11279	O	-2.963537	-1.475172	1.194566
11280	H	-2.064727	-1.758996	1.437444
11281	H	-3.016120	-1.524046	0.213377
11282	O	3.980794	4.050039	0.673258
11283	H	4.430830	4.459381	1.417681
11284	H	3.319828	3.426301	1.039818
11285	O	-3.035474	1.455911	-1.312555
11286	H	-2.159598	1.722058	-1.640385
11287	H	-2.990583	1.501751	-0.331169
11288	O	-5.825316	1.396607	-1.141736
11289	H	-6.006564	0.475373	-1.403214
11290	H	-4.930241	1.604336	-1.460186
11291	O	-0.195895	-1.483326	1.196123
11292	H	-0.125651	-0.519120	1.354277
11293	H	0.682862	-1.872005	1.373330
11294	O	2.476931	1.427658	-1.380366
11295	H	3.301349	1.833595	-1.701320
11296	H	2.466626	1.609099	-0.415631
11297	O	-3.082800	1.242106	1.421445
11298	H	-3.082041	0.258508	1.463237
11299	H	-3.976889	1.526000	1.684773
11300	O	2.315240	-1.330165	-1.508012
11301	H	2.441428	-0.357304	-1.537772
11302	H	1.416228	-1.507602	-1.832683
11303	O	3.800689	-0.151166	2.191388
11304	H	4.203224	-0.384575	3.033569
11305	H	3.319224	-0.957676	1.848696
11306				
11307	Cartesian coordinates of : W22_15			
11308				
11309	O	-3.928363	-2.198133	1.435068
11310	H	-2.987365	-2.250823	1.693000
11311	H	-3.975686	-2.520684	0.518113
11312	O	-3.948882	-2.478985	-1.404043
11313	H	-4.208615	-1.515465	-1.485010
11314	H	-4.563087	-2.988634	-1.941581
11315	O	-0.226193	0.069959	-1.228163
11316	H	-0.269221	0.180998	-0.242538
11317	H	-0.643936	-0.802010	-1.407416
11318	O	-1.121566	-2.200821	1.562479
11319	H	-0.812030	-1.295516	1.755720
11320	H	-1.137409	-2.258576	0.585361
11321	O	-0.478977	0.493658	1.415838

11322	H	0.215013	1.151208	1.634170
11323	H	-1.341513	0.963370	1.488894
11324	O	3.688117	1.186603	1.589745
11325	H	3.234460	0.322331	1.535978
11326	H	4.617845	0.929468	1.696734
11327	O	-4.984758	0.179629	1.414183
11328	H	-5.796315	0.228943	1.928570
11329	H	-4.605805	-0.742830	1.520999
11330	O	5.670685	-0.734549	0.943115
11331	H	6.571773	-1.053996	1.044792
11332	H	5.495894	-0.619645	-0.031638
11333	O	-1.073722	4.226004	-1.357704
11334	H	-1.096286	4.269031	-0.356720
11335	H	-1.193356	5.117576	-1.699210
11336	O	1.299179	2.574380	1.450131
11337	H	1.375791	2.597552	0.473174
11338	H	2.191041	2.394418	1.792689
11339	O	0.990036	-3.981192	-1.194526
11340	H	1.122728	-3.963392	-0.192835
11341	H	1.278509	-4.838826	-1.521270
11342	O	-1.235625	-2.431962	-1.218498
11343	H	-0.634657	-3.174413	-1.423767
11344	H	-2.161073	-2.637114	-1.461672
11345	O	-2.422248	1.807787	-1.499171
11346	H	-1.638209	1.227196	-1.563650
11347	H	-2.115838	2.713860	-1.693037
11348	O	3.927608	2.139912	-1.091273
11349	H	3.805885	1.944947	-0.145111
11350	H	3.063638	2.436834	-1.415064
11351	O	3.019027	-1.522028	1.179955
11352	H	3.990141	-1.589719	1.238695
11353	H	2.805057	-1.479192	0.223178
11354	O	1.124730	2.541852	-1.325996
11355	H	0.732299	1.687785	-1.571430
11356	H	0.459606	3.227138	-1.531778
11357	O	2.216659	-1.490574	-1.457938
11358	H	1.833543	-2.380848	-1.582271
11359	H	1.479630	-0.857792	-1.512022
11360	O	-4.622713	0.046210	-1.373536
11361	H	-4.911569	0.235844	-0.461734
11362	H	-3.965109	0.723666	-1.609168
11363	O	4.872091	-0.380247	-1.546988
11364	H	4.601711	0.562531	-1.581958
11365	H	4.061375	-0.878246	-1.737958
11366	O	-1.079902	4.063444	1.248650
11367	H	-1.770715	3.431173	1.514253
11368	H	-0.231500	3.714858	1.574427
11369	O	-2.806754	1.863789	1.230384
11370	H	-3.619912	1.395045	1.500717
11371	H	-2.803261	1.869414	0.249530
11372	O	1.266981	-3.674240	1.355143
11373	H	0.432351	-3.290729	1.683390
11374	H	1.950882	-2.990687	1.501601

11375

11376 Cartesian coordinates of : W22_16

11377

11378	O	-5.885943	0.117000	2.056607
11379	H	-5.936147	0.822170	1.351748
11380	H	-6.557352	0.308822	2.718266
11381	O	-3.001453	1.852183	-0.211607
11382	H	-3.030752	1.189757	-0.938758
11383	H	-2.100397	2.222929	-0.214962
11384	O	5.181769	-2.957063	-0.088398
11385	H	5.814698	-3.660169	-0.261918
11386	H	5.236904	-2.299500	-0.836249
11387	O	5.246843	-0.846796	1.848254
11388	H	4.393209	-0.841603	2.304981
11389	H	5.289969	-1.686644	1.360509
11390	O	4.609564	3.748747	-0.468167
11391	H	5.064658	2.894014	-0.303901
11392	H	4.907528	4.064149	-1.326568
11393	O	-0.440973	-0.096758	-2.000018
11394	H	-0.376112	0.726569	-1.472932
11395	H	-1.346286	-0.125028	-2.356026
11396	O	-5.787113	1.793041	0.036993

11397	H	-5.958719	1.280229	-0.774416
11398	H	-4.881568	2.137460	-0.047797
11399	O	-0.295196	-0.008863	1.774460
11400	H	-0.330358	-0.777935	1.163141
11401	H	-1.187822	0.055119	2.157867
11402	O	2.446367	-2.598745	0.050277
11403	H	2.484178	-1.955929	-0.690211
11404	H	3.315812	-3.040595	0.058635
11405	O	-0.244474	1.991570	-0.164426
11406	H	0.473839	2.646180	-0.155597
11407	H	-0.118547	1.395740	0.606133
11408	O	2.303961	-0.578209	-1.828446
11409	H	1.454573	-0.498089	-2.292128
11410	H	2.301551	0.117448	-1.135710
11411	O	-3.098750	0.098229	1.873753
11412	H	-3.115237	0.818791	1.202171
11413	H	-3.989985	0.080222	2.266609
11414	O	2.060878	3.621977	0.375092
11415	H	1.959778	4.250676	1.097145
11416	H	2.958343	3.775481	-0.010585
11417	O	-6.019917	-0.178896	-1.964056
11418	H	-6.740752	-0.354723	-2.576319
11419	H	-6.036624	-0.883578	-1.256630
11420	O	2.657863	0.939817	0.381502
11421	H	2.529417	0.329245	1.150801
11422	H	2.370294	1.837547	0.625702
11423	O	-0.275124	-2.058837	-0.062831
11424	H	0.548908	-2.574862	-0.032405
11425	H	-0.238579	-1.480113	-0.854794
11426	O	5.095940	-1.045284	-1.897229
11427	H	5.344417	-0.226359	-1.426957
11428	H	4.178083	-0.905264	-2.185892
11429	O	-3.030003	-1.978035	0.105881
11430	H	-2.995336	-1.312344	0.830197
11431	H	-2.146920	-2.384919	0.071733
11432	O	-3.229201	-0.215255	-1.976251
11433	H	-3.209072	-0.940564	-1.310599
11434	H	-4.144450	-0.183150	-2.308267
11435	O	2.336904	-0.936697	2.236191
11436	H	1.430419	-0.747289	2.529593
11437	H	2.283102	-1.659427	1.573240
11438	O	5.306273	1.132002	-0.111789
11439	H	4.340441	1.013477	0.043620
11440	H	5.677953	0.637246	0.642229
11441	O	-5.821462	-1.857317	0.044070
11442	H	-4.920294	-2.222381	0.069913
11443	H	-5.930785	-1.345290	0.866482

11444

11445 Cartesian coordinates of : W22_17

11446

11447	O	0.704752	-1.526201	-1.562365
11448	O	0.845802	-2.117791	1.091447
11449	O	0.737762	2.245552	0.633142
11450	O	0.987104	1.163430	-1.839506
11451	O	-2.073043	-1.487848	-1.717311
11452	O	-1.949449	-2.170239	0.900847
11453	O	-2.041846	2.226519	0.600810
11454	O	-1.797832	1.189859	-1.891999
11455	H	0.682196	-1.761508	-0.604579
11456	H	-1.080558	-2.572026	1.064252
11457	H	0.768764	1.873144	-0.281074
11458	H	-1.832586	0.203755	-1.837230
11459	H	-0.173324	-1.744020	-1.921659
11460	H	-1.944276	-1.337934	1.430858
11461	H	-0.158281	2.608749	0.749055
11462	H	-0.911578	1.418096	-2.217055
11463	H	1.895934	1.350843	-2.134967
11464	H	-2.973102	-1.649445	-2.057199
11465	H	1.742543	-2.467846	1.227853
11466	H	-2.950275	2.564020	0.708590
11467	H	0.924730	0.184763	-1.741834
11468	H	-2.093738	-1.745267	-0.764439
11469	H	0.838414	-1.269663	1.593658
11470	H	-2.005076	1.854969	-0.312547
11471	H	1.845293	0.267872	2.844678

11472	O	0.955472	0.244723	2.454747
11473	H	0.916414	0.979063	1.798360
11474	H	-0.983871	0.172916	2.778582
11475	O	-1.842841	0.143362	2.327332
11476	H	-1.859472	0.913448	1.710981
11477	O	-4.684505	0.047271	2.152202
11478	H	-4.808055	0.886301	1.673512
11479	H	-3.796428	0.083772	2.540735
11480	H	-5.507264	3.034788	0.576116
11481	O	-4.815401	2.368584	0.524190
11482	H	-4.834715	1.981980	-0.397299
11483	O	-4.611244	1.310524	-1.864266
11484	H	-4.792317	0.352298	-1.933623
11485	H	-3.691156	1.433208	-2.151569
11486	O	-4.839780	-1.479051	-1.926744
11487	H	-4.893225	-1.771841	-0.961764
11488	H	-5.519296	-1.951106	-2.417540
11489	H	-4.845345	-1.373816	1.150367
11490	O	-4.755932	-2.156034	0.556729
11491	H	-3.880298	-2.521015	0.762898
11492	H	3.562761	-1.719945	0.180532
11493	O	3.662674	-2.041411	1.106861
11494	H	4.348191	-2.723502	1.011634
11495	H	4.424813	0.123825	3.362842
11496	O	3.761010	0.138745	2.666383
11497	H	3.843029	-0.704412	2.153941
11498	O	3.514855	2.211589	0.782489
11499	H	3.685745	1.563901	1.492887
11500	H	2.587030	2.496207	0.873218
11501	O	3.761005	1.227441	-1.791737
11502	H	3.666473	1.478350	-0.846737
11503	H	4.465794	1.819066	-2.097978
11504	O	3.492624	-1.497678	-1.571718
11505	H	2.572301	-1.652815	-1.851402
11506	H	3.709894	-0.570094	-1.800181
11507	O	5.411251	3.294871	-0.981298
11508	H	5.810141	4.168829	-0.985360
11509	H	4.879379	3.215911	-0.172162
11510	O	5.295523	-3.404248	-0.627350
11511	H	5.809335	-4.069215	-1.092568
11512	H	4.811371	-2.880354	-1.287863

11513

11514 Cartesian coordinates of : W22_18

11515

11516	O	0.505751	-1.780910	-1.517080
11517	O	0.829687	-2.134715	1.201571
11518	O	0.793665	2.202966	0.291882
11519	O	0.885498	0.850719	-2.073622
11520	O	-2.266647	-1.648536	-1.552795
11521	O	-2.005793	-2.035181	1.112110
11522	O	-1.997275	2.285930	0.343535
11523	O	-1.898429	0.978399	-2.028106
11524	H	0.558999	-1.937782	-0.548647
11525	H	-1.142958	-2.441721	1.293277
11526	H	0.781733	1.736861	-0.577011
11527	H	-1.969447	0.005985	-1.866073
11528	H	-0.405510	-1.993492	-1.786464
11529	H	-1.980012	-1.154026	1.558317
11530	H	-0.086177	2.610029	0.387572
11531	H	-1.015632	1.133252	-2.401874
11532	H	1.766690	0.996579	-2.453204
11533	H	-3.183161	-1.820955	-1.839076
11534	H	1.662543	-2.566458	1.440270
11535	H	-2.888240	2.670282	0.440965
11536	H	0.806730	-0.114394	-1.883463
11537	H	-2.249634	-1.796419	-0.577006
11538	H	0.867145	-1.237481	1.611757
11539	H	-2.008949	1.815783	-0.524148
11540	H	1.761614	0.442639	2.719103
11541	O	0.894973	0.356470	2.285911
11542	H	0.884836	1.021348	1.557409
11543	H	-1.000499	0.434262	2.700962
11544	O	-1.881478	0.399839	2.293119
11545	H	-1.881060	1.093872	1.591896
11546	O	-4.714305	0.379153	2.219335

11547	H	-4.820882	1.166199	1.655629
11548	H	-3.814391	0.426991	2.578718
11549	H	-5.432834	3.213899	0.348084
11550	O	-4.770050	2.516764	0.350678
11551	H	-4.840012	2.029843	-0.519232
11552	O	-4.703791	1.194532	-1.911111
11553	H	-4.919589	0.241866	-1.871368
11554	H	-3.793896	1.253040	-2.246605
11555	O	-5.034244	-1.576688	-1.663178
11556	H	-5.044706	-1.760443	-0.670883
11557	H	-5.751916	-2.076336	-2.063950
11558	H	-4.900822	-1.139074	1.383732
11559	O	-4.836061	-1.980731	0.873701
11560	H	-3.960576	-2.338982	1.090600
11561	H	3.404859	-1.785352	0.290706
11562	O	3.726172	-1.916726	1.214528
11563	H	4.681698	-2.017509	1.051965
11564	H	4.286093	0.296963	3.306241
11565	O	3.628440	0.297948	2.603953
11566	H	3.684234	-0.577746	2.118773
11567	O	3.587517	2.046507	0.485163
11568	H	3.634172	1.474948	1.280865
11569	H	2.709282	2.467827	0.501332
11570	O	3.665388	0.905538	-2.017357
11571	H	3.605107	1.262942	-1.103207
11572	H	4.561425	1.131499	-2.300783
11573	O	3.287457	-1.749132	-1.463393
11574	H	2.425526	-2.068491	-1.775996
11575	H	3.372384	-0.826448	-1.778008
11576	O	6.060781	1.578894	-0.690837
11577	H	6.896527	2.047481	-0.603125
11578	H	5.398864	2.052978	-0.157251
11579	O	5.972985	-1.338329	-0.336436
11580	H	6.048582	-0.376446	-0.449515
11581	H	5.449918	-1.659512	-1.083846

11582

11583 Cartesian coordinates of : W22_19

11584

11585	O	-2.835517	-0.568537	-1.884395
11586	H	-2.854397	-1.521622	-2.115690
11587	H	-3.170235	-0.532629	-0.952195
11588	O	-2.547730	-3.295113	-1.812659
11589	H	-1.583009	-3.395953	-1.782776
11590	H	-2.857757	-3.421822	-0.900747
11591	O	-0.503007	-0.523017	1.217771
11592	H	-0.612347	-1.491719	1.317755
11593	H	-0.487396	-0.339520	0.252547
11594	O	-0.335768	-0.004187	-1.468371
11595	H	-1.283616	-0.168581	-1.755365
11596	H	-0.234426	0.972628	-1.337798
11597	O	2.558491	2.782420	-2.194764
11598	H	1.614219	2.854736	-1.958223
11599	H	2.677289	1.860415	-2.477006
11600	O	-4.186905	1.822943	-1.317113
11601	H	-3.850482	1.161878	-1.944339
11602	H	-4.499161	1.289750	-0.568902
11603	O	-1.521548	3.587586	1.940032
11604	H	-1.830105	3.813739	1.047874
11605	H	-0.552792	3.581489	1.921026
11606	O	1.759497	0.159552	2.360402
11607	H	0.901042	-0.113038	1.938808
11608	H	2.014774	-0.613049	2.888213
11609	O	-2.405037	3.716319	-0.782597
11610	H	-3.092790	3.017182	-0.953287
11611	H	-2.706498	4.516672	-1.224068
11612	O	3.662845	-2.385387	0.556107
11613	H	3.901495	-1.447052	0.456968
11614	H	3.464486	-2.703949	-0.341074
11615	O	2.397615	-0.113245	-2.104406
11616	H	2.715772	0.081955	-1.188489
11617	H	1.423040	-0.095179	-2.066662
11618	O	0.241981	-2.821695	-1.289028
11619	H	1.115021	-3.033689	-1.668535
11620	H	0.150067	-1.856369	-1.374015
11621	O	1.284125	2.821204	1.521031

11622	H	1.440916	2.039822	2.079237
11623	H	2.163098	3.121476	1.221066
11624	O	-0.426473	-3.256708	1.345916
11625	H	-0.094270	-3.307053	0.425644
11626	H	0.365198	-3.245926	1.920464
11627	O	2.009209	-2.703462	2.607064
11628	H	2.627838	-2.640830	1.830363
11629	H	2.432857	-3.284983	3.246956
11630	O	-3.904525	-0.351045	0.568538
11631	H	-3.893741	-1.260529	0.906895
11632	H	-3.461125	0.210744	1.258178
11633	O	3.470762	0.392617	0.321703
11634	H	2.845334	0.344782	1.087510
11635	H	3.846214	1.291343	0.331171
11636	O	2.893694	-2.727243	-2.162490
11637	H	3.378007	-3.119971	-2.895322
11638	H	2.823107	-1.751561	-2.321558
11639	O	0.084255	2.577510	-0.939977
11640	H	-0.767092	3.064369	-0.960803
11641	H	0.429851	2.618015	-0.020559
11642	O	3.708067	3.165755	0.136558
11643	H	4.389572	3.844329	0.160288
11644	H	3.353017	3.115386	-0.795172
11645	O	-3.170808	-3.159146	1.020122
11646	H	-3.707781	-3.815824	1.475624
11647	H	-2.256388	-3.266430	1.349446
11648	O	-2.519043	1.020732	2.363326
11649	H	-2.293678	1.970787	2.323093
11650	H	-1.696560	0.552938	2.141309
11651				
11652				
11653				
11654	Cartesian coordinates of the water 23-mer			
11655				
11656	Cartesian coordinates of : W23_ 1			
11657				
11658	O	1.089069	-0.324515	0.038376
11659	H	0.521488	-0.329964	-0.779293
11660	H	1.198457	-1.253425	0.324372
11661	O	-0.333199	0.488814	2.143197
11662	H	0.241268	0.306067	1.358422
11663	H	0.285310	0.653419	2.879174
11664	O	3.268363	1.170266	-0.350189
11665	H	3.200977	1.611659	-1.219849
11666	H	2.448700	0.621796	-0.268456
11667	O	-1.600387	-1.901525	1.769378
11668	H	-1.243029	-1.022525	2.019485
11669	H	-2.558456	-1.869568	1.952549
11670	O	-1.966689	2.360166	1.080114
11671	H	-1.419947	3.167390	1.063335
11672	H	-1.409678	1.701916	1.554930
11673	O	-0.531292	-0.363064	-2.064230
11674	H	-1.003649	-1.182328	-1.803655
11675	H	-1.155257	0.391023	-1.954739
11676	O	-2.150163	1.744558	-1.580512
11677	H	-2.125634	1.920886	-0.612548
11678	H	-3.066883	1.488502	-1.793978
11679	O	-1.470780	-2.630020	-0.890790
11680	H	-1.442420	-2.370747	0.056253
11681	H	-0.752810	-3.276309	-1.034079
11682	O	2.782019	-2.450445	-1.675938
11683	H	3.397613	-2.099117	-1.011284
11684	H	2.558408	-1.711391	-2.291977
11685	O	1.002775	-2.813284	1.387599
11686	H	0.097597	-2.762060	1.741527
11687	H	1.011888	-3.528536	0.722953
11688	O	0.918106	-4.101970	-1.013871
11689	H	1.089180	-4.973507	-1.383266
11690	H	1.652179	-3.488102	-1.331034
11691	O	0.193179	4.093127	0.749759
11692	H	0.322747	5.027973	0.938638
11693	H	0.976166	3.608365	1.147679
11694	O	3.055120	-1.348658	2.578112
11695	H	2.384064	-1.996236	2.294223
11696	H	3.677583	-1.268289	1.832746

11697	O	1.995099	0.804015	3.601031
11698	H	2.256248	0.890831	4.522788
11699	H	2.447691	-0.012804	3.237729
11700	O	2.473473	2.263009	-2.763348
11701	H	1.594442	2.651448	-2.492941
11702	H	2.876836	2.880156	-3.381354
11703	O	-4.330460	-1.390927	1.788187
11704	H	-4.396326	-0.406449	1.626228
11705	H	-5.023339	-1.628111	2.412016
11706	O	-4.673985	0.592214	-1.637203
11707	H	-4.489753	-0.378753	-1.491935
11708	H	-5.420913	0.661603	-2.239362
11709	O	2.281159	2.835394	1.676876
11710	H	2.755172	2.346203	0.976499
11711	H	2.209337	2.221470	2.430792
11712	O	0.194051	3.278289	-1.943532
11713	H	-0.660285	2.832961	-2.073913
11714	H	0.190858	3.618192	-1.028078
11715	O	-4.500223	1.141905	1.122208
11716	H	-3.725307	1.719737	1.242775
11717	H	-4.697888	1.133450	0.168229
11718	O	-4.187181	-1.902840	-0.983991
11719	H	-4.313806	-1.931727	-0.018266
11720	H	-3.322076	-2.313669	-1.157592
11721	O	1.946263	-0.479347	-3.312235
11722	H	0.994319	-0.434669	-3.111637
11723	H	2.256975	0.439750	-3.256608
11724	O	4.523088	-1.098834	0.184983
11725	H	5.473529	-1.210537	0.083872
11726	H	4.289193	-0.176607	-0.083247

11727

11728 Cartesian coordinates of : W23_2

11729

11730	O	-2.486591	-0.059315	2.070447
11731	H	-2.221571	-0.967143	2.368867
11732	H	-1.922064	0.103151	1.271988
11733	O	-0.810867	0.600735	0.127970
11734	H	-0.021723	0.636795	0.711496
11735	H	-0.608756	0.018550	-0.646551
11736	O	-0.224693	-0.847165	-2.023410
11737	H	-0.064530	-1.728063	-1.613501
11738	H	-1.043915	-0.878548	-2.559047
11739	O	1.951753	0.861931	-2.005093
11740	H	1.169319	0.282389	-2.101654
11741	H	2.714095	0.310937	-2.267944
11742	O	1.158503	-1.995105	1.916721
11743	H	1.160010	-1.024450	2.053391
11744	H	2.094825	-2.268100	1.964276
11745	O	0.323217	-2.988761	-0.485081
11746	H	0.566411	-2.575615	0.375739
11747	H	-0.482269	-3.514298	-0.313886
11748	O	1.075561	0.724845	2.076878
11749	H	1.772406	1.260958	1.628808
11750	H	0.574132	1.265968	2.710554
11751	O	2.772213	1.894174	0.397607
11752	H	2.401716	1.556915	-0.449979
11753	H	2.626566	2.861004	0.403781
11754	O	-1.620639	2.931855	-0.992949
11755	H	-1.264160	2.105915	-0.597323
11756	H	-0.901954	3.230432	-1.590452
11757	O	-2.743992	-0.701760	-3.082992
11758	H	-3.107773	0.143357	-2.667167
11759	H	-3.038262	-0.726976	-3.998776
11760	O	-2.176331	-3.944788	0.236320
11761	H	-2.558894	-4.826943	0.203896
11762	H	-2.802850	-3.329979	-0.245670
11763	O	1.740752	4.431835	0.361979
11764	H	2.065393	5.311304	0.576841
11765	H	0.867775	4.306361	0.831019
11766	O	4.029627	-0.975466	-2.212378
11767	H	4.610695	-1.186079	-2.949695
11768	H	3.630325	-1.832835	-1.888017
11769	O	3.867048	-2.440275	1.487526
11770	H	4.195103	-1.550847	1.169192
11771	H	4.556460	-2.822493	2.038942

11772	O	-3.756504	-2.284377	-1.002480
11773	H	-4.170661	-1.576999	-0.475827
11774	H	-3.428787	-1.862135	-1.818430
11775	O	-3.705988	1.337789	-1.838958
11776	H	-4.085428	1.028957	-0.997585
11777	H	-3.068297	2.052042	-1.628777
11778	O	-0.640265	4.017992	1.381226
11779	H	-0.840329	3.342780	2.052547
11780	H	-1.173046	3.796542	0.591495
11781	O	-1.114789	1.931131	3.293081
11782	H	-1.394128	2.185068	4.178182
11783	H	-1.717014	1.209163	2.986688
11784	O	4.664432	-0.186981	0.413111
11785	H	4.177292	0.641339	0.569185
11786	H	4.624781	-0.343207	-0.548276
11787	O	3.055093	-3.150017	-1.120040
11788	H	3.367453	-3.125522	-0.197207
11789	H	2.090770	-3.278625	-1.072798
11790	O	-4.628126	-0.040140	0.484098
11791	H	-3.953750	-0.029550	1.210014
11792	H	-5.494876	0.093953	0.879848
11793	O	-1.542697	-2.518850	2.596129
11794	H	-0.570636	-2.491485	2.575527
11795	H	-1.811739	-3.122918	1.880672
11796	O	0.805451	3.490316	-2.182006
11797	H	1.291022	2.664277	-2.340879
11798	H	1.253521	3.937833	-1.445172

11799

11800 Cartesian coordinates of : W23_ 3

11801

11802	O	0.455411	0.603567	2.734483
11803	H	1.395576	0.830251	2.603401
11804	H	0.410897	-0.337192	2.985501
11805	O	2.255679	-0.925525	-1.670956
11806	H	2.237659	0.047425	-1.507488
11807	H	3.126247	-1.120579	-2.065296
11808	O	-1.911914	-3.056569	1.366476
11809	H	-2.815418	-2.746864	1.561639
11810	H	-1.902582	-3.269827	0.415796
11811	O	-0.437025	-1.304495	-1.875289
11812	H	0.525942	-1.341770	-2.038518
11813	H	-0.524995	-0.837972	-1.009240
11814	O	4.964010	1.466897	-1.419600
11815	H	4.043916	1.785417	-1.380955
11816	H	5.299902	1.472295	-0.504973
11817	O	5.228363	-1.640250	0.503537
11818	H	4.334368	-1.906003	0.780644
11819	H	5.224671	-1.642819	-0.471350
11820	O	-2.053448	-3.318550	-1.445299
11821	H	-1.935617	-4.116848	-1.968631
11822	H	-1.367337	-2.655190	-1.725722
11823	O	-0.784816	0.244974	0.301137
11824	H	-0.246410	0.324937	1.117142
11825	H	-0.675323	1.103957	-0.174665
11826	O	-4.278453	0.718755	-2.266776
11827	H	-5.026604	0.939377	-2.831126
11828	H	-4.261855	1.390364	-1.519992
11829	O	0.242881	-2.190152	2.570780
11830	H	0.384880	-2.852128	3.255902
11831	H	-0.595525	-2.466535	2.100260
11832	O	-3.231326	0.455314	1.584881
11833	H	-3.764957	-0.348995	1.725576
11834	H	-2.441229	0.194225	1.067186
11835	O	-1.975583	3.959837	0.504503
11836	H	-1.796021	3.461548	1.351217
11837	H	-2.043821	4.892394	0.730923
11838	O	-4.443123	-1.854101	-1.153407
11839	H	-4.384501	-0.968224	-1.563067
11840	H	-3.664152	-2.368223	-1.431532
11841	O	-0.406726	2.463351	-1.197767
11842	H	-0.921911	3.184727	-0.791484
11843	H	-0.890873	2.106751	-1.984201
11844	O	5.697280	0.841703	1.230882
11845	H	6.508323	0.997175	1.723651
11846	H	5.635143	-0.132762	1.027478

11847	O	-1.606846	1.008078	-3.090812
11848	H	-2.564814	0.902467	-2.944779
11849	H	-1.210682	0.142385	-2.889773
11850	O	2.940955	0.895119	1.619820
11851	H	3.888333	1.089165	1.732958
11852	H	2.878963	-0.065457	1.408064
11853	O	2.218800	1.691694	-0.918834
11854	H	1.361711	2.135758	-1.080596
11855	H	2.330062	1.583653	0.048120
11856	O	-4.173323	2.301306	-0.214867
11857	H	-3.516379	3.013879	-0.127156
11858	H	-3.970133	1.675889	0.512121
11859	O	4.977056	-1.012720	-2.222866
11860	H	5.513782	-1.197519	-2.999292
11861	H	5.052322	-0.036201	-2.013123
11862	O	2.451720	-1.683427	0.945457
11863	H	1.665862	-1.992188	1.437983
11864	H	2.214360	-1.558184	0.001784
11865	O	-4.497078	-1.989123	1.429665
11866	H	-4.591900	-1.941617	0.430875
11867	H	-5.303953	-2.362995	1.795481
11868	O	-1.680593	2.477061	2.662030
11869	H	-0.863181	1.976716	2.829639
11870	H	-2.367974	1.793394	2.562182

11871

11872 Cartesian coordinates of : W23_ 4

11873

11874	O	-0.457369	2.618943	-1.297408
11875	H	-0.454401	2.719721	-0.322646
11876	H	-1.365098	2.368125	-1.549280
11877	O	-2.508900	-1.470694	1.325077
11878	H	-2.443591	-0.510349	1.515465
11879	H	-3.421889	-1.731321	1.553497
11880	O	2.555877	-3.293371	-1.911667
11881	H	3.274887	-2.639585	-1.965616
11882	H	2.608250	-3.693544	-1.029591
11883	O	0.086589	-2.389461	1.028888
11884	H	-0.834709	-2.325388	1.341825
11885	H	0.046578	-2.298111	0.041011
11886	O	-5.330261	0.912427	1.494637
11887	H	-5.560633	1.190381	0.589229
11888	H	-4.424732	1.232661	1.657888
11889	O	-5.287478	-1.456011	-1.303246
11890	H	-4.366801	-1.630180	-1.569944
11891	H	-5.366955	-1.762622	-0.381724
11892	O	2.309734	-3.936765	0.896848
11893	H	2.319266	-4.806517	1.308009
11894	H	1.447131	-3.515490	1.106931
11895	O	1.128014	0.437998	-1.070076
11896	H	0.515419	1.189074	-1.241232
11897	H	1.210764	0.360927	-0.092587
11898	O	3.802283	-0.137785	2.524775
11899	H	4.162808	-0.248047	3.409737
11900	H	4.121969	-0.906948	1.961046
11901	O	0.169379	-2.022781	-1.631935
11902	H	0.516576	-1.103302	-1.591118
11903	H	0.933861	-2.566832	-1.926624
11904	O	3.697116	1.136446	-1.606797
11905	H	2.763643	0.853459	-1.489104
11906	H	3.965667	1.486541	-0.722726
11907	O	2.188034	4.118215	0.943647
11908	H	2.184272	4.034833	-0.050215
11909	H	2.409464	5.030421	1.156012
11910	O	4.453651	-2.103706	0.983057
11911	H	3.758729	-2.785929	0.979193
11912	H	4.620805	-1.846809	0.055150
11913	O	-0.035305	2.522061	1.443704
11914	H	0.404518	1.669294	1.635418
11915	H	0.659891	3.204555	1.504052
11916	O	-5.670815	1.125448	-1.291055
11917	H	-5.627713	0.129661	-1.380835
11918	H	-6.392489	1.449120	-1.838394
11919	O	1.215912	0.051151	1.633655
11920	H	2.090427	-0.024669	2.068478
11921	H	0.819196	-0.844799	1.593410

11922	O	-2.902058	1.323367	-1.344514
11923	H	-3.855868	1.462577	-1.497504
11924	H	-2.727632	0.375460	-1.540310
11925	O	-2.557906	1.296883	1.367570
11926	H	-1.837764	1.879413	1.662688
11927	H	-2.617937	1.396742	0.390456
11928	O	4.171950	2.101125	0.873761
11929	H	3.545785	2.807397	1.106388
11930	H	4.116382	1.412308	1.558809
11931	O	-5.271822	-1.694393	1.507812
11932	H	-5.873880	-2.127508	2.120431
11933	H	-5.391313	-0.704093	1.594984
11934	O	-2.497335	-1.384279	-1.432075
11935	H	-1.670950	-1.751816	-1.797346
11936	H	-2.433958	-1.500286	-0.458966
11937	O	4.646512	-1.334396	-1.699792
11938	H	5.450187	-1.429443	-2.220665
11939	H	4.373035	-0.375428	-1.747190
11940	O	2.139945	3.651762	-1.650663
11941	H	1.236246	3.361537	-1.861546
11942	H	2.746581	2.937330	-1.908582

11943

11944 Cartesian coordinates of : W23_ 5

11945				
11946	O	-6.093011	-0.094235	-1.353402
11947	H	-6.086033	-0.080503	-0.356301
11948	H	-6.925243	0.283728	-1.653148
11949	O	6.028074	0.789751	1.238154
11950	H	6.193172	0.983187	0.297210
11951	H	5.155275	1.163605	1.448540
11952	O	-3.430349	0.733716	-1.474168
11953	H	-3.033670	-0.161505	-1.568523
11954	H	-4.385097	0.611250	-1.637039
11955	O	3.403838	1.129761	-1.367816
11956	H	4.323965	1.250302	-1.664336
11957	H	3.412861	1.232693	-0.388933
11958	O	0.631281	1.336536	-1.401424
11959	H	0.446953	0.377434	-1.517671
11960	H	1.560969	1.469728	-1.659338
11961	O	0.514962	1.499380	1.341787
11962	H	-0.177688	2.075020	1.719122
11963	H	0.472569	1.582171	0.363546
11964	O	6.152642	0.779596	-1.577106
11965	H	6.068277	-0.215393	-1.582279
11966	H	6.864199	1.022596	-2.176967
11967	O	5.741286	-1.805058	-1.341521
11968	H	5.877275	-2.029397	-0.403049
11969	H	4.811173	-2.006559	-1.542546
11970	O	2.959539	-1.573433	-1.406715
11971	H	2.038714	-1.772160	-1.653945
11972	H	3.067513	-0.601892	-1.515145
11973	O	3.251037	1.091939	1.355951
11974	H	2.378981	1.463987	1.583094
11975	H	3.169652	0.117692	1.462584
11976	O	0.206009	-1.371059	-1.338152
11977	H	0.210482	-1.445165	-0.359945
11978	H	-0.670400	-1.685058	-1.630231
11979	O	3.146954	-1.646448	1.315568
11980	H	4.034405	-1.941141	1.588747
11981	H	3.109958	-1.749273	0.337048
11982	O	-5.751726	-0.219404	1.246355
11983	H	-4.949925	0.295883	1.452692
11984	H	-5.545177	-1.141943	1.476862
11985	O	-4.733957	-2.855632	1.482481
11986	H	-3.795027	-2.595588	1.606955
11987	H	-4.933331	-3.550736	2.117055
11988	O	5.916844	-1.827894	1.474418
11989	H	6.586623	-2.216373	2.045187
11990	H	6.039884	-0.837320	1.479674
11991	O	-3.200811	0.921514	1.242932
11992	H	-3.228354	1.021493	0.264482
11993	H	-2.734198	1.694661	1.615438
11994	O	0.401419	-1.237626	1.435824
11995	H	1.281506	-1.576312	1.677913
11996	H	0.434988	-0.259972	1.537842

11997	O	-5.056280	-2.752221	-1.394270
11998	H	-5.136563	-2.953194	-0.447917
11999	H	-5.567056	-1.937595	-1.540543
12000	O	-1.653371	3.078197	2.110217
12001	H	-1.829458	3.513265	2.949990
12002	H	-1.762363	3.757156	1.380299
12003	O	-2.330898	-1.627747	1.431950
12004	H	-1.384036	-1.706700	1.652666
12005	H	-2.556808	-0.669630	1.492663
12006	O	-2.498565	-1.842595	-1.337979
12007	H	-3.330647	-2.315717	-1.563356
12008	H	-2.455060	-1.873469	-0.359791
12009	O	-1.986338	4.570436	0.025919
12010	H	-1.571640	5.408799	-0.194787
12011	H	-1.874326	3.957482	-0.758651
12012	O	-1.671990	2.858105	-1.906630
12013	H	-0.818914	2.387773	-1.870462
12014	H	-2.361087	2.168041	-1.923689

12015

12016 Cartesian coordinates of : W23_ 6

12017

12018	O	5.212900	-0.759558	1.673912
12019	H	5.575357	-0.656386	0.744582
12020	H	5.957129	-0.875208	2.272418
12021	O	-5.189379	1.880339	-1.323723
12022	H	-4.242638	2.077046	-1.206162
12023	H	-5.238053	1.126999	-1.940265
12024	O	3.382578	1.284481	1.474140
12025	H	2.484163	1.015343	1.772562
12026	H	4.027673	0.609860	1.766924
12027	O	-3.473449	0.722811	1.718472
12028	H	-4.426011	0.929309	1.729233
12029	H	-3.097412	1.196752	0.942948
12030	O	-1.283545	0.010400	3.349370
12031	H	-2.116684	0.355908	2.984897
12032	H	-1.298858	-0.950144	3.202778
12033	O	0.268543	1.841678	-0.606339
12034	H	0.921489	2.518815	-0.861823
12035	H	0.484953	1.535134	0.303784
12036	O	-6.139530	1.041369	0.965860
12037	H	-6.905294	1.517534	1.300383
12038	H	-5.869749	1.453400	0.095882
12039	O	-5.866462	-1.536533	-0.132954
12040	H	-6.112783	-0.752359	0.391391
12041	H	-5.061353	-1.898379	0.278834
12042	O	-3.245338	-1.824325	0.797388
12043	H	-2.576982	-2.332884	1.293151
12044	H	-3.297185	-0.940997	1.230049
12045	O	-2.485585	1.649909	-0.658279
12046	H	-1.566332	1.979371	-0.667584
12047	H	-2.458452	0.769407	-1.094348
12048	O	-1.048149	-2.661895	2.278415
12049	H	-0.871286	-3.485227	2.743824
12050	H	-0.283849	-2.494171	1.670128
12051	O	-2.618118	-0.888673	-1.685313
12052	H	-3.430354	-0.918633	-2.223865
12053	H	-2.820206	-1.366734	-0.848853
12054	O	5.858142	-0.525792	-0.836488
12055	H	5.322642	0.206639	-1.189623
12056	H	5.547411	-1.330569	-1.293183
12057	O	4.432003	-2.702750	-1.862609
12058	H	3.717652	-2.132095	-2.278523
12059	H	4.684010	-3.382355	-2.494413
12060	O	-5.260296	-0.671644	-2.524491
12061	H	-5.789524	-1.029018	-3.243686
12062	H	-5.581448	-1.075516	-1.667677
12063	O	3.678372	1.192023	-1.283891
12064	H	3.488780	1.167689	-0.321124
12065	H	3.382182	2.072237	-1.570063
12066	O	0.144529	-0.704983	-1.718925
12067	H	-0.790474	-0.874491	-1.939424
12068	H	0.201891	0.237471	-1.453250
12069	O	3.396658	-2.751959	0.734261
12070	H	4.003650	-2.159810	1.211453
12071	H	3.799092	-2.907815	-0.140345

12072	O	2.343772	3.668171	-1.217411
12073	H	2.276358	4.441426	-1.785665
12074	H	2.741837	3.953098	-0.358249
12075	O	2.724229	-0.972580	-2.725939
12076	H	1.765635	-1.044405	-2.570042
12077	H	3.000724	-0.153195	-2.267086
12078	O	0.908336	-1.878831	0.650374
12079	H	1.837329	-2.238426	0.648223
12080	H	0.660450	-1.624525	-0.263809
12081	O	3.482472	3.969202	1.170585
12082	H	3.562253	3.025007	1.431251
12083	H	3.127644	4.443410	1.928183
12084	O	0.814810	0.589987	1.752330
12085	H	0.099317	0.553283	2.430650
12086	H	0.865356	-0.328566	1.395564
12087				
12088	Cartesian coordinates of : W23_7			
12089				
12090	O	-0.971855	0.035398	1.450134
12091	H	-1.951119	0.059104	1.543429
12092	H	-0.651821	-0.876100	1.626644
12093	O	0.673216	2.201139	1.482785
12094	H	0.057985	1.446848	1.612114
12095	H	0.155355	3.003113	1.686165
12096	O	-0.722050	0.146640	-1.249961
12097	H	-0.100047	0.874053	-1.467815
12098	H	-0.778741	0.154167	-0.264491
12099	O	2.805487	-1.799077	1.762611
12100	H	3.580695	-2.170805	2.196950
12101	H	2.888223	-0.811164	1.795692
12102	O	-3.404847	0.449124	-1.502378
12103	H	-2.427272	0.379611	-1.585876
12104	H	-3.623102	1.372774	-1.729200
12105	O	0.094876	-2.447199	-1.301037
12106	H	-0.635567	-3.035181	-1.574917
12107	H	-0.207814	-1.526181	-1.463621
12108	O	3.392424	0.775380	-1.232768
12109	H	4.337583	0.899815	-1.446529
12110	H	3.183438	-0.177451	-1.337985
12111	O	3.090434	0.837300	1.486577
12112	H	2.361069	1.431881	1.743109
12113	H	3.177246	0.915007	0.508609
12114	O	2.804104	-1.913796	-1.026459
12115	H	2.753782	-1.993725	-0.053239
12116	H	1.966829	-2.272953	-1.371410
12117	O	-3.657908	0.228430	1.211965
12118	H	-3.659795	0.262969	0.227980
12119	H	-4.118721	-0.595789	1.456650
12120	O	0.100923	-2.464339	1.434357
12121	H	1.006229	-2.419956	1.788047
12122	H	0.187061	-2.517776	0.454435
12123	O	1.038397	2.239024	-1.248495
12124	H	1.017598	2.273598	-0.266521
12125	H	1.924488	1.910053	-1.486326
12126	O	-2.255187	-3.897603	-1.576449
12127	H	-2.457991	-4.630701	-2.165745
12128	H	-3.017952	-3.250795	-1.628013
12129	O	-3.541702	3.216758	-1.601189
12130	H	-2.594026	3.533949	-1.588803
12131	H	-4.040391	3.827793	-2.152236
12132	O	-1.206655	4.239513	1.513622
12133	H	-1.306526	5.030024	2.052866
12134	H	-2.090357	3.773183	1.502534
12135	O	-4.550049	-2.392950	1.339934
12136	H	-5.235525	-2.842315	1.843710
12137	H	-3.717648	-2.941517	1.406346
12138	O	6.165605	0.929604	-1.297166
12139	H	6.791456	1.576712	-1.634902
12140	H	6.227203	0.914161	-0.311528
12141	O	-1.083041	4.074857	-1.309026
12142	H	-0.987436	4.294114	-0.364391
12143	H	-0.302660	3.544219	-1.546853
12144	O	-4.251095	-2.214202	-1.465721
12145	H	-4.078962	-1.276967	-1.669954
12146	H	-4.570305	-2.246328	-0.545858

12147	O	-3.516135	3.035642	1.219214
12148	H	-3.666422	2.105807	1.463943
12149	H	-3.736762	3.110625	0.272880
12150	O	-2.354968	-3.819784	1.244791
12151	H	-1.502739	-3.470332	1.558532
12152	H	-2.229596	-4.043264	0.304305
12153	O	5.870901	0.277741	1.275930
12154	H	5.040360	0.626320	1.636335
12155	H	5.665808	-0.600706	0.903072
12156	O	5.564490	-1.785947	-0.579973
12157	H	4.719161	-2.063296	-0.967644
12158	H	5.964805	-1.169813	-1.210877

12159

12160 Cartesian coordinates of : W23_ 8

12161

12162	O	5.646826	0.550862	1.211742
12163	H	5.568371	-0.383975	1.479242
12164	H	4.839681	0.990183	1.539359
12165	O	-6.293564	0.568159	-1.211782
12166	H	-5.463347	1.009002	-1.460135
12167	H	-6.223844	-0.349925	-1.532449
12168	O	3.003855	1.461384	1.535578
12169	H	2.700758	0.547383	1.705596
12170	H	3.016443	1.533290	0.557557
12171	O	-3.805325	1.022638	1.385313
12172	H	-4.740270	1.009230	1.658542
12173	H	-3.802981	1.191282	0.415567
12174	O	-1.100143	1.621689	1.511038
12175	H	-0.753173	0.708379	1.612366
12176	H	-2.041646	1.595453	1.757432
12177	O	-0.870957	1.915190	-1.212498
12178	H	-0.192375	2.578508	-1.435768
12179	H	-0.934217	1.910807	-0.230943
12180	O	-6.524961	0.437799	1.400279
12181	H	-6.553148	0.558565	0.410066
12182	H	-7.335677	0.798542	1.771600
12183	O	-5.669107	-2.226830	1.081983
12184	H	-4.737846	-2.250407	1.361672
12185	H	-6.031194	-1.377813	1.396159
12186	O	-2.949974	-1.565464	1.296409
12187	H	-2.016837	-1.651170	1.560773
12188	H	-3.194016	-0.624503	1.447729
12189	O	-3.555225	1.183486	-1.333092
12190	H	-2.746344	1.682937	-1.542733
12191	H	-3.343702	0.234590	-1.485491
12192	O	-0.236786	-0.986289	1.328646
12193	H	0.661391	-1.238185	1.612732
12194	H	-0.234507	-1.013530	0.347705
12195	O	-3.139520	-1.509178	-1.430140
12196	H	-3.086259	-1.668410	-0.459930
12197	H	-3.974079	-1.914305	-1.727777
12198	O	5.706965	0.989550	-1.359541
12199	H	6.535357	1.388698	-1.642695
12200	H	5.772789	0.824986	-0.372233
12201	O	5.902417	-3.324942	-0.287530
12202	H	5.551485	-2.726055	-1.002434
12203	H	5.747975	-4.231547	-0.566805
12204	O	-5.834165	-2.194831	-1.534385
12205	H	-5.840177	-2.317556	-0.543090
12206	H	-6.380518	-2.883051	-1.925572
12207	O	4.892467	-1.637872	-2.033521
12208	H	3.929943	-1.531785	-1.925515
12209	H	5.266544	-0.742154	-1.949109
12210	O	-0.465435	-0.788861	-1.435677
12211	H	-0.596751	0.181477	-1.515996
12212	H	-1.291774	-1.213199	-1.725749
12213	O	5.139042	-2.150751	1.919297
12214	H	5.449403	-2.698316	1.145859
12215	H	5.566482	-2.494296	2.709761
12216	O	3.068228	1.692190	-1.220622
12217	H	4.006149	1.726730	-1.488757
12218	H	2.602167	2.524338	-1.429878
12219	O	2.285084	-0.919623	-1.292029
12220	H	1.362366	-1.089379	-1.556361
12221	H	2.422388	0.046672	-1.381372

12222	O	2.520579	-1.281275	1.425737
12223	H	3.330587	-1.726939	1.734655
12224	H	2.548147	-1.286015	0.444559
12225	O	1.263835	3.746089	-1.131150
12226	H	1.256570	4.667051	-1.409510
12227	H	1.189020	3.726200	-0.127342
12228	O	1.042937	3.423153	1.437379
12229	H	0.215861	2.955072	1.650341
12230	H	1.758213	2.812952	1.706893
12231				
12232	Cartesian coordinates of : W23_ 9			
12233				
12234	O	-5.169771	-2.527584	-0.637818
12235	H	-5.679080	-1.728245	-0.327322
12236	H	-5.798584	-3.163376	-0.992429
12237	O	5.443286	1.915227	0.504292
12238	H	5.851937	1.358134	-0.183482
12239	H	4.561704	2.159382	0.172332
12240	O	-2.830203	-1.257290	-1.531749
12241	H	-2.204037	-1.544882	-0.829605
12242	H	-3.601859	-1.850631	-1.477387
12243	O	3.556426	-0.273672	-1.844349
12244	H	4.526672	-0.245936	-1.926663
12245	H	3.293693	0.541650	-1.360781
12246	O	1.033033	-1.042284	-2.862896
12247	H	0.893025	-1.801777	-2.272880
12248	H	1.961694	-0.778342	-2.753720
12249	O	0.016288	2.027684	-0.522089
12250	H	-0.510797	2.817101	-0.301255
12251	H	-0.426608	1.570108	-1.279806
12252	O	6.262330	-0.185491	-1.177118
12253	H	7.104355	-0.372559	-1.602613
12254	H	6.137478	-0.838524	-0.431699
12255	O	5.674808	-1.727706	0.865864
12256	H	5.573575	-1.144278	1.639285
12257	H	4.799996	-2.125064	0.705937
12258	O	3.007971	-2.063314	0.127932
12259	H	2.268084	-2.648749	-0.116232
12260	H	3.179645	-1.496081	-0.659450
12261	O	2.747688	1.734841	-0.194296
12262	H	1.864092	2.061844	-0.447343
12263	H	2.604828	1.174974	0.600525
12264	O	0.659658	-3.149912	-0.895246
12265	H	0.442144	-4.043448	-1.178156
12266	H	-0.071127	-2.835842	-0.309527
12267	O	2.504889	-0.046959	1.895065
12268	H	3.317039	0.088635	2.417477
12269	H	2.643940	-0.867396	1.369033
12270	O	-6.161933	-0.288870	0.318429
12271	H	-5.554155	0.348347	-0.107325
12272	H	-5.945958	-0.205214	1.260897
12273	O	-4.613280	0.097678	2.707926
12274	H	-3.964280	0.799438	2.491810
12275	H	-4.837035	0.199992	3.638434
12276	O	5.147613	0.405900	2.631326
12277	H	5.607459	0.715551	3.417263
12278	H	5.313651	1.060080	1.894299
12279	O	-3.912251	1.028438	-0.607296
12280	H	-3.441589	1.231561	0.224630
12281	H	-3.508664	0.191730	-0.940593
12282	O	-0.211694	0.382498	1.577455
12283	H	0.655742	0.245497	2.001896
12284	H	-0.039643	0.949328	0.785989
12285	O	-3.593121	-2.408473	1.723186
12286	H	-4.187013	-2.643353	0.989117
12287	H	-3.954105	-1.597866	2.121702
12288	O	-1.925276	3.928627	0.138488
12289	H	-1.899431	4.884403	0.245006
12290	H	-2.293598	3.725461	-0.768273
12291	O	-2.612972	1.746379	1.785584
12292	H	-1.754080	1.297132	1.919936
12293	H	-2.417291	2.642182	1.451426
12294	O	-1.221379	-1.941335	0.568888
12295	H	-1.996050	-2.201764	1.124042
12296	H	-0.834649	-1.130476	0.970919

12297	O	-2.770034	2.987155	-2.151304
12298	H	-3.343945	2.296258	-1.758761
12299	H	-2.105850	2.493734	-2.658151
12300	O	-1.056408	0.687603	-2.603202
12301	H	-0.274483	0.141255	-2.850343
12302	H	-1.762160	0.036902	-2.444739
12303				
12304	Cartesian coordinates of : W23_10			
12305				
12306	O	-1.621252	-0.632947	1.812082
12307	O	-1.660070	1.968162	0.936957
12308	O	-4.403507	-0.524435	1.719487
12309	O	-4.635216	-1.344916	-0.870150
12310	O	-4.382383	1.322304	-1.504754
12311	O	-4.434381	2.084889	1.171725
12312	O	-1.597920	1.109527	-1.659778
12313	O	-1.884760	-1.480564	-0.793935
12314	O	-7.333147	-1.988653	-0.905867
12315	O	-7.228749	-0.586143	1.366460
12316	H	-4.449897	-0.931433	0.823004
12317	H	-3.530167	-0.755706	2.080760
12318	H	-2.532430	2.331313	1.165742
12319	H	-1.675568	1.783608	-0.029852
12320	H	-4.369101	1.739639	-0.620588
12321	H	-3.500477	1.462437	-1.889215
12322	H	-1.837254	-1.298542	0.170545
12323	H	-2.803113	-1.748874	-0.978128
12324	H	-1.574883	0.328575	1.612389
12325	H	-0.740152	-0.887700	2.135941
12326	H	-4.497392	1.147797	1.490712
12327	H	-4.645055	-0.432329	-1.231734
12328	H	-1.664771	0.146256	-1.471063
12329	H	-0.701591	1.259808	-2.007127
12330	H	-7.123710	0.176556	0.767043
12331	H	-6.390961	-0.675100	1.845213
12332	H	-7.438683	-1.700746	0.032046
12333	H	-5.514600	-1.737688	-1.030814
12334	H	-5.188695	2.573391	1.517451
12335	H	-7.870106	-2.772913	-1.050228
12336	H	1.214049	1.436320	-0.743692
12337	O	1.191475	1.063987	-1.653234
12338	H	2.086612	1.175911	-2.017691
12339	H	1.086086	0.861333	1.379368
12340	O	1.104340	1.770341	1.004983
12341	H	0.230591	2.158293	1.184162
12342	H	0.941540	-0.668235	-1.310305
12343	O	0.875018	-1.575292	-0.937956
12344	H	-0.040514	-1.867133	-1.090539
12345	H	1.091426	-1.256316	0.804274
12346	O	1.148789	-0.885770	1.712891
12347	H	2.040543	-1.097076	2.039805
12348	H	4.830449	-1.168835	1.971556
12349	O	3.926382	-0.917792	1.708271
12350	H	3.953661	0.045233	1.509674
12351	H	2.732863	-2.074547	-1.061030
12352	O	3.642030	-1.785074	-0.873116
12353	H	3.681318	-1.588232	0.089977
12354	H	3.012830	2.063293	1.053814
12355	O	3.874833	1.675123	0.826487
12356	H	3.849557	1.477531	-0.137108
12357	H	3.877566	-0.175289	-1.561531
12358	O	3.953970	0.785448	-1.758712
12359	H	4.871099	0.931576	-2.054043
12360	O	-7.127977	0.878200	-1.010020
12361	H	-6.349835	1.194731	-1.492630
12362	H	-7.401031	0.052304	-1.435914
12363	O	6.659128	1.409957	0.770687
12364	H	5.775094	1.746005	0.996567
12365	H	6.772085	0.573700	1.258331
12366	H	6.789502	1.125553	-0.841582
12367	O	6.733762	0.810176	-1.787092
12368	H	7.450013	1.217992	-2.283244
12369	H	6.666798	-1.591740	0.700156
12370	O	6.682738	-1.269552	1.644541
12371	H	7.354829	-1.766290	2.120873

12372	H	6.629299	-1.028679	-1.398583
12373	O	6.440124	-1.849843	-0.908656
12374	H	5.516348	-2.082821	-1.103175
12375				
12376	Cartesian coordinates of : W23_11			
12377				
12378	O	4.322828	-0.353833	0.826292
12379	H	4.510300	-0.535504	-0.128688
12380	H	4.606916	0.543065	1.059714
12381	O	-3.837401	1.506762	-2.215016
12382	H	-2.885596	1.670353	-2.084093
12383	H	-3.949768	0.553569	-2.392186
12384	O	1.712457	0.031475	0.640417
12385	H	1.256617	-0.731888	1.063718
12386	H	2.686778	-0.145998	0.729925
12387	O	-2.534552	1.274339	1.009750
12388	H	-3.419106	1.658711	0.862272
12389	H	-2.020392	1.443929	0.188717
12390	O	-0.851323	1.391816	3.249231
12391	H	-1.538089	1.458036	2.560099
12392	H	-0.833661	0.451969	3.497068
12393	O	0.577813	3.749971	-0.255451
12394	H	0.407057	4.684597	-0.102346
12395	H	0.740183	3.317099	0.628697
12396	O	-5.059975	1.931424	0.043030
12397	H	-5.662794	2.679504	0.081024
12398	H	-4.681093	1.869811	-0.882263
12399	O	-5.446586	-0.848030	0.211494
12400	H	-4.779602	-1.169011	0.845167
12401	H	-5.495118	0.117955	0.327733
12402	O	-2.998327	-1.381465	1.444560
12403	H	-2.541237	-1.602510	2.273876
12404	H	-2.753876	-0.446888	1.262050
12405	O	-1.190412	1.842053	-1.311902
12406	H	-0.670008	2.637363	-1.093966
12407	H	-0.533891	1.169984	-1.602880
12408	O	-1.048605	-1.491581	3.482597
12409	H	-1.008366	-1.981690	4.309642
12410	H	-0.373790	-1.879323	2.876722
12411	O	-2.467893	-2.820811	-0.908870
12412	H	-3.070340	-2.377589	-1.530932
12413	H	-2.654730	-2.415529	-0.039238
12414	O	4.307919	-1.138988	-1.707879
12415	H	3.927346	-0.479853	-2.315460
12416	H	3.729023	-1.921265	-1.721680
12417	O	2.671387	-3.442186	-1.320153
12418	H	1.697597	-3.282488	-1.322232
12419	H	2.829318	-4.259769	-1.802563
12420	O	-4.455427	-1.231193	-2.186563
12421	H	-5.077963	-1.628600	-2.803758
12422	H	-4.923579	-1.138157	-1.308072
12423	O	3.083403	0.975425	-3.086026
12424	H	3.358894	1.323856	-3.939140
12425	H	3.131620	1.717661	-2.424245
12426	O	0.143423	-2.572965	-1.107703
12427	H	-0.831993	-2.765662	-1.152813
12428	H	0.265591	-1.687526	-1.505275
12429	O	3.285697	-2.950348	1.410570
12430	H	3.838637	-2.154157	1.463883
12431	H	3.291984	-3.224243	0.476825
12432	O	3.064510	2.829110	-1.221205
12433	H	2.197117	3.225176	-1.018688
12434	H	3.501884	2.688706	-0.363528
12435	O	0.771166	0.027085	-1.856132
12436	H	1.230843	0.096652	-0.983755
12437	H	1.430249	0.275225	-2.528818
12438	O	0.685023	-2.291372	1.599232
12439	H	1.598744	-2.657101	1.683057
12440	H	0.377247	-2.532672	0.698967
12441	O	3.960935	2.424711	1.467537
12442	H	4.502233	3.088442	1.906682
12443	H	3.064935	2.471884	1.867289
12444	O	1.254245	2.325589	1.851367
12445	H	0.562367	2.123120	2.527165
12446	H	1.359071	1.454836	1.382927

12447
12448 Cartesian coordinates of : W23_12
12449
12450 O 0.376081 -1.677936 -1.458719
12451 O 0.513615 -1.979551 1.258446
12452 O 0.377263 2.292950 0.344753
12453 O 0.632817 0.963816 -2.038330
12454 O -2.411038 -1.648076 -1.527897
12455 O -2.268557 -2.033277 1.142715
12456 O -2.385686 2.285724 0.379679
12457 O -2.161283 0.992896 -1.993934
12458 H 0.374554 -1.791580 -0.479253
12459 H -1.388777 -2.406120 1.319609
12460 H 0.401848 1.832468 -0.525033
12461 H -2.189717 0.017916 -1.832481
12462 H -0.517839 -1.922385 -1.758565
12463 H -2.250645 -1.151608 1.584292
12464 H -0.521986 2.655100 0.439389
12465 H -1.284568 1.186297 -2.363688
12466 H 1.510669 1.133611 -2.415998
12467 H -3.313149 -1.851394 -1.838939
12468 H 1.372630 -2.403404 1.424121
12469 H -3.294288 2.626438 0.474898
12470 H 0.592934 -0.001677 -1.841671
12471 H -2.424265 -1.793400 -0.550330
12472 H 0.577112 -1.097430 1.689857
12473 H -2.366112 1.819676 -0.489375
12474 H 1.623040 0.639368 2.778002
12475 O 0.743558 0.520711 2.387407
12476 H 0.667041 1.172998 1.653515
12477 H -1.217718 0.490474 2.754029
12478 O -2.084350 0.413723 2.324106
12479 H -2.122483 1.113976 1.631590
12480 O -4.935873 0.271714 2.199376
12481 H -5.080997 1.060111 1.646370
12482 H -4.043551 0.356413 2.569581
12483 H -5.854700 3.064594 0.345206
12484 O -5.155178 2.404504 0.346309
12485 H -5.187356 1.923411 -0.528970
12486 O -4.976368 1.103903 -1.921392
12487 H -5.149194 0.142076 -1.888615
12488 H -4.063741 1.203100 -2.239456
12489 O -5.181519 -1.678158 -1.695711
12490 H -5.223301 -1.864867 -0.703917
12491 H -5.867447 -2.200189 -2.122804
12492 H -5.144320 -1.249658 1.354595
12493 O -5.071090 -2.089460 0.844491
12494 H -4.190409 -2.430256 1.070050
12495 H 3.194227 -1.972053 0.154334
12496 O 3.253443 -2.195800 1.110687
12497 H 4.104118 -2.648430 1.191587
12498 H 4.547346 0.363562 2.044583
12499 O 3.585809 0.327979 2.225756
12500 H 3.357234 -0.566431 1.898741
12501 O 3.132084 2.221154 0.375647
12502 H 3.220917 1.542698 1.091732
12503 H 2.241436 2.606201 0.451366
12504 O 3.434767 0.985920 -2.006604
12505 H 3.277814 1.392787 -1.119704
12506 H 4.293899 1.342804 -2.271649
12507 O 3.169970 -1.688887 -1.582264
12508 H 2.259703 -1.922986 -1.836207
12509 H 3.290867 -0.737191 -1.801306
12510 O 5.574269 2.456010 -0.812798
12511 H 6.214986 3.173455 -0.797463
12512 H 4.800322 2.736445 -0.288036
12513 O 5.590826 -2.424504 -0.512713
12514 H 6.312593 -2.935245 -0.891497
12515 H 4.878326 -2.376458 -1.175781
12516 H 5.918266 -0.713600 0.333191
12517 O 5.955868 0.124631 0.822577
12518 H 5.989248 0.840499 0.167402
12519
12520 Cartesian coordinates of : W23_13
12521

12522	O	-3.151182	-0.607173	1.226752
12523	H	-3.136316	-0.455972	2.190032
12524	H	-2.418319	-1.225981	1.036456
12525	O	-0.644477	-2.094945	3.430078
12526	H	-1.295026	-1.470384	3.794088
12527	H	0.126893	-1.562153	3.168324
12528	O	2.620837	3.351355	0.286174
12529	H	3.007082	2.559373	0.757451
12530	H	3.278359	4.053237	0.303858
12531	O	-1.216599	-2.627251	0.857227
12532	H	-1.071173	-2.627531	1.833059
12533	H	-0.325490	-2.696747	0.450464
12534	O	-0.821534	2.939982	-2.738453
12535	H	-1.189716	3.523578	-2.052389
12536	H	-1.513053	2.286751	-2.935988
12537	O	-1.869728	4.124159	-0.360263
12538	H	-2.177846	3.205766	-0.143419
12539	H	-2.614044	4.725337	-0.262342
12540	O	3.111944	-0.231115	-2.394860
12541	H	2.539107	-0.961676	-2.696289
12542	H	2.549497	0.566125	-2.308693
12543	O	-2.587382	0.664655	-2.685639
12544	H	-1.946144	-0.071234	-2.710504
12545	H	-3.423994	0.220538	-2.440834
12546	O	1.259603	-2.947740	-0.285163
12547	H	1.472360	-2.925144	-1.231783
12548	H	2.090860	-3.053673	0.203384
12549	O	1.451803	1.868013	-1.750587
12550	H	1.876067	2.544705	-1.189382
12551	H	0.672155	2.284561	-2.194871
12552	O	4.601651	-0.660100	-0.377748
12553	H	5.514133	-0.588778	-0.675694
12554	H	4.008887	-0.515285	-1.193828
12555	O	-2.423664	0.077126	3.824173
12556	H	-2.815915	0.499191	4.593629
12557	H	-1.739904	0.687733	3.438757
12558	O	-2.788530	-3.350035	-1.127246
12559	H	-2.937532	-4.273863	-1.349229
12560	H	-2.338477	-3.314491	-0.250382
12561	O	-2.203765	1.558079	-0.107245
12562	H	-2.360514	1.249769	-1.027191
12563	H	-2.651472	0.909657	0.478061
12564	O	1.412938	-2.344768	-3.041396
12565	H	0.478251	-2.055099	-2.871174
12566	H	1.442853	-2.797082	-3.889582
12567	O	3.495447	1.172918	1.437802
12568	H	2.777921	0.621493	1.799280
12569	H	3.977912	0.593118	0.819081
12570	O	1.481339	-0.759747	2.038518
12571	H	1.038993	-0.658155	1.160038
12572	H	2.145867	-1.466101	1.940728
12573	O	-0.503708	1.259087	2.519226
12574	H	-0.297515	2.175396	2.201485
12575	H	0.337966	0.797036	2.633756
12576	O	-0.902911	-1.499364	-2.129539
12577	H	-1.531959	-2.194384	-1.855936
12578	H	-0.559400	-1.057770	-1.312940
12579	O	-4.377779	-0.963794	-1.315628
12580	H	-4.291627	-0.751826	-0.372074
12581	H	-4.040051	-1.871610	-1.379127
12582	O	3.551900	-2.513671	1.265119
12583	H	4.162614	-3.028436	1.800923
12584	H	4.076457	-1.917249	0.680887
12585	O	0.176628	0.046076	-0.184696
12586	H	-0.544174	0.602015	0.175619
12587	H	0.715255	0.678496	-0.717909
12588	O	0.131114	3.673746	1.559830
12589	H	-0.505926	4.002153	0.901484
12590	H	1.004538	3.670641	1.129245

12591

12592

12593

12594 Cartesian coordinates of the water 24-mer

12595

12596 Cartesian coordinates of : W24_1

12597				
12598	O	1.103410	-0.003078	-1.404222
12599	H	2.067850	-0.111781	-1.562646
12600	H	0.650883	-0.862734	-1.551911
12601	O	-0.178682	2.398079	-1.378832
12602	H	0.299887	1.555162	-1.533738
12603	H	0.448945	3.109244	-1.610157
12604	O	1.048184	0.159188	1.300806
12605	H	0.540825	0.962018	1.545871
12606	H	1.036434	0.148872	0.313322
12607	O	-2.859279	-1.330269	-1.431931
12608	H	-3.785751	-1.555274	-1.639098
12609	H	-2.775692	-0.357907	-1.544851
12610	O	3.759465	0.113562	1.380323
12611	H	2.788189	0.175090	1.523542
12612	H	4.113476	0.998392	1.589669
12613	O	-0.090095	-2.309809	1.436392
12614	H	0.576394	-2.985117	1.668178
12615	H	0.336232	-1.434663	1.569028
12616	O	-2.950028	1.290820	1.450636
12617	H	-3.893259	1.462626	1.632501
12618	H	-2.814190	0.325751	1.570915
12619	O	-2.764825	1.408936	-1.290587
12620	H	-1.974226	1.900363	-1.578694
12621	H	-2.777050	1.458258	-0.308582
12622	O	-2.721131	-1.447317	1.315608
12623	H	-2.715753	-1.495642	0.333844
12624	H	-1.913279	-1.903153	1.613752
12625	O	3.809271	-0.149959	-1.343004
12626	H	3.875993	-0.112499	-0.361589
12627	H	4.146245	-1.026966	-1.605481
12628	O	-0.276717	-2.342855	-1.301594
12629	H	-1.194470	-2.189828	-1.591813
12630	H	-0.303438	-2.379541	-0.318347
12631	O	-0.428345	2.466503	1.359885
12632	H	-0.448399	2.500030	0.377546
12633	H	-1.339421	2.271129	1.643192
12634	O	2.068292	-4.048206	1.570337
12635	H	2.215623	-4.801065	2.151059
12636	H	2.909268	-3.505136	1.564336
12637	O	4.280190	2.837036	1.460241
12638	H	3.382298	3.273086	1.500908
12639	H	4.886037	3.375989	1.978087
12640	O	1.961887	4.148394	-1.524086
12641	H	2.127671	4.916900	-2.078665
12642	H	2.777349	3.570870	-1.559176
12643	O	4.350041	-2.864065	-1.503304
12644	H	4.939847	-3.399598	-2.042641
12645	H	3.450767	-3.299874	-1.512384
12646	O	-5.723709	1.375818	1.338583
12647	H	-6.406025	1.959920	1.682638
12648	H	-5.741319	1.424224	0.339469
12649	O	-5.629133	-1.549666	-1.387630
12650	H	-5.665464	-1.600264	-0.389527
12651	H	-6.275701	-2.165044	-1.746195
12652	O	1.931075	3.991354	1.298497
12653	H	1.819875	4.223049	0.358577
12654	H	1.101632	3.565383	1.576633
12655	O	4.254099	-2.638495	1.313522
12656	H	4.219155	-1.686696	1.520300
12657	H	4.505124	-2.713091	0.375145
12658	O	4.099968	2.649682	-1.356353
12659	H	4.096465	1.708204	-1.603834
12660	H	4.371335	2.688848	-0.421125
12661	O	1.995788	-3.984737	-1.255965
12662	H	1.176841	-3.528294	-1.518287
12663	H	1.900979	-4.192706	-0.308620
12664	O	-5.546659	1.259168	-1.269207
12665	H	-4.630703	1.475177	-1.521212
12666	H	-5.689819	0.329045	-1.521678
12667	O	-5.508934	-1.425941	1.225325
12668	H	-4.590887	-1.600566	1.500502
12669	H	-5.699855	-0.503348	1.473710
12670				
12671	Cartesian coordinates of : W24_ 2			

12672				
12673	O	-1.016612	3.010437	1.094628
12674	H	-0.456191	3.461291	0.401365
12675	H	-0.489904	3.016819	1.919008
12676	O	1.387809	0.222949	-0.080986
12677	H	0.418600	0.195953	0.118209
12678	H	1.443721	0.226165	-1.057685
12679	O	-1.199119	0.352709	0.486856
12680	H	-1.265156	-0.125102	1.344573
12681	H	-1.210248	1.317589	0.683043
12682	O	0.184423	-2.795122	0.749996
12683	H	1.053082	-3.214712	0.907038
12684	H	0.256685	-2.319065	-0.102614
12685	O	0.171757	-1.973192	-1.920315
12686	H	0.342366	-1.150499	-2.414805
12687	H	-0.607146	-2.420915	-2.299336
12688	O	1.334821	0.355909	-2.835925
12689	H	0.931617	1.226450	-3.031767
12690	H	2.304970	0.414540	-2.892537
12691	O	-1.087574	-1.284923	2.626513
12692	H	-2.012264	-1.583451	2.704508
12693	H	-0.610975	-1.936020	2.067451
12694	O	-2.819256	-0.435755	-1.587059
12695	H	-2.113869	-0.357701	-0.912017
12696	H	-2.744998	-1.312368	-2.005966
12697	O	-3.725517	-1.859568	1.994425
12698	H	-4.047592	-1.048175	1.501089
12699	H	-4.479424	-2.206584	2.481978
12700	O	-0.091499	2.717422	-3.061834
12701	H	-1.031364	2.524777	-2.765964
12702	H	-0.162106	3.205481	-3.888763
12703	O	0.862054	2.724544	3.113053
12704	H	0.971724	3.219983	3.930448
12705	H	0.947391	1.748972	3.340608
12706	O	2.949772	-0.919547	1.780168
12707	H	2.364718	-0.692789	1.022970
12708	H	3.085613	-1.881331	1.730039
12709	O	3.963483	-0.049617	-2.046442
12710	H	4.783133	-0.078383	-2.551221
12711	H	4.202474	0.340672	-1.150227
12712	O	1.111680	0.190630	3.581712
12713	H	0.304154	-0.335574	3.447095
12714	H	1.825754	-0.249613	3.078168
12715	O	-2.328993	-3.073523	-2.317777
12716	H	-2.744213	-3.709350	-2.907521
12717	H	-2.452163	-3.384491	-1.373706
12718	O	-2.526989	2.193546	-2.297710
12719	H	-2.698952	1.232347	-2.252263
12720	H	-2.900984	2.556085	-1.475451
12721	O	2.456032	2.594157	0.787399
12722	H	1.999188	1.763335	0.525881
12723	H	2.109427	2.806149	1.672945
12724	O	2.849172	-3.560741	0.862211
12725	H	2.988765	-3.268092	-0.084197
12726	H	3.268848	-4.417689	0.981709
12727	O	2.886909	-2.606506	-1.554942
12728	H	3.305838	-1.738751	-1.716362
12729	H	1.956098	-2.521019	-1.830501
12730	O	-4.529988	0.141165	0.515010
12731	H	-4.142541	-0.103526	-0.347767
12732	H	-4.240823	1.059966	0.653661
12733	O	-2.425776	-3.638138	0.217067
12734	H	-1.499005	-3.555203	0.507546
12735	H	-2.954791	-3.055259	0.794602
12736	O	4.585645	0.859887	0.319013
12737	H	4.085244	1.667928	0.539362
12738	H	4.276394	0.198927	0.966621
12739	O	0.611848	4.070417	-0.693079
12740	H	1.447782	3.713868	-0.337802
12741	H	0.484984	3.684128	-1.578103
12742	O	-3.539314	2.823377	0.321173
12743	H	-4.131834	3.566642	0.472127
12744	H	-2.680162	3.033460	0.759293
12745				
12746	Cartesian coordinates of : W24_3			

12747				
12748	O	1.290092	1.333087	1.409611
12749	O	1.486182	-1.408360	1.331005
12750	O	4.069225	1.415510	1.306817
12751	O	4.258813	1.311320	-1.422184
12752	O	4.069097	-1.415159	-1.306701
12753	O	4.258378	-1.311238	1.422326
12754	O	1.290010	-1.333104	-1.409114
12755	O	1.486641	1.407325	-1.329995
12756	O	7.033314	1.487692	-1.355407
12757	O	6.866713	1.323465	1.262103
12758	H	4.077085	1.501875	0.326958
12759	H	3.183793	1.685967	1.604326
12760	H	2.379952	-1.664676	1.616465
12761	H	1.464419	-1.508646	0.353020
12762	H	4.076771	-1.502321	-0.326718
12763	H	3.183803	-1.685187	-1.604470
12764	H	1.464593	1.509641	-0.352421
12765	H	2.380477	1.664442	-1.615995
12766	H	1.316303	0.355368	1.508875
12767	H	0.394716	1.612450	1.667910
12768	H	4.234203	-0.331615	1.506713
12769	H	4.234367	0.331352	-1.505892
12770	H	1.316516	-0.355285	-1.508471
12771	H	0.394871	-1.612322	-1.667906
12772	H	7.024999	0.392632	1.502507
12773	H	5.960679	1.534191	1.545670
12774	H	7.049225	1.522432	-0.357652
12775	H	5.170526	1.582159	-1.634016
12776	H	5.169917	-1.582605	1.634658
12777	H	7.727964	2.063973	-1.687828
12778	H	-1.464956	-1.508000	-0.352468
12779	O	-1.485689	-1.409940	-1.330548
12780	H	-2.380202	-1.664468	-1.616251
12781	H	-1.317146	-0.355684	1.507972
12782	O	-1.290140	-1.333388	1.410143
12783	H	-0.394462	-1.611578	1.668637
12784	H	-1.316928	0.355621	-1.508008
12785	O	-1.289908	1.333343	-1.409968
12786	H	-0.394301	1.611566	-1.668474
12787	H	-1.465110	1.508167	0.352579
12788	O	-1.485861	1.409630	1.330496
12789	H	-2.380442	1.664349	1.616242
12790	H	-5.170917	1.582490	1.634487
12791	O	-4.259692	1.311545	1.419990
12792	H	-4.234386	0.332179	1.507133
12793	H	-3.184681	1.685651	-1.605036
12794	O	-4.069778	1.416097	-1.306612
12795	H	-4.076603	1.502452	-0.326479
12796	H	-3.184612	-1.685450	1.605033
12797	O	-4.069520	-1.415677	1.306570
12798	H	-4.076535	-1.502498	0.326400
12799	H	-4.234108	-0.332065	-1.506999
12800	O	-4.259348	-1.311517	-1.420341
12801	H	-5.170524	-1.582504	-1.634719
12802	O	6.866781	-1.323443	-1.262456
12803	H	5.961210	-1.533973	-1.546843
12804	H	7.025175	-0.392022	-1.502699
12805	O	-6.865657	-1.322975	1.260097
12806	H	-5.960836	-1.533706	1.547374
12807	H	-7.025743	-0.392480	1.503014
12808	H	-7.050304	-1.521664	-0.356755
12809	O	-7.032546	-1.487725	-1.354489
12810	H	-7.727964	-2.062612	-1.687583
12811	H	-7.050202	1.522360	0.356315
12812	O	-7.033136	1.487740	1.354179
12813	H	-7.727878	2.063260	1.687380
12814	H	-7.025790	0.392862	-1.503382
12815	O	-6.865798	1.322853	-1.260443
12816	H	-5.961067	1.534052	-1.547311
12817	H	7.049714	-1.521082	0.357393
12818	O	7.032531	-1.487890	1.354931
12819	H	7.728772	-2.062561	1.687225

12820

12821 Cartesian coordinates of : W24_4

12822				
12823	O	-1.381461	0.379676	1.417489
12824	H	-2.358519	0.415805	1.535375
12825	H	-1.036600	1.284373	1.576627
12826	O	-0.324193	-2.126959	1.378539
12827	H	0.620526	-2.131497	1.619737
12828	H	-0.637335	-1.211939	1.543246
12829	O	3.084735	0.963200	-1.413057
12830	H	2.637948	0.104948	-1.568458
12831	H	4.028008	0.828516	-1.628740
12832	O	-1.283889	0.203703	-1.294427
12833	H	-0.967026	-0.686559	-1.552250
12834	H	-1.242116	0.218495	-0.309509
12835	O	2.393591	-1.558529	1.443012
12836	H	3.248260	-2.005318	1.598473
12837	H	2.540582	-0.605060	1.611229
12838	O	3.074374	1.114472	1.331202
12839	H	3.024815	1.146410	0.349573
12840	H	2.721497	1.967292	1.643494
12841	O	-0.507594	-2.423960	-1.350177
12842	H	-0.476008	-2.437106	-0.368033
12843	H	-1.265052	-2.981953	-1.606789
12844	O	-4.081356	0.529369	1.327900
12845	H	-4.500018	-0.299201	1.627545
12846	H	-4.156303	0.539442	0.347539
12847	O	-0.723285	3.016482	1.311366
12848	H	0.136695	3.362890	1.612186
12849	H	-0.702352	3.049743	0.329745
12850	O	2.146557	-1.621165	-1.314552
12851	H	1.306189	-2.008331	-1.618423
12852	H	2.128227	-1.655494	-0.333061
12853	O	-0.890469	2.898602	-1.448586
12854	H	-0.927588	1.933729	-1.610182
12855	H	-1.780442	3.240597	-1.654907
12856	O	-3.956752	0.646475	-1.409912
12857	H	-4.077151	1.582020	-1.651947
12858	H	-2.994935	0.462668	-1.512895
12859	O	-4.915950	-2.103286	1.589854
12860	H	-5.556152	-2.539490	2.160204
12861	H	-4.082200	-2.653552	1.597628
12862	O	1.842113	3.453827	-1.152673
12863	H	2.265948	2.622648	-1.437312
12864	H	0.919821	3.418745	-1.461810
12865	O	-2.946409	-3.755052	-1.476300
12866	H	-3.242342	-4.517141	-1.983635
12867	H	-3.685603	-3.083028	-1.487287
12868	O	-3.638515	3.433049	-1.417738
12869	H	-3.655688	3.453814	-0.419570
12870	H	-4.145903	4.185797	-1.736627
12871	O	4.982383	-2.540871	1.293705
12872	H	5.407809	-3.332984	1.635120
12873	H	4.977174	-2.591089	0.292975
12874	O	1.971624	3.701123	1.447177
12875	H	1.982002	3.711472	0.446652
12876	H	2.420349	4.494320	1.755472
12877	O	5.771597	0.264314	-1.438318
12878	H	5.857939	0.292952	-0.441216
12879	H	6.550608	0.676044	-1.823878
12880	O	-2.744445	-3.553982	1.337119
12881	H	-1.867867	-3.185413	1.547619
12882	H	-2.722587	-3.813228	0.398191
12883	O	-4.881469	-1.997177	-1.236110
12884	H	-4.720685	-1.070675	-1.487784
12885	H	-5.105497	-1.995513	-0.287926
12886	O	4.825883	-2.376795	-1.306073
12887	H	5.260174	-1.544166	-1.564926
12888	H	3.881309	-2.267377	-1.524473
12889	O	-3.515522	3.278541	1.207445
12890	H	-3.856220	2.420858	1.514732
12891	H	-2.584942	3.333185	1.489907
12892	O	5.694524	0.177329	1.171386
12893	H	5.604304	-0.759498	1.422303
12894	H	4.858349	0.609757	1.429896
12895				
12896	Cartesian coordinates of : W24_ 5			

12897				
12898	O	1.866808	0.232936	3.317318
12899	H	1.632061	-0.686630	3.526568
12900	H	1.046334	0.652621	3.021064
12901	O	0.971626	-2.442953	3.229269
12902	H	1.124838	-3.203640	3.797703
12903	H	1.463221	-2.586310	2.376530
12904	O	-1.332264	-1.338875	2.149593
12905	H	-0.660559	-1.827571	2.665932
12906	H	-0.990442	-0.427721	2.068478
12907	O	1.238761	3.594460	1.701319
12908	H	1.414095	3.987944	2.562611
12909	H	0.764601	2.747540	1.855505
12910	O	4.013618	0.450556	1.535906
12911	H	3.284727	0.374925	2.183360
12912	H	3.943838	1.338986	1.115599
12913	O	-4.138816	-1.040278	1.999894
12914	H	-4.332259	-1.630239	1.249776
12915	H	-3.208483	-1.192438	2.246077
12916	O	-0.231514	1.269319	1.698651
12917	H	-1.044273	1.669476	1.303503
12918	H	0.241821	0.808104	0.952098
12919	O	2.051014	-2.491611	0.839030
12920	H	2.993030	-2.392105	0.585163
12921	H	1.613982	-3.115183	0.198454
12922	O	-4.776774	1.326869	1.090532
12923	H	-5.516188	1.725607	1.559151
12924	H	-4.557255	0.458866	1.536622
12925	O	4.413074	-1.507296	-0.019119
12926	H	4.296356	-0.701389	0.597522
12927	H	5.327572	-1.797219	0.055179
12928	O	3.616920	2.824265	0.279462
12929	H	3.306886	2.565489	-0.606526
12930	H	2.848035	3.219977	0.721445
12931	O	1.018623	-0.124324	-0.133826
12932	H	0.425956	-0.510865	-0.822318
12933	H	1.473281	-0.886019	0.291123
12934	O	-1.760253	-2.705784	-0.240636
12935	H	-2.729679	-2.724852	-0.363632
12936	H	-1.588739	-2.237816	0.604560
12937	O	-2.312969	2.309309	0.352319
12938	H	-2.242979	1.864933	-0.524395
12939	H	-3.211540	2.133944	0.693974
12940	O	0.702754	-3.969524	-0.889239
12941	H	-0.235867	-3.782619	-0.718927
12942	H	0.910501	-3.626527	-1.778202
12943	O	-0.513754	4.313638	-0.396354
12944	H	-1.285255	3.841245	-0.034912
12945	H	0.161660	4.290030	0.303642
12946	O	-4.456890	-2.216934	-0.538941
12947	H	-5.160567	-2.766217	-0.897473
12948	H	-4.496162	-1.331281	-0.999079
12949	O	2.294648	1.581806	-1.874889
12950	H	1.589364	2.100570	-2.302861
12951	H	1.855198	1.046475	-1.182124
12952	O	-4.551168	0.227770	-1.494604
12953	H	-3.778285	0.638100	-1.920448
12954	H	-4.771432	0.769492	-0.715909
12955	O	-0.623574	-1.091563	-2.040966
12956	H	-0.040996	-1.579355	-2.659441
12957	H	-1.111254	-1.748318	-1.488824
12958	O	3.310644	-0.967243	-2.526394
12959	H	3.063064	-0.024045	-2.502608
12960	H	3.764007	-1.158880	-1.680213
12961	O	-1.983695	1.253949	-2.137944
12962	H	-1.412270	1.932062	-2.547099
12963	H	-1.488840	0.409164	-2.207338
12964	O	1.373977	-2.520927	-3.202205
12965	H	2.158282	-1.934353	-2.949871
12966	H	1.542625	-2.861158	-4.086170
12967	O	0.017967	3.125980	-2.678616
12968	H	-0.125138	3.648249	-1.839261
12969	H	0.073014	3.760578	-3.400477
12970				
12971	Cartesian coordinates of : W24_ 6			

12972				
12973	O	4.304585	-0.816837	-2.627082
12974	H	4.309911	-1.475392	-1.875029
12975	H	4.958709	-1.109193	-3.269238
12976	H	4.275588	0.956898	-2.123359
12977	O	4.086732	1.881792	-1.875605
12978	H	3.176211	2.063550	-2.163470
12979	O	4.300604	2.684426	0.610893
12980	H	4.303698	2.360898	-0.334577
12981	H	4.951190	3.390656	0.675011
12982	O	4.092750	0.686238	2.575087
12983	H	4.286687	1.359670	1.895504
12984	H	3.175526	0.840273	2.858065
12985	O	4.088276	-2.570511	-0.689983
12986	H	4.272914	-2.309295	0.232155
12987	H	3.172340	-2.895607	-0.706503
12988	H	4.312307	-0.886513	2.208872
12989	O	4.309323	-1.866506	2.013392
12990	H	4.967168	-2.275601	2.583917
12991	H	2.432183	-0.765422	-2.918624
12992	O	1.512650	-0.652836	-2.617072
12993	H	1.443134	0.277664	-2.301502
12994	H	1.307439	2.137403	-0.915349
12995	O	1.273045	1.952099	-1.884188
12996	H	0.393931	2.235066	-2.186042
12997	H	2.428259	2.906413	0.794387
12998	O	1.509465	2.588507	0.733886
12999	H	1.439153	1.842515	1.374685
13000	H	1.314075	-0.285449	2.288115
13001	O	1.279053	0.647506	2.607856
13002	H	0.398922	0.769846	3.001888
13003	H	2.438236	-2.149130	2.119942
13004	O	1.518815	-1.941708	1.873885
13005	H	1.447519	-2.127869	0.908762
13006	O	1.271094	-2.591866	-0.746725
13007	H	1.308157	-1.845786	-1.391335
13008	H	0.392179	-2.995376	-0.841685
13009	H	-0.397495	-0.876437	-2.985952
13010	O	-1.278525	-0.783230	-2.586360
13011	H	-1.309151	-1.414897	-1.829052
13012	H	-1.446287	0.886176	-2.134233
13013	O	-1.519491	1.852848	-1.959354
13014	H	-2.440402	2.094415	-2.166310
13015	H	-0.391972	3.018893	0.732641
13016	O	-1.273479	2.626355	0.616234
13017	H	-1.310668	2.294016	-0.312243
13018	H	-1.441184	1.407528	1.829339
13019	O	-1.504813	0.779285	2.585970
13020	H	-2.421542	0.843568	2.908960
13021	O	-1.269815	-1.846451	1.961010
13022	H	-0.389591	-2.144030	2.245908
13023	H	-1.310530	-0.878368	2.145368
13024	O	-1.515616	-2.627069	-0.620914
13025	H	-2.434256	-2.932885	-0.727160
13026	H	-1.446440	-2.288746	0.302082
13027	H	-3.176660	-0.748636	-2.880206
13028	O	-4.090115	-0.729633	-2.547961
13029	H	-4.277908	0.198104	-2.309029
13030	H	-4.980796	2.547325	-2.300037
13031	O	-4.312097	1.991475	-1.887836
13032	H	-4.312701	2.199097	-0.909567
13033	O	-4.313028	-2.639231	-0.772097
13034	H	-4.977166	-3.277877	-1.049558
13035	H	-4.312580	-1.897500	-1.442860
13036	H	-4.279153	-2.113390	0.992067
13037	O	-4.085996	-1.853516	1.912921
13038	H	-3.170585	-2.128632	2.089705
13039	O	-4.295063	0.646712	2.672092
13040	H	-4.957518	0.720171	3.366099
13041	H	-4.295590	-0.302760	2.360029
13042	H	-3.170996	2.875521	0.798835
13043	O	-4.086473	2.581246	0.654989
13044	H	-4.269315	1.906369	1.336295
13045				
13046	Cartesian coordinates of : W24_ 7			

13047				
13048	O	1.864070	-1.443770	-1.348571
13049	H	2.728767	-1.878777	-1.496413
13050	H	1.989196	-0.494703	-1.561037
13051	O	-1.720536	0.351033	-1.450210
13052	H	-2.662599	0.611976	-1.570686
13053	H	-1.161897	1.154252	-1.565120
13054	O	-1.662215	0.189218	1.226619
13055	H	-1.644544	0.176687	0.238114
13056	H	-1.420665	-0.721968	1.499936
13057	O	2.034338	1.374622	1.345599
13058	H	1.296386	1.955893	1.603483
13059	H	1.770548	0.451475	1.547758
13060	O	2.248152	1.312367	-1.404039
13061	H	3.142201	1.598714	-1.671525
13062	H	2.238877	1.370026	-0.422359
13063	O	-0.819388	-2.194655	-1.351348
13064	H	0.130763	-2.186286	-1.568014
13065	H	-1.120599	-1.274875	-1.517847
13066	O	-4.292326	1.160076	-1.359394
13067	H	-4.369481	1.203609	-0.380044
13068	H	-4.848891	0.413543	-1.648034
13069	O	1.555120	-1.340486	1.370713
13070	H	0.763101	-1.808998	1.685708
13071	H	1.556372	-1.430028	0.389860
13072	O	-0.221778	2.587517	-1.342312
13073	H	-0.192641	2.679477	-0.365130
13074	H	0.680549	2.337723	-1.618837
13075	O	-0.462816	2.587399	1.422435
13076	H	-1.161699	3.224496	1.653479
13077	H	-0.881630	1.701691	1.512401
13078	O	-1.022722	-2.447112	1.381663
13079	H	-1.859744	-2.877067	1.635823
13080	H	-0.969366	-2.508114	0.401805
13081	O	-4.131767	1.269406	1.380730
13082	H	-3.990252	2.200644	1.625883
13083	H	-3.250743	0.840589	1.474365
13084	O	-5.441301	-1.362157	-1.591935
13085	H	-6.139660	-1.741550	-2.134573
13086	H	-4.679695	-2.004568	-1.599011
13087	O	-3.684900	-3.257791	1.506590
13088	H	-4.121822	-3.960476	1.998161
13089	H	-4.302004	-2.474306	1.505495
13090	O	4.392350	-2.530470	-1.346881
13091	H	4.720575	-3.248480	-1.896775
13092	H	5.060824	-1.781635	-1.386726
13093	O	6.086531	-0.459529	1.589902
13094	H	6.755657	-0.675727	2.246473
13095	H	5.369121	-1.157331	1.638724
13096	O	4.765373	1.940722	1.122317
13097	H	3.837234	1.806455	1.390000
13098	H	5.265753	1.166335	1.444218
13099	O	-2.981508	3.853083	1.395603
13100	H	-3.291894	4.720751	1.673110
13101	H	-2.969128	3.846155	0.401517
13102	O	4.949812	1.998901	-1.463985
13103	H	4.925503	2.085877	-0.463333
13104	H	5.376581	2.783833	-1.821404
13105	O	6.072880	-0.559257	-1.217452
13106	H	5.745493	0.317899	-1.491329
13107	H	6.306897	-0.477493	-0.274303
13108	O	4.203993	-2.253089	1.454237
13109	H	3.283840	-1.980756	1.630070
13110	H	4.219161	-2.574396	0.534407
13111	O	-3.481859	-3.107584	-1.308590
13112	H	-3.491495	-3.349293	-0.364492
13113	H	-2.551119	-2.962169	-1.549528
13114	O	-5.371632	-1.247224	1.233451
13115	H	-5.142378	-0.339451	1.496133
13116	H	-5.595322	-1.217589	0.285628
13117	O	-2.868998	3.601359	-1.247746
13118	H	-1.968461	3.409664	-1.558700
13119	H	-3.446662	2.887651	-1.566519
13120				

13121 Cartesian coordinates of : W24_ 8

13122				
13123	H	5.015581	1.463922	-3.092098
13124	O	4.341377	1.233839	-2.445369
13125	H	4.336802	0.237624	-2.358823
13126	H	4.254966	2.162366	-0.864072
13127	O	4.068976	2.655371	-0.041751
13128	H	3.153108	2.973168	-0.113225
13129	H	5.015198	1.947538	2.812551
13130	O	4.341760	1.502506	2.289006
13131	H	4.336669	1.927596	1.383981
13132	H	4.256738	-0.330993	2.298174
13133	O	4.070884	-1.289632	2.316834
13134	H	3.154985	-1.385978	2.627913
13135	H	5.015577	-3.413224	0.278284
13136	O	4.342385	-2.736471	0.156758
13137	H	4.338227	-2.166028	0.978151
13138	O	4.073516	-1.360693	-2.273593
13139	H	4.258168	-1.826178	-1.435127
13140	H	3.158110	-1.582576	-2.514374
13141	H	2.459700	1.397595	-2.672913
13142	O	1.544950	1.212434	-2.395076
13143	H	1.489629	0.234481	-2.282054
13144	H	1.276293	2.101226	-0.957174
13145	O	1.249475	2.681746	-0.158646
13146	H	0.371442	3.097568	-0.149546
13147	H	2.458536	1.617693	2.547273
13148	O	1.543269	1.471761	2.248683
13149	H	1.488092	1.863446	1.345702
13150	H	1.277077	-0.217853	2.296154
13151	O	1.251272	-1.200006	2.397972
13152	H	0.373678	-1.416704	2.753755
13153	O	1.545628	-2.683947	0.149872
13154	H	2.461079	-3.015371	0.128066
13155	H	1.489872	-2.094890	0.938422
13156	O	1.253085	-1.477048	-2.239914
13157	H	0.375311	-1.676564	-2.605358
13158	H	1.278831	-1.880667	-1.338824
13159	H	-0.373160	1.416072	-2.753227
13160	O	-1.250929	1.199111	-2.397920
13161	H	-1.276366	0.217104	-2.295484
13162	H	-2.460842	3.015385	-0.128554
13163	O	-1.545508	2.683627	-0.150476
13164	H	-1.489982	2.094093	-0.938765
13165	O	-1.543610	-1.473526	-2.248179
13166	H	-2.459065	-1.619040	-2.546483
13167	H	-1.488123	-1.865338	-1.345212
13168	H	-1.276080	-2.101338	0.957562
13169	O	-1.249679	-2.682517	0.159466
13170	H	-0.371695	-3.098424	0.150150
13171	O	-1.545088	-1.212110	2.395225
13172	H	-2.460105	-1.397048	2.672489
13173	H	-1.489513	-0.234249	2.281768
13174	H	-0.375206	1.677072	2.605801
13175	O	-1.252929	1.477941	2.239966
13176	H	-1.278609	1.881709	1.338915
13177	H	-4.338177	2.166328	-0.978605
13178	O	-4.342428	2.736792	-0.157221
13179	H	-5.015751	3.413391	-0.278874
13180	O	-4.070296	1.289553	-2.316812
13181	H	-4.256226	0.330919	-2.298033
13182	H	-3.154390	1.385736	-2.627966
13183	O	-4.341689	-1.502380	-2.288912
13184	H	-5.015209	-1.947059	-2.812647
13185	H	-4.336852	-1.927626	-1.383913
13186	H	-4.255357	-2.161701	0.864115
13187	O	-4.069227	-2.654817	0.041903
13188	H	-3.153462	-2.972864	0.113665
13189	O	-4.341500	-1.233178	2.445032
13190	H	-5.015515	-1.463253	3.091956
13191	H	-4.336889	-0.237017	2.358712
13192	H	-3.158510	1.583432	2.514298
13193	O	-4.073781	1.361596	2.273047
13194	H	-4.257882	1.826889	1.434324
13195				
13196	Cartesian coordinates of : W24_ 9			

13197				
13198	O	-2.414340	1.390005	-1.852130
13199	O	-2.862177	2.099249	0.728721
13200	O	-2.258675	-2.225026	0.618967
13201	O	-2.459722	-1.323925	-1.928095
13202	O	0.372835	1.521167	-1.823806
13203	O	-0.099240	2.356109	0.739172
13204	O	0.485643	-2.023228	0.844286
13205	O	0.315240	-1.214117	-1.760378
13206	H	-2.506118	1.672158	-0.911915
13207	H	-1.016065	2.669527	0.803828
13208	H	-2.273393	-1.902436	-0.313477
13209	H	0.347294	-1.521412	-0.824636
13210	H	-1.534685	1.681014	-2.149093
13211	H	0.041238	2.071812	-0.193121
13212	H	-1.350411	-2.531854	0.789915
13213	H	-0.542908	-1.499179	-2.116013
13214	H	-3.340429	-1.608214	-2.229607
13215	H	1.272079	1.814263	-2.054342
13216	H	-3.800894	2.351246	0.763186
13217	H	1.397785	-2.345898	0.958755
13218	H	-2.468276	-0.338124	-1.921130
13219	H	0.399504	0.537143	-1.813622
13220	H	-2.779340	1.297835	1.298099
13221	H	0.399134	-1.227437	1.419203
13222	H	-3.605015	-0.198761	2.600357
13223	O	-2.692433	-0.129930	2.275138
13224	H	-2.550342	-0.905593	1.680764
13225	H	-0.786024	0.094601	2.777353
13226	O	0.104915	0.188818	2.401606
13227	H	0.049650	0.976477	1.812402
13228	O	2.934211	0.214270	2.412939
13229	H	3.013405	-0.591688	1.854936
13230	H	2.064659	0.164632	2.841619
13231	H	4.148913	-2.284075	0.949530
13232	O	3.239019	-1.974569	0.793266
13233	H	3.226120	-1.614398	-0.125392
13234	O	3.079509	-0.942340	-1.706080
13235	H	3.062395	0.046218	-1.635845
13236	H	2.218075	-1.210269	-2.067310
13237	O	3.141959	1.740313	-1.533767
13238	H	2.983981	2.063460	-0.604780
13239	H	4.087181	1.906425	-1.695176
13240	H	2.750735	1.725481	1.503509
13241	O	2.678167	2.524749	0.941926
13242	H	1.761630	2.829178	1.035396
13243	H	-5.542538	1.614019	-0.453933
13244	O	-5.664585	1.956807	0.486611
13245	H	-6.354233	2.627768	0.460942
13246	H	-6.236019	-0.174592	2.860802
13247	O	-5.523110	-0.139367	2.215192
13248	H	-5.680402	0.647038	1.642619
13249	O	-5.042163	-2.367478	0.520107
13250	H	-5.273566	-1.645245	1.131242
13251	H	-4.115352	-2.600498	0.704880
13252	O	-5.226100	-1.707507	-2.009232
13253	H	-5.238017	-2.007693	-1.056117
13254	H	-5.851094	-2.249704	-2.500059
13255	O	-5.199797	1.076017	-1.898048
13256	H	-4.296145	1.306812	-2.175293
13257	H	-5.296895	0.110811	-2.018569
13258	H	4.930111	-1.274028	-1.976691
13259	O	5.864925	-1.112353	-1.758876
13260	H	6.034995	-1.587220	-0.925533
13261	O	6.013869	-1.945319	0.926718
13262	H	6.729815	-2.360344	1.416715
13263	H	5.943317	-0.996435	1.225985
13264	O	5.624739	0.590520	1.494995
13265	H	5.617181	1.112807	0.671826
13266	H	4.801409	0.758778	1.978165
13267	H	6.698310	1.924599	-1.461037
13268	O	5.896847	1.466630	-1.189976
13269	H	5.982942	0.515052	-1.473377
13270				
13271	Cartesian coordinates of : W24_10			

13272				
13273	O	-0.905031	4.797245	-0.819622
13274	H	-1.085249	5.636062	-1.255363
13275	H	-0.940592	4.088172	-1.522721
13276	O	1.586369	-2.665586	-0.684463
13277	H	2.448937	-2.632396	-1.150519
13278	H	1.734228	-2.344695	0.234029
13279	O	-2.545093	-2.550660	1.581527
13280	H	-1.931864	-3.079596	2.122001
13281	H	-2.488494	-2.892616	0.663462
13282	O	4.062149	-2.250364	-1.719596
13283	H	4.563469	-2.785150	-2.342393
13284	H	4.007253	-1.311164	-2.079325
13285	O	-0.057562	3.129166	3.075777
13286	H	0.300803	2.218141	2.941689
13287	H	-0.057454	3.307657	4.021248
13288	O	-4.692143	-0.884544	0.658232
13289	H	-4.332991	0.018113	0.748111
13290	H	-4.168374	-1.461677	1.236886
13291	O	-2.286839	3.708601	1.360090
13292	H	-1.863478	4.223045	0.648460
13293	H	-1.599338	3.517891	2.021583
13294	O	0.878054	0.719003	2.254286
13295	H	0.038063	0.407487	1.839133
13296	H	1.409567	1.119330	1.526706
13297	O	-4.502160	-1.474764	-1.894547
13298	H	-4.673311	-1.271187	-0.931792
13299	H	-5.352066	-1.637747	-2.315457
13300	O	-0.410730	-1.017092	-1.338102
13301	H	-0.653013	-0.705652	-0.426289
13302	H	0.359269	-1.628163	-1.224554
13303	O	-0.193970	-3.867037	2.447345
13304	H	-0.069577	-4.588763	3.072305
13305	H	-0.197542	-4.264892	1.532341
13306	O	1.802055	-1.906213	1.937089
13307	H	1.183492	-2.548201	2.334562
13308	H	1.512114	-1.008111	2.202337
13309	O	-1.296823	-0.230425	1.047830
13310	H	-2.015479	0.433042	0.854409
13311	H	-1.740139	-1.047228	1.377382
13312	O	1.217715	1.170980	-2.126793
13313	H	0.673564	0.383236	-1.940001
13314	H	1.514792	1.502680	-1.248054
13315	O	-2.589928	0.569307	-2.237856
13316	H	-3.347634	-0.031659	-2.366314
13317	H	-1.816817	-0.012912	-2.145011
13318	O	3.873407	0.231855	-2.406961
13319	H	2.962077	0.568374	-2.512057
13320	H	4.262827	0.708492	-1.652192
13321	O	-3.200428	1.439062	0.365861
13322	H	-2.958094	2.337791	0.716904
13323	H	-3.037383	1.410416	-0.595281
13324	O	-0.246241	-4.640133	-0.067694
13325	H	0.467101	-4.106539	-0.467724
13326	H	-1.056270	-4.415777	-0.554207
13327	O	4.779626	1.044203	0.145466
13328	H	5.624705	1.410481	0.423103
13329	H	4.694599	0.136143	0.545611
13330	O	1.277235	4.375867	0.904457
13331	H	0.581596	4.640308	0.273960
13332	H	0.836914	4.185173	1.750044
13333	O	-0.936364	2.895030	-2.628029
13334	H	-1.670209	2.262666	-2.687470
13335	H	-0.119471	2.357551	-2.596020
13336	O	-2.330965	-3.044786	-1.128956
13337	H	-1.697815	-2.337513	-1.364873
13338	H	-3.170669	-2.785679	-1.550364
13339	O	2.209543	2.004032	0.263146
13340	H	3.177354	1.879713	0.300312
13341	H	1.977981	2.952114	0.460098
13342	O	4.458493	-1.447885	0.950734
13343	H	4.438627	-1.937541	0.109314
13344	H	3.671048	-1.708113	1.458223

13345

13346 Cartesian coordinates of : W24_11

13347				
13348	O	-1.908924	-1.376475	-1.332559
13349	H	-1.896908	-0.407426	-1.510666
13350	H	-2.772011	-1.694923	-1.668876
13351	O	1.692993	0.347814	-1.457274
13352	H	2.644470	0.564855	-1.582191
13353	H	1.169251	1.172737	-1.594726
13354	O	-1.679213	-1.280085	1.363700
13355	H	-1.774110	-1.407382	0.386829
13356	H	-0.876480	-1.766176	1.627278
13357	O	-2.129738	1.363959	-1.474273
13358	H	-3.046087	1.374026	-1.841954
13359	H	-2.218752	1.495434	-0.508878
13360	O	1.591419	0.223552	1.218538
13361	H	1.587295	0.199635	0.229205
13362	H	1.326076	-0.675600	1.501892
13363	O	0.748400	-2.180672	-1.324710
13364	H	1.071951	-1.270738	-1.505137
13365	H	-0.201746	-2.151775	-1.543497
13366	O	0.868789	-2.406067	1.395286
13367	H	0.855590	-2.462908	0.411982
13368	H	1.684548	-2.855591	1.682590
13369	O	0.308146	2.649632	-1.430475
13370	H	-0.593577	2.405794	-1.717147
13371	H	0.261589	2.772049	-0.458699
13372	O	4.306810	1.036992	-1.367057
13373	H	4.831382	0.257719	-1.627082
13374	H	4.370869	1.105008	-0.388767
13375	O	-1.973349	1.499658	1.302428
13376	H	-1.246364	2.103874	1.534538
13377	H	-1.664872	0.586425	1.468353
13378	O	0.533202	2.702264	1.349458
13379	H	1.257560	3.318306	1.556562
13380	H	0.913398	1.804448	1.465140
13381	O	4.104185	1.226489	1.370340
13382	H	3.209457	0.831069	1.468348
13383	H	3.993395	2.172287	1.574201
13384	O	3.509936	-3.278498	1.580280
13385	H	3.924086	-3.971893	2.103360
13386	H	4.144517	-2.509102	1.567360
13387	O	5.374992	-1.529276	-1.527518
13388	H	4.597744	-2.153261	-1.531376
13389	H	6.067444	-1.930255	-2.061842
13390	O	3.105068	3.854889	1.282597
13391	H	3.474665	4.707284	1.533108
13392	H	3.092480	3.818088	0.288096
13393	O	-6.295573	1.129981	0.027789
13394	H	-7.091639	1.656652	0.147298
13395	H	-5.693014	1.300955	0.806142
13396	O	-4.499960	-1.914380	-2.104087
13397	H	-4.848966	-2.611079	-2.668214
13398	H	-5.029902	-1.908245	-1.255470
13399	O	-5.833641	-1.628926	0.116492
13400	H	-6.194617	-0.722701	0.098915
13401	H	-5.296519	-1.692987	0.926489
13402	O	-4.654534	1.270687	2.055795
13403	H	-3.743573	1.554925	1.854068
13404	H	-4.564750	0.359844	2.386186
13405	O	-4.143467	-1.499887	2.394314
13406	H	-4.227754	-2.081469	3.156346
13407	H	-3.201086	-1.529003	2.096957
13408	O	5.255367	-1.330691	1.284496
13409	H	5.495722	-1.338802	0.340252
13410	H	5.059007	-0.407169	1.517246
13411	O	3.362708	-3.211911	-1.241581
13412	H	2.442095	-3.028205	-1.495612
13413	H	3.350863	-3.432023	-0.292533
13414	O	2.989588	3.535733	-1.346381
13415	H	3.536002	2.788816	-1.643223
13416	H	2.082217	3.377322	-1.657145
13417	O	-4.665484	0.943156	-2.280651
13418	H	-5.306431	1.110933	-1.566857
13419	H	-4.696267	-0.013259	-2.448411
13420				
13421	Cartesian coordinates of : W24_12			

13422				
13423	O	-1.071276	-0.208322	0.349468
13424	H	-1.848779	-0.749925	0.074925
13425	H	-0.598371	0.128601	-0.444374
13426	O	-3.425766	-1.468035	0.087899
13427	H	-3.352319	-2.319798	-0.378194
13428	H	-3.958063	-0.836784	-0.457057
13429	O	2.357107	2.339060	-0.335926
13430	H	2.350229	1.926979	0.551775
13431	H	3.237232	2.124359	-0.733353
13432	O	0.359354	1.081823	-1.545641
13433	H	1.110565	1.568527	-1.121685
13434	H	-0.344458	1.736036	-1.719794
13435	O	0.720139	-1.016289	2.109701
13436	H	-0.016504	-0.774989	1.491350
13437	H	0.323614	-1.627593	2.756741
13438	O	2.168100	1.261464	2.228635
13439	H	1.586546	1.979415	2.540803
13440	H	1.647839	0.429457	2.304479
13441	O	1.831434	-2.514912	0.111537
13442	H	1.576114	-1.948187	0.869444
13443	H	2.814598	-2.545040	0.129074
13444	O	1.485911	-1.277231	-2.305293
13445	H	1.140563	-0.375116	-2.143777
13446	H	1.518769	-1.722491	-1.425110
13447	O	-2.055137	1.542969	2.087162
13448	H	-1.361620	2.138240	2.428680
13449	H	-1.608726	0.970169	1.413333
13450	O	-1.754571	2.892238	-1.729264
13451	H	-2.126259	2.406653	-2.487530
13452	H	-2.434570	2.853505	-1.028397
13453	O	-2.650448	0.785106	-3.342329
13454	H	-2.850108	0.696710	-4.279516
13455	H	-2.132059	-0.021428	-3.084993
13456	O	-2.331447	-3.630610	-1.198168
13457	H	-2.601234	-4.482266	-1.554287
13458	H	-1.630684	-3.802537	-0.500046
13459	O	-1.352471	-1.394543	-2.550671
13460	H	-1.737664	-2.220490	-2.201149
13461	H	-0.397321	-1.543738	-2.657987
13462	O	-1.068068	-2.812654	3.169633
13463	H	-1.841474	-2.179992	3.099842
13464	H	-1.213932	-3.369825	3.940119
13465	O	0.159576	3.242147	2.476881
13466	H	0.144637	3.612264	1.549767
13467	H	0.192038	3.996012	3.075009
13468	O	-0.513347	-3.968077	0.626671
13469	H	-0.718261	-3.634183	1.519742
13470	H	0.378834	-3.647389	0.397379
13471	O	-3.658957	2.681302	0.313218
13472	H	-4.178232	3.427698	0.627846
13473	H	-3.140258	2.321650	1.081120
13474	O	-2.997649	-1.096178	2.799398
13475	H	-2.746983	-0.157950	2.836693
13476	H	-3.323855	-1.253059	1.890476
13477	O	4.136605	-0.961548	-2.561455
13478	H	4.504915	-1.233055	-3.407694
13479	H	3.154600	-1.095855	-2.602238
13480	O	0.271358	4.112099	-0.014752
13481	H	1.117463	3.723442	-0.305536
13482	H	-0.388863	3.890988	-0.691513
13483	O	4.728702	0.448719	1.552224
13484	H	3.893641	0.796774	1.927626
13485	H	5.392759	0.506867	2.246588
13486	O	-4.570516	0.514683	-1.280991
13487	H	-4.041321	0.659831	-2.084973
13488	H	-4.430156	1.294129	-0.716612
13489	O	4.733124	1.421593	-1.150203
13490	H	4.610242	0.650516	-1.732461
13491	H	5.021378	1.083414	-0.287657
13492	O	4.507765	-2.026103	0.046970
13493	H	4.601804	-1.727260	-0.873437
13494	H	4.627492	-1.242870	0.608938
13495				
13496	Cartesian coordinates of : W24_13			

13497				
13498	O	2.323226	1.468113	1.775800
13499	O	2.820049	2.079247	-0.817749
13500	O	2.291753	-2.232747	-0.506501
13501	O	2.471951	-1.233022	1.993525
13502	O	-0.467898	1.654015	1.716862
13503	O	0.045166	2.314035	-0.874163
13504	O	-0.466067	-2.052842	-0.687187
13505	O	-0.309687	-1.056017	1.849531
13506	H	2.401969	1.718266	0.825438
13507	H	0.958055	2.636209	-0.950782
13508	H	2.273324	-1.876258	0.414301
13509	H	-0.295045	-0.070281	1.821220
13510	H	1.442343	1.754696	2.072365
13511	H	0.011745	1.497326	-1.426011
13512	H	1.390794	-2.548774	-0.695957
13513	H	0.541526	-1.338846	2.222169
13514	H	3.348802	-1.493099	2.325558
13515	H	-1.365082	1.904436	1.996962
13516	H	3.746646	2.365252	-0.871319
13517	H	-1.373632	-2.358505	-0.865830
13518	H	2.476771	-0.248978	1.932622
13519	H	-0.379814	1.921375	0.772167
13520	H	2.786247	1.243698	-1.344135
13521	H	-0.477957	-1.696415	0.231275
13522	H	3.728920	-0.317694	-2.544464
13523	O	2.811915	-0.223884	-2.236453
13524	H	2.656599	-0.970177	-1.607955
13525	H	0.900304	-0.047910	-2.746267
13526	O	0.005873	0.037342	-2.377785
13527	H	-0.118518	-0.735304	-1.778370
13528	O	-2.831276	0.260516	-2.380089
13529	H	-2.906048	-0.558634	-1.839866
13530	H	-1.962051	0.225693	-2.809968
13531	H	-4.111876	-2.287376	-0.977912
13532	O	-3.217773	-1.937954	-0.814777
13533	H	-3.236330	-1.568641	0.100830
13534	O	-3.092731	-0.902828	1.678982
13535	H	-3.093935	0.087824	1.626558
13536	H	-2.233858	-1.163702	2.050875
13537	O	-3.263782	1.770312	1.546061
13538	H	-3.098270	2.106110	0.621106
13539	H	-4.217361	1.900318	1.681784
13540	H	-2.794716	1.777533	-1.456250
13541	O	-2.736024	2.579806	-0.896140
13542	H	-1.818398	2.881932	-0.984918
13543	H	6.386187	2.472936	-0.986645
13544	O	5.640849	1.899011	-0.783391
13545	H	5.745692	1.075510	-1.315035
13546	H	6.301007	-0.765669	-2.749962
13547	O	5.632505	-0.463590	-2.126793
13548	H	5.489307	-1.203205	-1.456013
13549	O	5.089029	-2.320455	-0.418961
13550	H	5.227043	-2.095191	0.522313
13551	H	4.158992	-2.593489	-0.507786
13552	O	5.255179	-1.427447	2.219206
13553	H	5.298887	-0.432496	2.142682
13554	H	5.893498	-1.703481	2.883900
13555	O	5.116603	1.166844	1.906741
13556	H	5.336401	1.468268	1.006494
13557	H	4.213362	1.475810	2.093415
13558	H	-5.807671	1.253268	0.007888
13559	O	-5.996072	1.487796	0.952841
13560	H	-6.732903	2.106382	0.946131
13561	H	-6.071566	-0.280688	1.590683
13562	O	-5.873943	-1.233698	1.650410
13563	H	-4.939504	-1.284170	1.919731
13564	O	-5.986940	-2.152537	-0.800738
13565	H	-6.047563	-1.894522	0.162484
13566	H	-6.693922	-2.774749	-0.994337
13567	O	-5.564546	0.544679	-1.512300
13568	H	-4.755348	0.646533	-2.036001
13569	H	-5.761908	-0.408685	-1.480630
13570				

13571 Cartesian coordinates of : W24_14

13572				
13573	O	-4.406434	0.296269	1.844086
13574	H	-4.839535	0.551343	1.008079
13575	H	-3.674163	0.924176	1.980084
13576	O	3.626561	-1.227070	0.181140
13577	H	3.740504	-2.180645	0.349814
13578	H	3.011739	-1.132876	-0.577868
13579	O	1.178942	2.774729	-1.705316
13580	H	1.992183	2.550659	-2.191252
13581	H	1.458968	3.074913	-0.799446
13582	O	3.133857	-3.870730	0.763166
13583	H	3.620599	-4.636554	1.082184
13584	H	2.460656	-3.616322	1.461129
13585	O	-4.310959	-1.758599	-1.136781
13586	H	-4.125857	-2.111526	-0.249582
13587	H	-3.454470	-1.728596	-1.619562
13588	O	3.457588	2.112071	2.240026
13589	H	2.986016	1.255001	2.419214
13590	H	3.920502	2.374019	3.041615
13591	O	-5.215045	0.621546	-0.821914
13592	H	-4.943395	-0.330837	-1.019157
13593	H	-6.070518	0.787305	-1.228751
13594	O	-1.885279	-1.718759	-2.374253
13595	H	-1.289737	-0.960188	-2.298214
13596	H	-1.395802	-2.503479	-2.067353
13597	O	-1.241706	4.172293	-1.262286
13598	H	-0.416962	3.879746	-1.686481
13599	H	-1.898222	3.465820	-1.406947
13600	O	2.209682	-0.216993	2.277696
13601	H	1.322759	-0.056671	1.880122
13602	H	2.745120	-0.596050	1.544065
13603	O	3.523239	1.499959	-2.553950
13604	H	4.160280	1.701026	-3.246577
13605	H	4.012973	1.512093	-1.683226
13606	O	2.040415	-0.801094	-2.029191
13607	H	2.549836	-0.071348	-2.436422
13608	H	1.135796	-0.463570	-1.914802
13609	O	-0.386163	0.660628	-1.530742
13610	H	-1.308603	1.006201	-1.482952
13611	H	0.193649	1.466115	-1.633944
13612	O	-0.224390	-0.087531	1.082721
13613	H	-0.201076	0.162014	0.130519
13614	H	-0.569310	-1.009232	1.112842
13615	O	-0.923211	4.354254	1.335032
13616	H	-1.077179	4.380827	0.346640
13617	H	-1.190636	5.206113	1.693846
13618	O	1.408944	-2.979506	2.508265
13619	H	1.654538	-2.063923	2.728148
13620	H	0.481206	-2.955549	2.205798
13621	O	-2.761397	1.857476	-1.006490
13622	H	-3.666563	1.521704	-1.158526
13623	H	-2.634597	1.865962	-0.031186
13624	O	4.695402	1.303888	-0.210202
13625	H	4.609289	0.358402	0.005304
13626	H	4.371308	1.775371	0.577195
13627	O	-0.634194	-3.923860	-1.207080
13628	H	0.344252	-3.879724	-1.424743
13629	H	-0.956744	-4.788395	-1.480508
13630	O	-3.762985	-2.222123	1.624248
13631	H	-3.985000	-1.256964	1.785506
13632	H	-4.317262	-2.741029	2.215759
13633	O	-2.094454	1.852916	1.648965
13634	H	-1.366990	1.196286	1.630240
13635	H	-1.703413	2.737658	1.780972
13636	O	1.720924	3.674594	0.720570
13637	H	0.898702	3.943614	1.165173
13638	H	2.288715	3.206766	1.357953
13639	O	-1.077338	-2.675170	1.236581
13640	H	-1.004325	-3.177040	0.399544
13641	H	-2.028768	-2.614453	1.463906
13642	O	1.888738	-3.638011	-1.722461
13643	H	2.409239	-3.783928	-0.909500
13644	H	2.064380	-2.733651	-2.033303
13645				
13646				

13647 Cartesian coordinates of the water 26-mer

13648

13649 Cartesian coordinates of : W25_ 1

13650

13651	O	-4.284499	1.775776	-1.463403
13652	H	-3.363596	2.047521	-1.638185
13653	H	-4.442214	1.973246	-0.522726
13654	O	-4.849607	-0.755145	-1.738426
13655	H	-5.554650	-0.911103	-2.373942
13656	H	-4.648274	0.226506	-1.734008
13657	O	-2.338917	-1.870117	-1.363954
13658	H	-2.386210	-1.877724	-0.381225
13659	H	-3.229534	-1.624791	-1.679034
13660	O	-0.536562	-0.230267	2.151112
13661	H	-0.002038	-0.316223	2.958481
13662	H	0.101943	-0.390018	1.406914
13663	O	-1.543693	2.311326	-1.371384
13664	H	-1.534035	2.236472	-0.390680
13665	H	-0.982922	3.080096	-1.593133
13666	O	0.059830	4.285689	1.271265
13667	H	-0.616377	3.605705	1.454015
13668	H	0.004063	4.485945	0.319223
13669	O	2.546081	3.624182	1.636266
13670	H	1.580234	3.893322	1.583945
13671	H	3.009284	4.291405	2.151481
13672	O	-0.597466	-4.180825	1.452352
13673	H	-0.675455	-5.063907	1.827122
13674	H	0.239249	-3.773291	1.834177
13675	O	4.728542	-0.467446	0.088120
13676	H	4.510699	0.043780	-0.714218
13677	H	4.360658	0.053871	0.821085
13678	O	-1.711842	2.124797	1.362154
13679	H	-1.302418	1.315104	1.736209
13680	H	-2.675951	2.054939	1.513119
13681	O	-0.394217	-3.889348	-1.346545
13682	H	-0.444301	-4.060839	-0.386767
13683	H	-1.128759	-3.284701	-1.554800
13684	O	2.001080	-0.767732	-3.173912
13685	H	2.055309	-1.721189	-2.975039
13686	H	1.083926	-0.499531	-2.972471
13687	O	1.773705	-0.643979	3.655127
13688	H	2.185746	-0.625423	4.524177
13689	H	2.277252	-0.026095	3.066109
13690	O	-4.860132	-0.837624	1.075846
13691	H	-4.100857	-1.399800	1.318200
13692	H	-5.017632	-0.978769	0.124498
13693	O	3.721443	0.889357	-2.151610
13694	H	4.319456	1.119002	-2.871004
13695	H	3.061556	0.234734	-2.533492
13696	O	-4.454154	1.722657	1.361205
13697	H	-5.103318	2.120525	1.949530
13698	H	-4.631560	0.735788	1.336019
13699	O	1.972402	-3.458944	-2.356963
13700	H	1.055658	-3.642176	-1.998189
13701	H	2.192396	-4.180167	-2.954405
13702	O	2.959493	-2.470213	0.016001
13703	H	2.881943	-2.946055	-0.830860
13704	H	3.744424	-1.868139	-0.005600
13705	O	0.318331	4.344102	-1.531299
13706	H	0.379542	5.095718	-2.128401
13707	H	1.222116	3.914792	-1.491266
13708	O	-2.380794	-2.072895	1.366954
13709	H	-1.939336	-2.933057	1.509450
13710	H	-1.774561	-1.408862	1.762432
13711	O	2.856364	0.897669	1.758704
13712	H	2.237707	0.629900	1.044512
13713	H	2.792952	1.871422	1.838229
13714	O	2.664098	3.278202	-1.164807
13715	H	2.858115	3.354851	-0.214919
13716	H	2.987035	2.412132	-1.483697
13717	O	-0.409873	-0.074363	-2.032699
13718	H	-1.136605	-0.719290	-1.879867
13719	H	-0.806966	0.818082	-1.927711
13720	O	1.160330	-0.444208	0.121704
13721	H	1.718698	-1.245545	-0.007887

13722	H	0.645631	-0.286507	-0.706688
13723	O	1.616397	-3.151325	2.313767
13724	H	2.208129	-3.013137	1.546613
13725	H	1.653138	-2.333129	2.840089
13726				
13727	Cartesian coordinates of : W25_ 2			
13728				
13729	O	-1.537063	2.438712	-2.728031
13730	H	-2.464507	2.163361	-2.620859
13731	H	-1.029420	1.610036	-2.841657
13732	O	-4.523471	-0.671428	1.975029
13733	H	-5.392317	-1.017411	2.197228
13734	H	-4.062627	-1.322845	1.387132
13735	O	-2.931440	-2.003662	0.327245
13736	H	-2.195174	-1.344861	0.287781
13737	H	-2.510858	-2.848403	0.587538
13738	O	-1.200330	-3.975447	1.099420
13739	H	-0.768929	-3.402736	1.809277
13740	H	-1.276198	-4.868837	1.447513
13741	O	1.866948	2.414455	-0.172645
13742	H	1.438311	1.916393	0.564200
13743	H	1.198739	3.058601	-0.476595
13744	O	-1.918611	-0.181027	2.827249
13745	H	-2.874264	-0.317234	2.914790
13746	H	-1.695548	0.671138	3.241213
13747	O	-3.623271	-1.489791	-2.328313
13748	H	-3.812021	-0.534645	-2.359436
13749	H	-3.536779	-1.734071	-1.386175
13750	O	-1.214524	0.034768	-0.038022
13751	H	-0.555034	0.267399	0.654355
13752	H	-0.772543	0.057554	-0.913931
13753	O	-0.393991	3.900738	-0.902759
13754	H	-0.859348	3.353720	-1.605725
13755	H	-0.344164	4.799627	-1.244220
13756	O	0.232539	-3.435050	-1.269642
13757	H	-0.375439	-3.108940	-1.955347
13758	H	-0.297928	-3.697713	-0.496138
13759	O	-0.156570	0.063649	-2.598646
13760	H	-0.433010	-0.771202	-3.026397
13761	H	0.818635	0.132162	-2.619160
13762	O	4.884108	-0.367935	1.885166
13763	H	5.635075	-0.505394	2.470709
13764	H	5.045626	-0.904231	1.052665
13765	O	4.615789	1.962645	0.299568
13766	H	4.640756	1.295041	1.009894
13767	H	3.708027	2.312158	0.248765
13768	O	2.298248	-1.901039	-0.551654
13769	H	1.560993	-2.491265	-0.852020
13770	H	2.237360	-1.064938	-1.058102
13771	O	-0.854627	2.303570	3.445443
13772	H	-0.735587	2.853927	4.224435
13773	H	-1.243109	2.868403	2.711991
13774	O	-1.925944	3.537574	1.432833
13775	H	-1.355280	3.723000	0.661908
13776	H	-2.619324	2.931834	1.111331
13777	O	-3.470147	1.418049	0.412055
13778	H	-2.614041	0.933927	0.283105
13779	H	-3.992278	0.864648	1.022534
13780	O	2.235935	-1.245285	2.033088
13781	H	2.254522	-1.551135	1.088103
13782	H	3.157873	-1.015482	2.252417
13783	O	2.433632	0.473831	-1.956027
13784	H	2.259940	1.233808	-1.349237
13785	H	3.362289	0.546371	-2.240374
13786	O	0.721002	0.890364	1.700237
13787	H	0.358597	1.326828	2.493657
13788	H	1.312326	0.136696	1.954019
13789	O	5.205069	0.703593	-1.918926
13790	H	5.083973	1.265863	-1.101649
13791	H	5.901644	1.093253	-2.455077
13792	O	5.057597	-1.647191	-0.378654
13793	H	4.160505	-1.994115	-0.546763
13794	H	5.229423	-0.984388	-1.071608
13795	O	-0.215877	-2.361904	2.848963
13796	H	-0.783593	-1.565878	2.912594

13797	H	0.700260	-2.059954	2.717764
13798	O	-4.082131	1.327450	-2.152784
13799	H	-4.917758	1.708007	-2.440697
13800	H	-4.018113	1.432170	-1.167727
13801	O	-1.354716	-2.277864	-3.326551
13802	H	-1.446362	-2.747121	-4.161126
13803	H	-2.268536	-1.997331	-3.026030
13804				
13805	Cartesian coordinates of : W25_ 3			
13806				
13807	O	-2.612582	-2.291647	0.318369
13808	O	-2.888750	-0.994160	-2.051599
13809	O	-2.609175	2.011510	1.132223
13810	O	-2.808001	-0.427030	2.283513
13811	O	0.160735	-2.281390	0.392683
13812	O	-0.100683	-1.096675	-2.053693
13813	O	0.162128	2.095001	1.002137
13814	O	-0.025255	-0.312779	2.278883
13815	H	-2.648285	-1.833481	-0.553870
13816	H	-0.987501	-1.300911	-2.393392
13817	H	-2.623981	1.124067	1.564914
13818	H	0.015518	0.565449	1.833622
13819	H	-1.724682	-2.684062	0.387713
13820	H	-0.031602	-1.537563	-1.174931
13821	H	-1.722096	2.379890	1.288605
13822	H	-0.909687	-0.379470	2.675926
13823	H	-3.711534	-0.464097	2.644108
13824	H	1.062927	-2.647580	0.414201
13825	H	-3.804660	-1.184123	-2.318061
13826	H	1.063320	2.420898	1.175119
13827	H	-2.760623	-1.115599	1.579511
13828	H	0.133937	-1.578688	1.082567
13829	H	-2.867348	-0.024291	-1.872927
13830	H	0.106583	1.934916	0.031508
13831	H	-3.815581	1.923971	-1.768979
13832	O	-2.906194	1.675806	-1.533912
13833	H	-2.818683	1.814383	-0.560159
13834	H	-1.006627	1.905365	-1.926413
13835	O	-0.114617	1.614761	-1.673602
13836	H	-0.100700	0.641281	-1.825425
13837	O	2.675001	1.707031	-1.620558
13838	H	2.729392	1.835392	-0.644589
13839	H	1.790702	2.005015	-1.889622
13840	H	3.853364	2.340819	1.172564
13841	O	2.934273	2.029834	1.069709
13842	H	2.902999	1.139387	1.491489
13843	O	2.756299	-0.430450	2.206011
13844	H	2.775393	-1.110789	1.490767
13845	H	1.880435	-0.490063	2.622045
13846	O	2.926881	-2.271192	0.225994
13847	H	2.883017	-1.805276	-0.643294
13848	H	3.840491	-2.601903	0.313484
13849	H	2.706054	0.000895	-1.970493
13850	O	2.697587	-0.970575	-2.137473
13851	H	1.811971	-1.168137	-2.484450
13852	H	-5.644133	-1.544896	-1.032615
13853	O	-5.706725	-1.129650	-1.949728
13854	H	-6.352316	-1.639691	-2.449493
13855	H	-6.417076	2.025701	-2.156898
13856	O	-5.720859	1.575546	-1.668010
13857	H	-5.818854	0.608407	-1.831832
13858	O	-5.404875	1.965829	1.131861
13859	H	-5.590171	1.893007	0.178582
13860	H	-4.490984	2.289271	1.216010
13861	O	-5.594652	-0.299696	2.435565
13862	H	-5.604204	0.585176	1.971473
13863	H	-6.263110	-0.279424	3.127266
13864	O	-5.403474	-2.181339	0.390865
13865	H	-4.494766	-2.516266	0.486344
13866	H	-5.567811	-1.590109	1.151762
13867	H	4.657953	-0.358603	2.488123
13868	O	5.562209	-0.366907	2.132618
13869	H	5.716188	0.520236	1.751814
13870	O	5.696170	2.147151	0.916218
13871	H	6.394145	2.783907	1.097607

13872	H	5.687297	1.972944	-0.078996
13873	O	5.498109	1.641345	-1.602432
13874	H	5.615735	0.685424	-1.809567
13875	H	4.600689	1.863362	-1.899266
13876	H	4.627653	-1.249546	-2.363673
13877	O	5.531379	-1.046943	-2.074892
13878	H	5.683551	-1.565604	-1.265218
13879	H	6.368047	-2.997232	0.677801
13880	O	5.688193	-2.360900	0.436899
13881	H	5.724685	-1.611612	1.098053
13882				
13883	Cartesian coordinates of : W25_4			
13884				
13885	O	-0.841850	1.847747	3.490673
13886	H	-1.767221	2.139650	3.428527
13887	H	-0.846385	0.947564	3.861748
13888	O	1.140128	-1.944758	2.606880
13889	H	0.799614	-1.614876	1.742703
13890	H	2.002135	-1.481982	2.748675
13891	O	0.523810	-4.099979	-1.389300
13892	H	0.439595	-4.981618	-1.765563
13893	H	-0.390937	-3.767105	-1.183916
13894	O	0.048023	1.503828	1.034597
13895	H	-0.317659	1.704086	1.939992
13896	H	-0.099098	2.263983	0.436468
13897	O	4.514371	-2.179008	0.407114
13898	H	5.305941	-2.723624	0.357305
13899	H	3.731825	-2.796015	0.452337
13900	O	-0.939924	-0.945614	3.845044
13901	H	-0.104629	-1.372469	3.497518
13902	H	-1.259150	-1.491613	4.570332
13903	O	-0.600686	0.179858	-2.839536
13904	H	-0.172492	1.015638	-3.110778
13905	H	-1.137955	0.383859	-2.043468
13906	O	-1.720958	-2.793728	-0.863073
13907	H	-2.009986	-2.428735	-1.739185
13908	H	-1.262673	-2.066168	-0.391409
13909	O	-4.189374	-2.165685	0.333859
13910	H	-3.410184	-2.657570	0.012295
13911	H	-3.832133	-1.561645	1.011573
13912	O	0.747188	2.570878	-3.250092
13913	H	1.715030	2.447181	-3.016788
13914	H	0.712227	3.052326	-4.082916
13915	O	3.486483	-0.133203	-1.152839
13916	H	4.071548	-0.789593	-0.726965
13917	H	2.776119	-0.665284	-1.570017
13918	O	2.845747	3.891335	-0.092954
13919	H	2.906422	3.048793	0.433386
13920	H	3.371124	4.563148	0.352257
13921	O	2.749701	1.469861	0.941605
13922	H	2.951793	0.883354	0.177171
13923	H	1.773243	1.424857	1.070393
13924	O	-2.728374	-0.259917	1.784312
13925	H	-3.073890	0.593404	2.110475
13926	H	-2.092194	-0.578630	2.455238
13927	O	0.102450	3.636428	-0.726220
13928	H	0.982018	3.975482	-0.475683
13929	H	0.192092	3.349520	-1.655543
13930	O	0.051417	-1.048208	0.309032
13931	H	0.659382	-1.143989	-0.454373
13932	H	-0.049043	-0.083075	0.494502
13933	O	-4.672993	-0.655284	-1.733199
13934	H	-5.581710	-0.375609	-1.877033
13935	H	-4.649358	-1.276481	-0.947647
13936	O	-2.596969	3.284815	0.085484
13937	H	-1.766101	3.749163	-0.103983
13938	H	-2.533672	2.429214	-0.384750
13939	O	3.534022	-0.681306	2.629854
13940	H	3.379876	0.195153	2.236051
13941	H	4.076243	-1.165816	1.983959
13942	O	-3.356529	2.400305	2.439892
13943	H	-4.190129	2.796899	2.709997
13944	H	-3.074328	2.845112	1.592551
13945	O	3.212299	2.364689	-2.439342
13946	H	3.287248	2.997242	-1.702692

13947	H	3.506010	1.499454	-2.100192
13948	O	2.378507	-3.685683	0.711753
13949	H	1.725248	-3.874668	0.013218
13950	H	1.891104	-3.355226	1.486807
13951	O	-2.399085	0.664521	-0.819840
13952	H	-3.248620	0.332237	-1.175153
13953	H	-2.303305	0.259284	0.067686
13954	O	1.337244	-1.532084	-2.069536
13955	H	0.626913	-1.028341	-2.527206
13956	H	1.161246	-2.486969	-2.141494
13957	O	-2.561803	-1.777911	-3.201215
13958	H	-1.957952	-1.053249	-3.435216
13959	H	-3.415960	-1.371434	-2.974831
13960				
13961	Cartesian coordinates of : W25_ 5			
13962				
13963	O	-2.510475	-1.969555	1.189730
13964	O	-2.843301	-1.729640	-1.488337
13965	O	-2.656657	2.269997	0.251154
13966	O	-2.832046	0.496517	2.273358
13967	O	0.272782	-1.958602	1.201335
13968	O	-0.042238	-1.773472	-1.498904
13969	O	0.128426	2.312598	0.147412
13970	O	-0.041094	0.549511	2.221515
13971	H	-2.536354	-1.895671	0.206571
13972	H	-0.922326	-2.123258	-1.714745
13973	H	-2.637071	1.632463	1.005610
13974	H	0.006024	-0.368768	1.866376
13975	H	-1.619950	-2.284500	1.422756
13976	H	-0.087908	-0.818286	-1.740880
13977	H	-1.777270	2.684732	0.217532
13978	H	-0.922578	0.648326	2.617774
13979	H	-3.731670	0.583197	2.634316
13980	H	1.172913	-2.246035	1.434589
13981	H	-3.743199	-2.045876	-1.671816
13982	H	1.023093	2.693283	0.098151
13983	H	-2.772197	-0.410734	1.891568
13984	H	0.244822	-1.903263	0.217540
13985	H	-2.875436	-0.766514	-1.704997
13986	H	0.140193	1.685987	0.908018
13987	H	-3.950404	1.042881	-2.354074
13988	O	-3.034964	0.912920	-2.054509
13989	H	-2.943712	1.421225	-1.212604
13990	H	-1.131446	1.019944	-2.487950
13991	O	-0.237882	0.872383	-2.136932
13992	H	-0.167433	1.411019	-1.314127
13993	O	2.568899	0.816669	-2.189355
13994	H	2.631125	1.376769	-1.380041
13995	H	1.679914	0.956169	-2.554501
13996	H	3.809385	2.671953	-0.001215
13997	O	2.905638	2.310252	0.051073
13998	H	2.910027	1.691335	0.819205
13999	O	2.754587	0.593825	2.145573
14000	H	2.792457	-0.334137	1.808322
14001	H	1.880680	0.706045	2.554191
14002	O	3.051838	-1.911916	1.194128
14003	H	3.012904	-1.876192	0.207849
14004	H	3.970885	-2.148930	1.418693
14005	H	2.723108	-0.849247	-1.761048
14006	O	2.759850	-1.798364	-1.491129
14007	H	1.882541	-2.151558	-1.712344
14008	H	-6.367711	-2.268667	-1.936560
14009	O	-5.677929	-1.742852	-1.519261
14010	H	-5.841953	-0.800237	-1.754821
14011	H	-6.533980	1.379208	-2.517545
14012	O	-5.857427	0.930202	-2.000787
14013	H	-5.778036	1.414302	-1.120563
14014	O	-5.462415	2.151149	0.242049
14015	H	-5.600621	1.623296	1.053351
14016	H	-4.555386	2.500378	0.286962
14017	O	-5.623519	0.435644	2.434546
14018	H	-5.603639	-0.478872	2.033001
14019	H	-6.295335	0.444466	3.123079
14020	O	-5.313034	-1.897836	1.291681
14021	H	-5.485195	-1.898222	0.332496

14022	H	-4.393331	-2.192401	1.409249
14023	H	4.690066	-2.156769	-1.578564
14024	O	5.580746	-1.857367	-1.334211
14025	H	5.636911	-0.937127	-1.683165
14026	H	5.818247	-1.922287	0.219646
14027	O	5.826837	-1.922316	1.229335
14028	H	6.539632	-2.499084	1.520027
14029	H	5.752527	-0.183169	1.784946
14030	O	5.571253	0.750375	2.012254
14031	H	4.668344	0.773605	2.370035
14032	O	5.678248	2.450978	0.020504
14033	H	5.738907	1.819140	0.792079
14034	H	6.376904	3.104770	0.118859
14035	O	5.419473	0.714835	-2.210302
14036	H	4.509909	0.854871	-2.516585
14037	H	5.577854	1.372960	-1.509980
14038				
14039	Cartesian coordinates of : W25_ 6			
14040				
14041	O	-1.087154	1.699348	-1.250037
14042	O	-0.914243	1.434230	1.481031
14043	O	1.678463	1.477300	-1.330022
14044	O	1.740191	-1.274192	-1.411025
14045	O	1.536314	-1.346230	1.329347
14046	O	1.861755	1.387105	1.411770
14047	O	-1.238795	-1.284079	1.223509
14048	O	-1.023366	-1.041357	-1.505334
14049	O	4.515313	-1.315232	-1.485310
14050	O	4.451529	1.410703	-1.233275
14051	O	4.623485	1.151480	1.485634
14052	O	4.307638	-1.554766	1.232707
14053	H	1.657356	0.506980	-1.485286
14054	H	0.798620	1.815208	-1.571497
14055	H	-0.007869	1.653316	1.758103
14056	H	-0.986554	0.454147	1.514058
14057	H	1.610418	-0.378639	1.485995
14058	H	0.624657	-1.594470	1.562023
14059	H	-1.000167	-0.059612	-1.545759
14060	H	-0.141916	-1.351374	-1.776009
14061	H	-1.069102	1.732418	-0.267391
14062	H	-1.968079	2.011485	-1.519997
14063	H	1.849191	1.544192	0.441264
14064	H	1.707175	-1.428965	-0.440540
14065	H	-1.213174	-1.319314	0.241409
14066	H	-2.150460	-1.509170	1.481816
14067	H	3.410162	-1.801330	1.513655
14068	H	4.315067	-1.589417	0.249384
14069	H	4.551345	0.171005	1.519156
14070	H	4.459275	1.442968	-0.249842
14071	H	3.581112	1.740170	-1.514831
14072	H	4.535852	-0.332581	-1.522586
14073	H	2.622842	-1.556763	-1.706702
14074	H	2.767419	1.580058	1.710476
14075	H	5.414169	-1.617152	-1.709612
14076	H	5.545599	1.367449	1.715161
14077	H	-3.923971	-0.128548	1.448366
14078	O	-4.001360	-1.098969	1.310031
14079	H	-4.882255	-1.353046	1.643387
14080	H	-3.680300	1.783680	0.419524
14081	O	-3.684067	1.623226	1.390503
14082	H	-2.792795	1.841563	1.711314
14083	H	-3.880498	-1.197936	-0.463486
14084	O	-3.801468	-1.016094	-1.426475
14085	H	-2.913002	-1.304411	-1.697704
14086	H	-3.859576	0.743490	-1.482059
14087	O	-3.857044	1.716543	-1.334170
14088	H	-4.768242	2.012248	-1.511651
14089	H	-7.325856	2.440963	-1.466001
14090	O	-6.630634	1.823486	-1.219423
14091	H	-6.652867	1.719636	-0.226665
14092	H	-5.586892	-1.074175	-2.043380
14093	O	-6.541198	-0.885651	-2.022466
14094	H	-6.628202	0.070578	-1.854367
14095	H	-5.575135	1.685339	1.660241
14096	O	-6.479548	1.464017	1.380408

14097	H	-6.650764	0.553401	1.684195
14098	H	-7.176164	-1.710460	1.259158
14099	O	-6.698707	-1.278996	2.021614
14100	H	-7.051190	-1.650120	2.836155
14101	H	-8.648981	-2.465576	-0.378796
14102	O	-7.730449	-2.298679	-0.151019
14103	H	-7.316710	-1.799154	-0.907333
14104	H	6.345442	1.454905	-1.465466
14105	O	7.238883	1.187235	-1.190295
14106	H	7.352344	0.261405	-1.472974
14107	H	7.952544	-2.202071	-1.778963
14108	O	7.277964	-1.619885	-1.416609
14109	H	7.290875	-1.707244	-0.422446
14110	O	7.399690	1.212809	1.430915
14111	H	8.117537	1.739193	1.795194
14112	H	7.423197	1.297642	0.436307
14113	H	7.302047	-0.667556	1.488999
14114	O	7.109406	-1.580183	1.206307
14115	H	6.195678	-1.769702	1.479480
14116				
14117	Cartesian coordinates of : W25_ 7			
14118				
14119	O	2.148250	-0.062835	-0.739249
14120	H	1.628400	-0.885435	-0.898891
14121	H	1.746411	0.667392	-1.256819
14122	O	-2.757064	-1.975247	0.797444
14123	H	-3.559492	-2.475593	0.559370
14124	H	-3.058343	-1.101734	1.141973
14125	O	2.524693	-2.900205	2.161819
14126	H	1.554887	-2.952615	2.142251
14127	H	2.853375	-3.324898	1.348861
14128	O	3.002828	-0.282856	1.867388
14129	H	2.697847	-0.137164	0.943529
14130	H	2.887868	-1.254712	2.031622
14131	O	2.616607	3.562669	-0.609214
14132	H	3.486116	3.074475	-0.508607
14133	H	2.812540	4.501835	-0.535808
14134	O	-0.128921	-2.159963	1.579964
14135	H	-0.037219	-1.209488	1.804708
14136	H	-1.087021	-2.324974	1.498082
14137	O	4.245214	0.266983	-2.437061
14138	H	3.869783	0.620766	-3.252666
14139	H	3.468630	0.057468	-1.868942
14140	O	-4.252199	-1.460039	-2.444915
14141	H	-3.280240	-1.410985	-2.410524
14142	H	-4.603531	-0.553722	-2.381596
14143	O	0.939632	-2.460640	-0.895665
14144	H	1.741557	-3.015873	-0.899003
14145	H	0.586212	-2.461129	0.023678
14146	O	0.339181	2.365763	0.384932
14147	H	1.151579	2.861602	0.154720
14148	H	-0.354464	2.988022	0.719991
14149	O	3.464705	-3.565883	-0.408081
14150	H	4.160107	-2.865682	-0.559194
14151	H	3.860639	-4.403219	-0.669571
14152	O	-1.805425	3.609096	1.341598
14153	H	-1.954634	3.131262	2.173818
14154	H	-2.518530	3.351615	0.731538
14155	O	5.323551	-1.731523	-0.792998
14156	H	5.511500	-1.118839	-0.057717
14157	H	5.195276	-1.174697	-1.578495
14158	O	5.503518	0.207563	1.271565
14159	H	6.154115	0.213753	1.980211
14160	H	4.606055	0.032529	1.668970
14161	O	-5.134867	-2.784589	-0.374460
14162	H	-5.578383	-3.616009	-0.566264
14163	H	-4.842278	-2.373740	-1.238876
14164	O	-1.557217	-1.407162	-1.603084
14165	H	-0.746255	-1.933109	-1.709303
14166	H	-1.915073	-1.632974	-0.714235
14167	O	-3.318824	2.141274	-0.526884
14168	H	-4.134953	1.966964	-1.032061
14169	H	-2.561096	1.883780	-1.102221
14170	O	-1.034423	1.297529	-1.719134
14171	H	-1.154823	0.323952	-1.702733

14172	H	-0.500210	1.544369	-0.934083
14173	O	-1.785850	1.650523	3.440917
14174	H	-1.833721	1.747133	4.396892
14175	H	-0.932327	1.208093	3.222323
14176	O	-6.038574	-0.305901	0.571871
14177	H	-5.898349	-1.254234	0.396805
14178	H	-5.334362	-0.031064	1.185440
14179	O	-5.543156	0.947936	-1.681684
14180	H	-5.847811	0.510981	-0.836652
14181	H	-6.317146	1.309692	-2.124062
14182	O	-3.549629	0.478839	1.599446
14183	H	-3.071170	0.838603	2.368091
14184	H	-3.402640	1.097468	0.843609
14185	O	1.607728	1.860345	-2.593033
14186	H	1.856544	2.688064	-2.146247
14187	H	0.641488	1.866798	-2.696849
14188	O	0.366920	0.493177	2.299361
14189	H	0.413700	1.131503	1.543394
14190	H	1.301737	0.329581	2.527282
14191	O	4.866809	2.244365	-0.564046
14192	H	5.166672	1.697021	0.183857
14193	H	4.823136	1.633429	-1.323993
14194				
14195	Cartesian coordinates of : W25_ 8			
14196				
14197	O	-4.017655	-0.506404	2.849948
14198	H	-3.902155	-1.363768	2.345460
14199	H	-4.631018	-0.679228	3.570866
14200	H	-4.193065	0.971875	1.803296
14201	O	-4.124116	1.741852	1.204735
14202	H	-3.233250	2.116128	1.328537
14203	O	-4.300235	1.431004	-1.557897
14204	H	-4.228603	1.349397	-0.583895
14205	H	-5.035141	2.055839	-1.664392
14206	O	-3.754709	-1.040839	-2.724287
14207	H	-4.090841	-0.192402	-2.375656
14208	H	-2.846697	-0.872174	-3.028001
14209	O	-3.497520	-2.736403	1.593727
14210	H	-3.679738	-2.859220	0.642129
14211	H	-2.553747	-2.930276	1.723552
14212	H	-3.792721	-2.330174	-1.757401
14213	O	-3.681799	-3.137765	-1.174369
14214	H	-4.248127	-3.828817	-1.531720
14215	H	-2.182150	-0.089893	3.048336
14216	O	-1.277282	0.026072	2.707200
14217	H	-1.322147	0.758070	2.049686
14218	H	-1.382548	1.969302	0.046632
14219	O	-1.366931	2.153866	1.017383
14220	H	-0.547339	2.647864	1.188202
14221	H	-2.491030	1.909915	-1.830318
14222	O	-1.544435	1.763932	-1.646993
14223	H	-1.346182	0.856377	-1.975905
14224	H	-0.897527	-1.414193	-2.032204
14225	O	-0.961108	-0.676678	-2.683979
14226	H	-0.081895	-0.592615	-3.089433
14227	H	-1.798226	-3.194433	-1.152538
14228	O	-0.918338	-2.801462	-1.006451
14229	H	-0.864413	-2.603607	-0.043615
14230	O	-0.706845	-2.412005	1.677387
14231	H	-0.862097	-1.497231	2.011272
14232	H	0.210406	-2.636789	1.906347
14233	H	0.619735	0.215314	3.103746
14234	O	1.493629	0.275694	2.683252
14235	H	1.644039	-0.585041	2.224635
14236	H	1.456410	1.662627	1.641028
14237	O	1.399386	2.499917	1.125584
14238	H	2.266587	2.933594	1.222381
14239	H	0.279337	2.425001	-1.816743
14240	O	1.196916	2.230217	-1.561633
14241	H	1.225895	2.272707	-0.576676
14242	H	1.590695	0.680072	-2.227189
14243	O	1.780098	-0.172532	-2.683102
14244	H	2.698314	-0.109874	-3.002397
14245	O	1.836406	-2.390289	-1.136673
14246	H	1.012664	-2.883499	-1.286973

14247	H	1.760772	-1.556136	-1.658458
14248	O	2.063085	-2.112169	1.552203
14249	H	3.008984	-2.219714	1.759098
14250	H	1.990762	-2.159670	0.570470
14251	H	3.339746	0.699822	2.939103
14252	O	4.260830	0.730969	2.628909
14253	H	4.333769	1.518666	2.056931
14254	H	4.705440	3.766876	1.145501
14255	O	4.144066	3.002560	0.982677
14256	H	4.168464	2.819721	-0.000484
14257	O	4.814040	-1.651812	1.696844
14258	H	5.544402	-2.034446	2.192856
14259	H	4.682908	-0.719014	2.033123
14260	H	4.790211	-1.853324	-0.130435
14261	O	4.621982	-2.001301	-1.080671
14262	H	3.759080	-2.444724	-1.143805
14263	O	4.561821	0.040005	-2.716830
14264	H	5.248785	-0.048062	-3.384936
14265	H	4.666016	-0.722127	-2.077422
14266	H	3.052614	2.638370	-1.835974
14267	O	3.988180	2.543660	-1.588818
14268	H	4.288449	1.691423	-1.958556
14269	H	-5.511750	2.859563	0.503882
14270	O	-5.990243	3.193718	-0.274051
14271	H	-6.775859	3.651450	0.035313

14272

14273 Cartesian coordinates of : W25_ 9

14274

14275	O	1.768619	0.619680	3.190123
14276	H	1.861129	-0.250039	3.612529
14277	H	2.372140	0.623778	2.421450
14278	O	1.140034	3.338752	2.546100
14279	H	1.209356	2.532171	3.077145
14280	H	0.195587	3.475572	2.291985
14281	O	1.803028	1.636000	-3.487521
14282	H	2.164956	1.862935	-4.349682
14283	H	2.473980	1.050903	-3.018470
14284	O	-0.707514	0.063397	2.103384
14285	H	0.070626	0.366011	2.613655
14286	H	-0.801323	-0.906897	2.253688
14287	O	-1.307725	4.165898	-1.160423
14288	H	-0.344788	4.002203	-1.392217
14289	H	-1.553355	5.010209	-1.551154
14290	O	2.796991	3.397955	0.583734
14291	H	3.443172	4.097851	0.723159
14292	H	2.153997	3.424765	1.363795
14293	O	-0.701514	-2.434282	-2.457742
14294	H	-1.665115	-2.593333	-2.435340
14295	H	-0.387957	-2.696316	-1.568712
14296	O	3.348423	0.009985	-2.217097
14297	H	2.952352	-0.878717	-2.357493
14298	H	3.476014	0.139407	-1.264837
14299	O	3.441019	-2.034405	1.388440
14300	H	3.545378	-1.093032	1.168056
14301	H	2.770743	-2.100975	2.090827
14302	O	-3.389925	-2.647836	-1.751695
14303	H	-4.025652	-3.236172	-2.172013
14304	H	-3.805914	-1.739565	-1.742235
14305	O	-2.459536	1.661965	-1.411789
14306	H	-2.210082	2.606316	-1.464567
14307	H	-1.737740	1.173104	-1.857712
14308	O	-4.910694	-0.315869	1.276712
14309	H	-5.673940	-0.113441	1.826006
14310	H	-4.225899	0.392869	1.416787
14311	O	-2.909301	1.387967	1.287998
14312	H	-2.714142	1.443275	0.325274
14313	H	-2.144672	0.911520	1.679295
14314	O	3.092742	0.664421	0.666241
14315	H	2.185524	0.481363	0.302959
14316	H	3.229822	1.632183	0.604275
14317	O	-3.330783	-2.684356	1.166295
14318	H	-3.943468	-1.942575	1.312946
14319	H	-3.298499	-2.814635	0.202886
14320	O	0.763796	-0.179663	-0.147803
14321	H	0.379627	0.073696	-1.023866

14322	H	0.100690	0.015010	0.551660
14323	O	3.120593	-3.868013	-0.498275
14324	H	3.668296	-4.653929	-0.415641
14325	H	3.409999	-3.213598	0.186282
14326	O	-0.838399	-2.637908	2.239528
14327	H	-1.795282	-2.760048	2.037609
14328	H	-0.375681	-2.882127	1.407106
14329	O	-1.371838	3.783014	1.648904
14330	H	-2.050796	3.091603	1.716354
14331	H	-1.358581	4.034250	0.707443
14332	O	1.519282	-2.195271	3.541933
14333	H	1.774143	-2.797646	4.248634
14334	H	0.612506	-2.449565	3.266154
14335	O	-4.507301	-0.283307	-1.508089
14336	H	-4.851745	-0.247232	-0.597518
14337	H	-3.941912	0.501954	-1.619510
14338	O	1.187243	3.705308	-1.701241
14339	H	1.418205	3.016090	-2.352365
14340	H	1.784535	3.606017	-0.935378
14341	O	0.568807	-2.893101	-0.048874
14342	H	1.350394	-3.467249	-0.136781
14343	H	0.883503	-1.961862	-0.088111
14344	O	-0.350841	0.254914	-2.522478
14345	H	-0.463111	-0.703185	-2.716220
14346	H	0.304808	0.658634	-3.124167
14347	O	2.208391	-2.400707	-2.749637
14348	H	1.266399	-2.560382	-2.910295
14349	H	2.522994	-3.077465	-2.127482
14350				
14351	Cartesian coordinates of : W25_10			
14352				
14353	O	-0.096492	-3.081160	2.866806
14354	H	0.756185	-3.531063	2.733180
14355	H	0.054902	-2.377948	3.522824
14356	O	-0.998329	1.213475	3.221408
14357	H	-0.722873	1.092258	2.284206
14358	H	-1.978010	1.105485	3.205370
14359	O	1.895686	3.791972	-1.817537
14360	H	2.159913	4.697460	-2.008007
14361	H	2.393672	3.200936	-2.421799
14362	O	-0.620103	-1.759830	0.648296
14363	H	-0.413752	-2.313695	1.451945
14364	H	-0.600390	-2.319329	-0.153296
14365	O	-3.121027	3.343923	0.946418
14366	H	-3.597119	4.175396	1.039668
14367	H	-2.189196	3.522697	1.243470
14368	O	0.562334	-0.669064	4.151030
14369	H	-0.088659	0.053438	3.923959
14370	H	0.939669	-0.455205	5.009881
14371	O	0.936975	0.148851	-2.765184
14372	H	0.317801	-0.416717	-3.271327
14373	H	1.282715	-0.381254	-1.993009
14374	O	1.789758	2.868545	0.890367
14375	H	1.938661	3.206311	-0.009587
14376	H	1.337314	2.007971	0.787687
14377	O	4.067855	1.135195	1.326310
14378	H	3.444998	1.879869	1.361227
14379	H	3.586555	0.373774	1.696950
14380	O	-1.042919	-1.399766	-3.862589
14381	H	-1.928837	-1.000789	-3.613208
14382	H	-1.103201	-1.681141	-4.781126
14383	O	-2.998318	1.515933	-1.156690
14384	H	-2.126217	1.834490	-1.469574
14385	H	-3.284049	2.207291	-0.529758
14386	O	-3.787181	-2.663764	-1.256312
14387	H	-3.667544	-2.014816	-0.512992
14388	H	-4.546697	-3.218033	-1.051483
14389	O	-3.123014	-0.742632	0.435043
14390	H	-2.988413	0.041103	-0.141757
14391	H	-2.223775	-1.085568	0.648094
14392	O	2.318789	-1.015615	1.965768
14393	H	2.511118	-1.971409	2.007464
14394	H	1.719446	-0.826316	2.713208
14395	O	-1.026692	-3.194457	-1.679745
14396	H	-1.989117	-3.283829	-1.552682

14397	H	-0.926343	-2.679551	-2.501919
14398	O	-0.016711	0.818273	0.723992
14399	H	-0.377097	1.263547	-0.065743
14400	H	-0.105242	-0.157233	0.604456
14401	O	4.348721	0.222005	-1.223247
14402	H	4.411509	0.661508	-0.345126
14403	H	4.122030	0.900182	-1.876438
14404	O	1.617329	-3.848814	-0.724964
14405	H	0.713949	-3.981397	-1.050630
14406	H	1.847728	-2.919434	-0.929726
14407	O	-3.631187	1.055097	2.609923
14408	H	-3.656777	0.318827	1.974712
14409	H	-3.671992	1.867601	2.077475
14410	O	2.354557	-3.837047	1.803361
14411	H	2.061934	-3.957098	0.858598
14412	H	3.069724	-4.459748	1.964990
14413	O	-3.372136	-0.553266	-3.065486
14414	H	-3.726115	-1.293957	-2.540316
14415	H	-3.447714	0.246347	-2.515347
14416	O	-0.703713	3.758954	2.008182
14417	H	0.174257	3.652487	1.596632
14418	H	-0.723429	3.107312	2.730337
14419	O	2.124464	-1.139523	-0.812774
14420	H	3.023973	-0.739671	-0.980870
14421	H	1.937178	-0.963328	0.132165
14422	O	-0.422052	2.176117	-1.680401
14423	H	0.078874	1.477327	-2.166225
14424	H	0.117460	2.981925	-1.725128
14425	O	2.997024	1.766859	-3.290229
14426	H	3.390082	1.764701	-4.168638
14427	H	2.261975	1.106180	-3.286763

14428

14429

14430 Cartesian coordinates of the water 26-mer

14431

14432 Cartesian coordinates of : W26_ 1

14433

14434	O	-2.232093	1.943348	-1.325599
14435	H	-1.542725	2.501583	-1.765395
14436	H	-1.739289	1.252027	-0.822570
14437	O	-1.025828	-0.128592	-0.080204
14438	H	-0.482789	0.054737	0.726949
14439	H	-1.663127	-0.850537	0.119779
14440	O	0.588780	0.488752	1.963155
14441	H	0.994930	1.318092	1.625638
14442	H	1.307693	-0.184589	1.975339
14443	O	2.491369	-2.287805	-0.799039
14444	H	1.857586	-1.753237	-1.330833
14445	H	2.093728	-3.177276	-0.728100
14446	O	0.681262	-0.708735	-2.056505
14447	H	0.163707	-1.071711	-2.800115
14448	H	0.022675	-0.548894	-1.334452
14449	O	1.972567	1.703107	-1.917984
14450	H	2.935732	1.604981	-2.051113
14451	H	1.563595	0.829138	-2.093136
14452	O	-2.751869	-2.200014	0.320626
14453	H	-2.684782	-2.442285	1.265354
14454	H	-3.662905	-1.917674	0.104218
14455	O	1.773475	2.573311	0.669360
14456	H	1.315848	3.436751	0.674315
14457	H	1.760371	2.253918	-0.261851
14458	O	2.483948	-1.436134	1.787124
14459	H	2.519679	-1.686803	0.835008
14460	H	3.381266	-1.130562	2.021984
14461	O	-1.871511	-2.624251	2.875669
14462	H	-0.937139	-2.918004	2.648567
14463	H	-2.177284	-3.202188	3.582014
14464	O	0.855363	-4.467368	-0.327267
14465	H	0.023217	-4.200722	-0.827276
14466	H	0.984921	-5.410735	-0.465507
14467	O	-3.390219	1.894656	2.552424
14468	H	-3.904932	2.200885	3.306016
14469	H	-2.768921	1.180076	2.893124
14470	O	-1.307537	-3.701722	-1.511793
14471	H	-1.270748	-3.155564	-2.318495

14472	H	-1.891620	-3.233538	-0.883067
14473	O	-1.303001	-1.833633	-3.617935
14474	H	-1.400936	-2.035330	-4.553447
14475	H	-2.060951	-1.232055	-3.359093
14476	O	-1.709553	0.139881	3.435233
14477	H	-1.841655	-0.816909	3.301796
14478	H	-0.818588	0.338164	3.085424
14479	O	4.721544	1.294834	-1.806266
14480	H	5.381709	1.508258	-2.472756
14481	H	4.865213	0.342587	-1.527642
14482	O	0.528475	-3.384811	2.245559
14483	H	1.267262	-2.752988	2.313375
14484	H	0.637098	-3.841894	1.389156
14485	O	5.017263	-0.319051	1.842171
14486	H	4.837075	0.630160	1.572535
14487	H	5.714259	-0.311413	2.504915
14488	O	-4.967149	-1.002690	-0.703217
14489	H	-4.939708	-0.070547	-0.329281
14490	H	-5.887422	-1.250064	-0.833534
14491	O	0.158567	4.795527	0.362336
14492	H	0.264263	5.723449	0.591394
14493	H	-0.735543	4.495078	0.683937
14494	O	4.504949	2.055559	0.906612
14495	H	4.685505	2.005975	-0.049428
14496	H	3.578529	2.355293	0.984381
14497	O	5.017972	-1.119798	-0.863098
14498	H	4.218526	-1.672747	-0.950068
14499	H	5.178310	-1.015937	0.092315
14500	O	-4.623976	1.419109	0.112105
14501	H	-3.975944	1.813429	-0.495425
14502	H	-4.265589	1.548388	1.013769
14503	O	-3.213683	-0.260890	-2.813109
14504	H	-3.871318	-0.620685	-2.190832
14505	H	-2.927144	0.599500	-2.452374
14506	O	-2.196654	3.788217	0.859894
14507	H	-2.505143	3.242426	1.605984
14508	H	-2.327989	3.237957	0.067313
14509	O	-0.189183	3.494775	-2.155781
14510	H	0.629162	2.985011	-2.288146
14511	H	-0.003911	4.122361	-1.436420

14512

14513 Cartesian coordinates of : W26_ 2

14514

14515	O	-0.746972	2.293695	-1.394534
14516	H	-1.110077	1.499510	-1.841083
14517	H	0.040610	2.595024	-1.923487
14518	O	-1.262960	-0.614889	0.239114
14519	H	-1.416500	-1.587926	0.324837
14520	H	-1.649197	-0.169835	1.025751
14521	O	-2.243764	0.507053	2.521960
14522	H	-1.625604	0.080466	3.146370
14523	H	-2.080720	1.490874	2.504826
14524	O	1.372224	-0.381468	-0.040471
14525	H	0.383054	-0.369996	0.016252
14526	H	1.669929	-0.010124	0.810677
14527	O	0.662203	2.654015	1.001469
14528	H	0.182835	2.321209	0.213468
14529	H	1.460747	3.099302	0.650526
14530	O	1.683148	0.656238	2.549050
14531	H	1.259953	1.454616	2.164133
14532	H	1.011135	0.144213	3.046240
14533	O	-1.763148	-3.247329	0.169078
14534	H	-2.691923	-3.089249	-0.116778
14535	H	-1.245699	-3.585030	-0.588394
14536	O	-1.840407	-0.054319	-2.312743
14537	H	-1.834510	-0.326652	-1.368227
14538	H	-2.765597	-0.123004	-2.613238
14539	O	2.316794	0.184464	-2.516036
14540	H	3.248586	-0.098529	-2.524805
14541	H	2.037825	0.080395	-1.579463
14542	O	-0.220923	-0.943060	3.729935
14543	H	-0.163104	-1.802506	3.196017
14544	H	-0.146865	-1.188076	4.658021
14545	O	1.809079	-3.035066	0.288410
14546	H	1.632374	-2.088568	0.080549

14547	H	1.375450	-3.534647	-0.429299
14548	O	0.120493	-3.818636	-1.795276
14549	H	0.139452	-4.572111	-2.393400
14550	H	0.200398	-2.988215	-2.360582
14551	O	0.267992	-1.634380	-3.170849
14552	H	-0.512537	-1.065843	-3.015368
14553	H	1.051412	-1.055926	-3.099068
14554	O	-0.050381	-3.113861	2.362709
14555	H	-0.811895	-3.313296	1.787831
14556	H	0.719860	-3.163916	1.759267
14557	O	2.988778	3.548326	-0.211721
14558	H	3.465746	4.370993	-0.065085
14559	H	3.652680	2.804474	-0.126424
14560	O	4.898720	-0.585979	-1.739307
14561	H	5.707088	-0.842655	-2.193249
14562	H	4.743472	-1.248139	-1.006293
14563	O	4.688728	1.584107	0.023333
14564	H	4.635143	1.055592	0.839444
14565	H	4.829052	0.950660	-0.705244
14566	O	-4.840364	1.472946	-0.552527
14567	H	-4.172017	2.181273	-0.493351
14568	H	-4.826034	0.982303	0.288738
14569	O	-4.589150	-0.306355	-2.438380
14570	H	-5.276292	-0.286622	-3.110753
14571	H	-4.761040	0.436334	-1.792153
14572	O	4.444134	-2.120602	0.333920
14573	H	4.377191	-1.543025	1.113721
14574	H	3.625630	-2.652432	0.310083
14575	O	-2.859129	3.479519	-0.376715
14576	H	-2.046526	3.148941	-0.848426
14577	H	-3.100427	4.323186	-0.772201
14578	O	-4.636563	-0.270141	1.655481
14579	H	-5.325274	-0.348485	2.322986
14580	H	-3.799312	-0.022443	2.117579
14581	O	4.239263	-0.043192	2.281450
14582	H	3.322020	0.233375	2.519453
14583	H	4.775711	0.008832	3.078615
14584	O	1.551614	2.874361	-2.561590
14585	H	1.912698	1.983634	-2.738424
14586	H	2.121610	3.250281	-1.868393
14587	O	-4.210330	-2.250408	-0.382407
14588	H	-4.383531	-1.747231	-1.196594
14589	H	-4.420185	-1.647115	0.350929
14590	O	-1.808040	3.092182	2.218406
14591	H	-0.874382	3.188755	1.958401
14592	H	-2.310734	3.369582	1.430994

14593

14594 Cartesian coordinates of : W26_ 3

14595

14596	O	1.399102	0.180137	0.025880
14597	H	1.612843	0.540067	-0.861223
14598	H	0.457027	-0.119452	-0.044440
14599	O	-1.101738	-0.702910	-0.184341
14600	H	-1.508041	-0.308318	-0.992185
14601	H	-1.083014	-1.681296	-0.296410
14602	O	-2.126892	0.515521	-2.354198
14603	H	-1.963316	1.415400	-1.984242
14604	H	-3.078326	0.252558	-2.236580
14605	O	1.356730	2.091981	2.021648
14606	H	1.665525	1.693972	2.856296
14607	H	1.389593	1.365478	1.360646
14608	O	-1.997038	-0.136135	2.296444
14609	H	-1.739166	-0.360131	1.374321
14610	H	-2.924820	-0.454032	2.364152
14611	O	2.633530	-2.121549	0.643412
14612	H	3.018613	-2.489809	-0.176763
14613	H	2.190543	-1.278695	0.364712
14614	O	-1.398304	2.750550	-1.059711
14615	H	-1.268200	2.537357	-0.108127
14616	H	-0.569901	3.164131	-1.369969
14617	O	-1.022732	-3.388670	-0.395499
14618	H	-0.500836	-3.612535	0.399596
14619	H	-0.394696	-3.363015	-1.160271
14620	O	1.719188	1.079418	-2.591267
14621	H	1.482524	2.027901	-2.583038

14622	H	1.065233	0.595137	-3.132333
14623	O	-0.209377	-0.511022	-3.789083
14624	H	-1.025686	-0.137578	-3.358529
14625	H	-0.388535	-0.597639	-4.730697
14626	O	1.138590	3.655604	-1.880852
14627	H	1.793209	3.611141	-1.114079
14628	H	1.274197	4.498970	-2.323934
14629	O	0.147872	-1.297225	3.541558
14630	H	0.281489	-2.098493	3.006518
14631	H	-0.677838	-0.877450	3.217751
14632	O	2.790845	3.422934	0.089823
14633	H	2.318246	3.198188	0.914839
14634	H	3.475015	2.729906	0.012151
14635	O	2.135211	0.300842	4.001331
14636	H	1.372922	-0.338612	3.858103
14637	H	2.285516	0.361386	4.949533
14638	O	-5.427131	1.151614	0.322328
14639	H	-6.322887	1.495692	0.396019
14640	H	-4.814219	1.932193	0.388412
14641	O	4.638189	1.299404	0.180867
14642	H	4.418203	0.728558	0.978122
14643	H	5.545455	1.596745	0.309218
14644	O	0.647935	-2.862290	-2.419624
14645	H	0.365586	-2.075966	-2.919326
14646	H	1.612447	-2.792346	-2.299069
14647	O	-1.377881	2.440491	1.673071
14648	H	-0.449734	2.530987	1.963627
14649	H	-1.666934	1.568086	2.019866
14650	O	4.141730	-0.315240	2.161047
14651	H	3.521939	-0.068410	2.874784
14652	H	3.765944	-1.113407	1.747143
14653	O	-4.490556	-0.474076	-1.755616
14654	H	-4.935930	0.073859	-1.082742
14655	H	-4.275186	-1.325037	-1.335882
14656	O	-3.729839	-2.864849	-0.350156
14657	H	-4.241991	-3.664572	-0.509030
14658	H	-2.785703	-3.133453	-0.375646
14659	O	0.704568	-3.494573	1.797036
14660	H	1.013830	-4.289493	2.243320
14661	H	1.494339	-3.062678	1.368857
14662	O	-4.494364	-1.081637	1.822182
14663	H	-4.925267	-0.339223	1.364181
14664	H	-4.305825	-1.759276	1.152758
14665	O	-3.772481	3.230473	0.432185
14666	H	-3.101692	3.187999	1.135680
14667	H	-3.240510	3.343994	-0.371323
14668	O	4.157608	-0.134998	-2.165413
14669	H	3.394064	0.375047	-2.496302
14670	H	4.421651	0.309883	-1.335798
14671	O	3.429551	-2.600630	-1.936120
14672	H	3.769658	-1.660702	-2.065621
14673	H	4.044118	-3.198334	-2.372504
14674				
14675	Cartesian coordinates of : W26_ 4			
14676				
14677	O	-1.481131	-0.731863	1.437099
14678	O	0.207029	3.605948	1.334743
14679	O	-0.056373	3.439574	-1.557842
14680	O	-1.287302	-0.930908	-1.325713
14681	O	-2.233509	1.646379	-1.525988
14682	O	1.275823	-0.823596	1.336628
14683	O	2.175618	1.747602	1.401700
14684	O	2.072881	1.779899	-1.400522
14685	O	1.482333	-0.870777	-1.412029
14686	H	1.295091	-0.933715	0.359440
14687	H	0.347557	-0.952946	1.607189
14688	H	-0.362087	-1.079327	-1.595633
14689	H	-1.292502	-0.957352	-0.344783
14690	H	1.350358	2.396553	-1.663105
14691	H	2.127553	1.867071	-0.427354
14692	H	0.985459	3.022602	1.482896
14693	H	0.335061	4.398667	1.864997
14694	H	-1.675461	0.230350	1.493882
14695	H	-2.286994	-1.200039	1.718737
14696	H	1.685063	0.083798	-1.556269

14697	H	2.279608	-1.368401	-1.663853
14698	H	1.825460	0.834085	1.520131
14699	H	3.124873	1.716432	1.622014
14700	H	-0.881605	2.951412	-1.721524
14701	H	-0.078793	3.714631	-0.627449
14702	H	-3.172969	1.603362	-1.777252
14703	H	-1.872883	0.737175	-1.617366
14704	H	-2.107475	1.935256	0.203330
14705	O	-2.042741	1.938086	1.185631
14706	H	-1.340550	2.573688	1.415141
14707	H	3.014800	-1.562379	1.680759
14708	O	3.952314	-1.529048	1.422342
14709	H	4.219065	-0.585022	1.485042
14710	H	5.775357	1.021694	1.564622
14711	O	4.846196	1.063040	1.272402
14712	H	4.867646	1.127509	0.289328
14713	H	4.953206	-2.177746	-1.565535
14714	O	4.126864	-1.730537	-1.307564
14715	H	4.069659	-1.798896	-0.328625
14716	H	3.915160	1.461753	-1.720279
14717	O	4.697111	0.948800	-1.445724
14718	H	4.442693	0.001760	-1.519807
14719	H	-5.851815	0.889931	-1.653938
14720	O	-4.917617	0.958349	-1.385618
14721	H	-4.917111	1.115981	-0.414803
14722	H	-4.426761	0.155796	1.483842
14723	O	-4.685795	1.093565	1.338516
14724	H	-3.901100	1.630560	1.546156
14725	H	-3.040522	-1.658605	-1.591291
14726	O	-3.974392	-1.609973	-1.321077
14727	H	-4.257908	-0.679643	-1.468333
14728	H	-4.070966	-1.726436	0.433226
14729	O	-4.114775	-1.582986	1.406115
14730	H	-4.931038	-2.018481	1.712178
14731	H	-7.584007	0.396313	0.358854
14732	O	-7.368124	0.282040	1.302378
14733	H	-6.576303	0.819379	1.474645
14734	H	-7.301508	-0.856146	-1.472278
14735	O	-7.560004	0.107275	-1.503023
14736	H	-8.318850	0.197567	-2.087148
14737	H	-6.746730	-2.543717	-0.218744
14738	O	-6.671200	-2.344468	-1.169633
14739	H	-5.724027	-2.379544	-1.387374
14740	H	-7.089849	-1.306737	1.611977
14741	O	-6.795443	-2.259936	1.645277
14742	H	-7.368224	-2.730004	2.258575
14743	H	7.562272	0.375192	-0.362723
14744	O	7.378059	0.178226	-1.299046
14745	H	6.583267	0.685701	-1.537721
14746	H	7.412084	-2.902077	-2.005119
14747	O	6.825801	-2.387182	-1.442467
14748	H	7.114957	-1.432502	-1.483464
14749	O	7.486402	0.249617	1.519453
14750	H	7.245977	-0.719014	1.557109
14751	H	8.234628	0.396653	2.105724
14752	H	6.751418	-2.511342	0.433639
14753	O	6.656192	-2.236103	1.363942
14754	H	5.706011	-2.268991	1.568486

14755

14756 Cartesian coordinates of : W26_ 5

14757

14758	O	-0.977364	-0.839987	-1.423126
14759	O	-3.363519	3.185965	-1.386711
14760	O	-3.102774	3.119953	1.517875
14761	O	-1.152221	-1.030557	1.338128
14762	O	-0.675012	1.675146	1.518925
14763	O	-3.689073	-1.369224	-1.333093
14764	O	-4.975427	1.016565	-1.443387
14765	O	-4.894886	1.091788	1.341476
14766	O	-3.889258	-1.419104	1.400470
14767	H	-3.678114	-1.461430	-0.352948
14768	H	-2.756652	-1.370667	-1.617264
14769	H	-2.040047	-1.334278	1.603775
14770	H	-1.136171	-1.064214	0.357171
14771	H	-4.316418	1.836386	1.623571

14772	H	-4.927924	1.161748	0.365325
14773	H	-4.027723	2.473459	-1.527756
14774	H	-3.610511	3.926416	-1.949496
14775	H	-0.957081	0.140256	-1.493976
14776	H	-0.098262	-1.162078	-1.689867
14777	H	-4.234174	-0.504072	1.530411
14778	H	-4.625521	-2.025133	1.602186
14779	H	-4.481407	0.170107	-1.548975
14780	H	-5.916628	0.817616	-1.613773
14781	H	-2.212004	2.769258	1.689930
14782	H	-3.118654	3.387610	0.585405
14783	H	0.256329	1.793542	1.776569
14784	H	-0.878699	0.719910	1.622476
14785	H	-0.840800	1.907263	-0.209324
14786	O	-0.887853	1.889980	-1.192911
14787	H	-1.677389	2.404899	-1.440975
14788	H	-5.335560	-2.291587	-1.575523
14789	O	-6.248722	-2.496851	-1.308813
14790	H	-6.780010	-1.708952	-1.523453
14791	H	-8.404582	0.266291	-1.670067
14792	O	-7.542963	0.007801	-1.329400
14793	H	-7.589506	0.001211	-0.327317
14794	H	-6.699789	-3.575511	1.634407
14795	O	-6.334385	-2.747772	1.307798
14796	H	-6.335313	-2.777731	0.310238
14797	H	-6.637172	0.426983	1.554024
14798	O	-7.382229	-0.133160	1.267994
14799	H	-7.136938	-1.049801	1.489821
14800	H	3.005891	1.605602	1.711011
14801	O	2.089733	1.452297	1.422110
14802	H	2.074195	1.599884	0.449957
14803	H	1.791077	0.555358	-1.454400
14804	O	1.860166	1.525508	-1.312929
14805	H	0.984213	1.895407	-1.523736
14806	H	0.683441	-1.439900	1.621829
14807	O	1.608228	-1.258221	1.375478
14808	H	1.746442	-0.296232	1.520951
14809	H	1.746745	-1.368023	-0.388182
14810	O	1.768273	-1.225226	-1.361562
14811	H	2.626400	-1.561893	-1.672501
14812	H	4.653098	1.352425	-0.279152
14813	O	4.627586	1.311878	-1.262057
14814	H	3.773182	1.688431	-1.533114
14815	H	4.702539	0.095024	1.504796
14816	O	4.833546	1.068544	1.455970
14817	H	5.771296	1.230672	1.665848
14818	H	4.349465	-1.665737	0.256649
14819	O	4.360321	-1.622187	1.239380
14820	H	3.454915	-1.815334	1.536659
14821	H	4.605455	-0.438147	-1.533755
14822	O	4.533061	-1.417785	-1.486742
14823	H	5.411846	-1.768416	-1.720418
14824	H	6.519401	1.248162	-1.526843
14825	O	7.401050	0.932136	-1.265236
14826	H	7.455932	-0.001320	-1.540247
14827	O	7.608520	0.965674	1.352493
14828	H	8.362032	1.451230	1.701225
14829	H	7.620391	1.042221	0.357069
14830	O	7.154106	-1.806016	1.161580
14831	H	7.401551	-0.902259	1.429864
14832	H	6.237126	-1.942904	1.454570
14833	H	7.297665	-1.954466	-0.467060
14834	O	7.273873	-1.874847	-1.461956
14835	H	7.900220	-2.505674	-1.829651
14836				
14837	Cartesian coordinates of : W26_ 6			
14838				
14839	O	-0.861161	-1.520648	-1.203135
14840	O	-0.657242	1.193238	-1.580512
14841	O	1.907874	-1.605472	-1.090202
14842	O	2.076455	-1.066773	1.606175
14843	O	1.900256	1.624736	1.068773
14844	O	2.117424	1.084941	-1.620471
14845	O	-0.874517	1.567113	1.134795
14846	O	-0.696003	-1.149907	1.510631

14847	O	4.846738	-1.172632	1.552354
14848	O	4.685042	-1.543924	-1.155372
14849	O	4.888054	1.161034	-1.523263
14850	O	4.676094	1.534009	1.181375
14851	H	1.925412	-1.539985	-0.109710
14852	H	1.012403	-1.900939	-1.330163
14853	H	0.238899	1.400939	-1.896717
14854	H	-0.687536	1.454451	-0.633267
14855	H	1.937253	1.557959	0.088592
14856	H	1.004150	1.931498	1.290666
14857	H	-0.711183	-1.407363	0.561176
14858	H	0.193290	-1.364820	1.841391
14859	H	-0.826429	-0.573129	-1.462989
14860	H	-1.762881	-1.826941	-1.409322
14861	H	2.087624	0.104284	-1.555146
14862	H	2.056702	-0.085999	1.539579
14863	H	-0.849774	0.618407	1.391358
14864	H	-1.778545	1.876669	1.321917
14865	H	3.791672	1.878248	1.392578
14866	H	4.675641	0.583531	1.435542
14867	H	4.850954	1.419952	-0.575243
14868	H	4.699076	-0.593836	-1.410611
14869	H	3.801119	-1.879221	-1.382605
14870	H	4.825445	-1.431232	0.603639
14871	H	2.968246	-1.304443	1.914036
14872	H	3.015729	1.314144	-1.915415
14873	H	5.756844	-1.336504	1.860213
14874	H	5.805070	1.317372	-1.814101
14875	H	-3.606352	1.533547	0.047891
14876	O	-3.644398	1.621675	1.028204
14877	H	-4.509548	2.017747	1.239183
14878	H	-3.516769	0.120849	-1.619527
14879	O	-3.437242	1.101002	-1.641924
14880	H	-2.537073	1.304474	-1.949035
14881	H	-3.531127	-0.069863	1.510961
14882	O	-3.467149	-1.050543	1.558222
14883	H	-2.568251	-1.261234	1.865472
14884	H	-3.596170	-1.496838	-0.167392
14885	O	-3.622479	-1.582329	-1.145133
14886	H	-4.484101	-1.993677	-1.356565
14887	H	-6.642425	-3.176183	-1.697890
14888	O	-6.233443	-2.457495	-1.206282
14889	H	-6.793224	-1.628427	-1.339821
14890	H	-5.169055	-1.742865	1.737542
14891	O	-6.106704	-1.929685	1.546189
14892	H	-6.138057	-2.331400	0.657461
14893	H	-5.181876	1.806751	-1.871445
14894	O	-6.119245	1.974295	-1.675738
14895	H	-6.150368	2.359904	-0.785965
14896	H	-6.862772	1.645753	1.385202
14897	O	-6.314592	2.435162	1.166080
14898	H	-6.707765	3.195961	1.604556
14899	H	-8.406998	-0.024407	2.130579
14900	O	-7.681451	0.119703	1.514942
14901	H	-7.058875	-0.669137	1.596589
14902	H	6.579872	-1.816586	-1.212377
14903	O	7.483659	-1.500157	-1.042937
14904	H	7.626271	-1.565545	-0.080992
14905	H	8.297864	-1.312066	2.377290
14906	O	7.615119	-1.080774	1.740422
14907	H	7.640531	-0.092498	1.600048
14908	O	7.658075	1.046758	-1.660540
14909	H	8.352459	1.270973	-2.287261
14910	H	7.671190	0.058246	-1.519894
14911	H	7.639334	1.532731	0.161362
14912	O	7.476284	1.467947	1.120079
14913	H	6.571492	1.790698	1.271383
14914	H	-7.099720	0.513580	-1.589167
14915	O	-7.609485	-0.282079	-1.313947
14916	H	-7.895357	-0.097078	-0.403866

14917

14918 Cartesian coordinates of : W26_ 7

14919

14920	O	3.047721	-2.222203	0.333122
14921	O	3.190837	-0.297755	2.244638

Cartesian coordinates			SI_Geometries.dat		200
14922	O	2.784690	1.672238	-1.646653	
14923	O	3.172504	-0.971470	-2.078038	
14924	O	0.280880	-2.427296	0.252941	
14925	O	0.419556	-0.598454	2.276569	
14926	O	0.014602	1.598923	-1.545338	
14927	O	0.386059	-1.050657	-2.104588	
14928	H	3.032988	-1.535376	1.040217	
14929	H	1.311869	-0.635421	2.658984	
14930	H	2.867664	0.703486	-1.816942	
14931	H	0.280681	-0.088696	-1.918684	
14932	H	2.189515	-2.679077	0.373813	
14933	H	0.397616	-1.268546	1.554058	
14934	H	1.878447	1.921277	-1.899705	
14935	H	1.280327	-1.165464	-2.466955	
14936	H	4.084377	-1.043322	-2.411250	
14937	H	-0.594562	-2.847060	0.328625	
14938	H	4.110773	-0.344041	2.556994	
14939	H	-0.900724	1.803618	-1.808323	
14940	H	3.154765	-1.440107	-1.211214	
14941	H	0.280137	-1.945137	-0.606195	
14942	H	3.111408	0.580506	1.802785	
14943	H	0.055063	1.720639	-0.569068	
14944	H	3.928921	2.483617	1.164603	
14945	O	3.043228	2.117817	1.004627	
14946	H	2.969849	1.971451	0.030502	
14947	H	1.129431	2.310450	1.321386	
14948	O	0.261192	1.902770	1.165098	
14949	H	0.310524	1.009948	1.578098	
14950	O	-2.525376	1.784845	1.078065	
14951	H	-2.573440	1.644526	0.102788	
14952	H	-1.666486	2.203167	1.254537	
14953	H	-3.668864	1.558231	-1.809278	
14954	O	-2.739874	1.344219	-1.599600	
14955	H	-2.646232	0.376818	-1.763014	
14956	O	-2.387809	-1.321233	-2.015991	
14957	H	-2.377730	-1.777326	-1.141219	
14958	H	-1.501570	-1.435588	-2.396952	
14959	O	-2.484336	-2.556880	0.400225	
14960	H	-2.483314	-1.868856	1.107313	
14961	H	-3.377359	-2.949761	0.404768	
14962	H	-2.439095	0.240117	1.884079	
14963	O	-2.373591	-0.642320	2.317747	
14964	H	-1.481506	-0.678981	2.701395	
14965	H	5.995818	-0.918221	1.429725	
14966	O	6.013606	-0.259951	2.194098	
14967	H	6.683641	-0.562907	2.815472	
14968	H	6.516867	2.865260	1.493340	
14969	O	5.855942	2.249444	1.161109	
14970	H	6.016188	1.377604	1.592245	
14971	O	5.576844	1.817024	-1.634488	
14972	H	5.742587	2.022658	-0.697061	
14973	H	4.646048	2.040895	-1.808886	
14974	O	5.946944	-0.702823	-2.253327	
14975	H	5.889586	0.275210	-2.057389	
14976	H	6.624872	-0.833298	-2.923608	
14977	O	5.825536	-1.940252	0.241341	
14978	H	4.942900	-2.350287	0.239893	
14979	H	5.971046	-1.577696	-0.654599	
14980	H	-4.289349	-1.487742	-2.329447	
14981	O	-5.201650	-1.471638	-1.995595	
14982	H	-5.446218	-0.528163	-1.912485	
14983	O	-5.493384	1.245768	-1.489448	
14984	H	-6.243146	1.840657	-1.643969	
14985	H	-5.408572	1.260157	-0.506889	
14986	O	-5.319412	1.522757	1.220485	
14987	H	-5.362671	0.647031	1.676996	
14988	H	-4.431635	1.874716	1.401868	
14989	H	-4.265725	-0.998779	2.640609	
14990	O	-5.183355	-0.934059	2.331071	
14991	H	-5.297183	-1.633656	1.662288	
14992	H	-5.873071	-3.561185	0.193755	
14993	O	-5.234985	-2.842252	0.231949	
14994	H	-5.301793	-2.333303	-0.627955	
14995	O	-7.246475	2.958698	-0.184502	
14996	H	-6.752203	2.609173	0.577363	

14997	H	-8.060599	3.344706	0.148450
14998				
14999	Cartesian coordinates of : W26_ 8			
15000				
15001	O	-2.030593	-1.523942	3.389030
15002	H	-1.415588	-0.817428	3.638584
15003	H	-2.897709	-1.112398	3.231602
15004	O	1.225223	-0.613527	1.511083
15005	H	0.659041	-0.196577	2.202493
15006	H	1.030073	-1.568767	1.431730
15007	O	-0.659279	1.917080	-2.264068
15008	H	-1.170414	1.463742	-2.960602
15009	H	-0.118059	1.228512	-1.801404
15010	O	1.206710	3.843589	-2.023643
15011	H	0.500555	3.220679	-2.315843
15012	H	1.221353	4.579995	-2.643030
15013	O	1.232220	3.135446	2.750682
15014	H	0.766453	3.504358	1.950031
15015	H	1.362532	3.881787	3.345335
15016	O	-3.155979	-3.388074	-1.046332
15017	H	-3.890557	-2.787632	-0.842361
15018	H	-2.700172	-3.539286	-0.199747
15019	O	1.191597	-3.242437	0.703540
15020	H	2.110920	-3.516712	0.868835
15021	H	1.133538	-3.028060	-0.253971
15022	O	1.052103	0.297214	-1.033442
15023	H	1.849784	0.871975	-1.036399
15024	H	0.892056	0.056259	-0.092217
15025	O	3.136328	2.064802	-1.048630
15026	H	2.682812	2.822278	-1.459976
15027	H	3.301728	2.268764	-0.088874
15028	O	-2.330941	3.170583	-0.441956
15029	H	-1.752928	2.696028	-1.073412
15030	H	-2.436077	2.571504	0.323519
15031	O	-1.485943	-1.909263	-2.579039
15032	H	-0.582584	-2.279094	-2.610156
15033	H	-2.082819	-2.571497	-2.153175
15034	O	-2.343471	1.268285	1.549755
15035	H	-3.180809	0.959049	1.941396
15036	H	-2.037294	0.549721	0.953025
15037	O	4.002457	-3.302893	0.961823
15038	H	4.096567	-2.360299	1.242384
15039	H	4.613626	-3.833243	1.482148
15040	O	3.598732	2.244990	1.549228
15041	H	3.857214	1.345432	1.805326
15042	H	2.815684	2.495626	2.076918
15043	O	-2.370338	0.309542	-3.746093
15044	H	-2.076609	-0.583478	-3.438580
15045	H	-2.602777	0.234796	-4.676720
15046	O	-4.204552	1.307769	-1.757576
15047	H	-3.802868	2.104705	-1.374437
15048	H	-3.647272	1.045255	-2.509528
15049	O	4.798894	0.001390	-1.366392
15050	H	4.286821	0.831953	-1.487693
15051	H	5.729313	0.224713	-1.471854
15052	O	3.842312	-2.673120	-1.844514
15053	H	4.034719	-3.049905	-0.969971
15054	H	4.222363	-1.779695	-1.838567
15055	O	-1.512304	-0.777131	-0.038131
15056	H	-1.390514	-1.640172	0.428660
15057	H	-1.370717	-0.965971	-0.986831
15058	O	-1.481287	-3.130282	1.266647
15059	H	-1.653179	-2.735901	2.149856
15060	H	-0.575688	-3.487971	1.264509
15061	O	1.134766	-2.310768	-1.904602
15062	H	1.184796	-1.354075	-1.692747
15063	H	2.059880	-2.564188	-2.111923
15064	O	0.091169	4.193376	0.608867
15065	H	-0.834365	4.015712	0.350192
15066	H	0.590066	4.194289	-0.224935
15067	O	3.925428	-0.629304	1.268573
15068	H	4.190855	-0.401110	0.357947
15069	H	2.944589	-0.564395	1.329586
15070	O	-4.306461	-0.896911	-0.131106
15071	H	-4.527059	-0.128511	-0.701684

15072	H	-3.327253	-0.874121	-0.125001
15073	O	-0.282683	0.804820	3.241194
15074	H	0.285719	1.585711	3.367964
15075	H	-1.033011	1.127127	2.695581
15076	O	-4.450235	-0.319707	2.458902
15077	H	-4.609043	-0.613179	1.525851
15078	H	-5.298681	-0.258554	2.907759
15079				
15080	Cartesian coordinates of : W26_ 9			
15081				
15082	O	2.332091	0.095690	1.148982
15083	H	1.865296	0.931593	1.365034
15084	H	2.154734	-0.056447	0.185852
15085	O	-1.391062	-1.269821	1.644841
15086	H	-0.601462	-1.721746	1.991026
15087	H	-1.566581	-1.672660	0.763253
15088	O	-2.109635	-2.365518	-0.744567
15089	H	-2.893563	-2.927101	-0.614464
15090	H	-2.441167	-1.569702	-1.235761
15091	O	-5.585789	-1.520381	-2.214331
15092	H	-5.841135	-0.662651	-1.828818
15093	H	-4.782504	-1.316237	-2.716119
15094	O	4.851499	1.114696	1.136343
15095	H	3.949132	0.715773	1.145380
15096	H	4.717842	2.025977	1.452492
15097	O	-4.753629	-3.135491	-0.272422
15098	H	-5.156350	-2.584005	-0.994981
15099	H	-5.251918	-3.957007	-0.220342
15100	O	3.186629	-3.751203	-1.155728
15101	H	3.695137	-3.075992	-1.633453
15102	H	2.243826	-3.558232	-1.307200
15103	O	4.457710	-1.255646	-1.651570
15104	H	4.807409	-1.392468	-0.735298
15105	H	4.961496	-0.498155	-1.991204
15106	O	-5.400358	0.901370	-0.812850
15107	H	-5.574265	0.841179	0.147689
15108	H	-5.197401	1.836109	-1.001778
15109	O	-5.507393	0.623223	1.939194
15110	H	-6.262132	0.582002	2.534178
15111	H	-4.998866	-0.237419	2.034038
15112	O	-4.135036	3.400505	-0.866372
15113	H	-4.423867	4.305077	-1.020367
15114	H	-4.003827	3.278802	0.120698
15115	O	-3.095920	-0.189014	-1.916864
15116	H	-3.829472	0.168918	-1.374725
15117	H	-2.456451	0.548423	-1.962909
15118	O	-4.173185	-1.595191	2.036070
15119	H	-4.368175	-2.174862	1.276637
15120	H	-3.203861	-1.520121	2.105678
15121	O	-3.735219	2.764340	1.620366
15122	H	-4.376113	2.083893	1.897876
15123	H	-2.854424	2.346457	1.681587
15124	O	5.378091	-1.636736	0.851334
15125	H	4.813364	-2.272576	1.325318
15126	H	5.407296	-0.808370	1.351397
15127	O	3.595871	-3.718226	1.459820
15128	H	3.472592	-3.808874	0.475039
15129	H	3.963311	-4.549220	1.777376
15130	O	-1.296655	1.476372	1.302395
15131	H	-0.456062	1.887752	1.572408
15132	H	-1.249751	0.512742	1.485593
15133	O	1.214745	-2.302547	1.775132
15134	H	1.928885	-2.941223	1.952005
15135	H	1.659236	-1.428373	1.711987
15136	O	3.635613	3.402723	-1.307970
15137	H	2.746307	3.112768	-1.579976
15138	H	4.265486	2.713097	-1.584958
15139	O	0.613193	-2.734774	-0.884500
15140	H	-0.348225	-2.804797	-1.034254
15141	H	0.740058	-2.656639	0.086982
15142	O	1.098468	2.223796	-1.476980
15143	H	0.157518	2.348604	-1.704986
15144	H	1.305516	1.277943	-1.624766
15145	O	1.233918	2.586354	1.244065
15146	H	1.201671	2.601236	0.260958

15147	H	1.987044	3.147196	1.504393
15148	O	-1.665475	2.124207	-1.361781
15149	H	-2.421736	2.738496	-1.400281
15150	H	-1.562222	1.893603	-0.411954
15151	O	1.913743	-0.408679	-1.447925
15152	H	1.346069	-1.209332	-1.415499
15153	H	2.831876	-0.715608	-1.645596
15154	O	5.559982	1.330860	-1.455548
15155	H	6.480253	1.584568	-1.579636
15156	H	5.412862	1.219247	-0.482351
15157	O	3.794081	3.728034	1.291026
15158	H	4.103772	4.597201	1.563363
15159	H	3.773298	3.709628	0.292157
15160				
15161	Cartesian coordinates of : W26_10			
15162				
15163	O	-2.307900	-1.661085	-3.081427
15164	H	-1.428960	-2.059322	-2.940855
15165	H	-2.903095	-2.178844	-2.509012
15166	O	0.940275	-0.010974	-1.196494
15167	H	0.456336	-0.799963	-1.520931
15168	H	0.639611	0.790649	-1.679442
15169	O	0.710132	-0.830580	3.403451
15170	H	-0.195131	-1.079462	3.138593
15171	H	0.939233	-0.091932	2.804847
15172	O	2.506453	-2.607752	2.821012
15173	H	2.808185	-3.078921	3.604481
15174	H	1.794677	-1.959421	3.117701
15175	O	2.465232	-3.780231	-1.568071
15176	H	2.136825	-4.012053	-0.652789
15177	H	2.849721	-4.570612	-1.958585
15178	O	-4.507370	1.483192	-1.321364
15179	H	-3.624163	1.311164	-1.748506
15180	H	-5.094765	1.838380	-1.995817
15181	O	0.125328	2.365670	-2.292429
15182	H	1.042209	2.650214	-2.535310
15183	H	-0.078505	2.903639	-1.505524
15184	O	1.644442	0.763968	1.318103
15185	H	2.488116	0.259266	1.354694
15186	H	1.201927	0.441895	0.501695
15187	O	3.955689	-0.719479	1.343243
15188	H	3.872139	-1.026052	0.407980
15189	H	3.678041	-1.458059	1.918086
15190	O	-1.686708	-1.192744	2.047761
15191	H	-2.558071	-0.992030	2.429182
15192	H	-1.502004	-0.418461	1.460848
15193	O	-2.387836	4.618735	1.231596
15194	H	-1.487001	4.363233	0.937759
15195	H	-2.296964	5.319194	1.883392
15196	O	-1.296897	-3.292587	0.332242
15197	H	-2.162252	-3.465188	-0.083498
15198	H	-1.466100	-2.582014	0.989458
15199	O	2.691069	3.093054	-2.264582
15200	H	3.410903	2.441391	-2.366836
15201	H	2.703471	3.278682	-1.308368
15202	O	3.435436	-1.175808	-1.248838
15203	H	2.580385	-0.700129	-1.334695
15204	H	3.258125	-2.103647	-1.492035
15205	O	-3.734408	2.300800	1.189456
15206	H	-4.174653	2.253406	0.318911
15207	H	-3.386680	3.214656	1.307447
15208	O	-4.202661	0.040556	2.576931
15209	H	-4.783919	0.069789	3.343242
15210	H	-4.081103	0.964216	2.260984
15211	O	5.145930	1.737224	1.065272
15212	H	4.856523	0.849335	1.358441
15213	H	6.040250	1.864537	1.396738
15214	O	2.693261	3.182157	0.593867
15215	H	3.623335	3.168791	0.864592
15216	H	2.358350	2.297399	0.861075
15217	O	-1.376878	1.007301	0.530406
15218	H	-1.489196	0.790765	-0.419862
15219	H	-2.207047	1.469137	0.778204
15220	O	-2.117536	0.780020	-2.144796
15221	H	-2.167419	-0.120538	-2.577827

15222	H	-1.443921	1.330437	-2.583986
15223	O	-0.072464	3.458652	0.357972
15224	H	0.850664	3.682364	0.569986
15225	H	-0.223246	2.535720	0.640529
15226	O	1.390248	-4.187909	0.777630
15227	H	0.426592	-4.057719	0.761202
15228	H	1.752364	-3.663913	1.518463
15229	O	4.765669	1.271438	-1.799193
15230	H	4.511727	0.334978	-1.792955
15231	H	4.989319	1.489707	-0.880227
15232	O	-4.919850	-0.972085	0.023851
15233	H	-4.754657	-0.733532	0.952166
15234	H	-4.878353	-0.143596	-0.487889
15235	O	0.032625	-2.468572	-1.905425
15236	H	0.845668	-2.989545	-2.037843
15237	H	-0.380452	-2.791212	-1.072191
15238	O	-3.733890	-3.057067	-1.055540
15239	H	-4.196616	-2.291316	-0.616710
15240	H	-4.409553	-3.712622	-1.256078
15241				
15242	Cartesian coordinates of : W26_11			
15243				
15244	O	3.544747	-1.525851	2.932975
15245	H	3.541928	-0.522178	2.953033
15246	H	4.108110	-1.824003	3.653837
15247	H	3.690500	-2.288014	1.293118
15248	O	3.613304	-2.672686	0.396913
15249	H	2.691436	-2.971506	0.298612
15250	O	4.061782	-1.199773	-1.915835
15251	H	3.912337	-1.546726	-1.010735
15252	H	4.736770	-1.804544	-2.264018
15253	O	3.859003	1.554515	-1.789830
15254	H	4.076728	0.608336	-1.912804
15255	H	2.948115	1.675979	-2.112401
15256	O	3.328595	1.065640	3.020594
15257	H	3.635003	1.626592	2.281089
15258	H	2.393582	1.287652	3.166934
15259	H	3.827362	2.092825	-0.052512
15260	O	3.796605	2.633139	0.765699
15261	H	4.458710	3.320350	0.588600
15262	H	1.674867	-1.770613	2.828025
15263	O	0.797784	-1.598002	2.440661
15264	H	0.836600	-1.928340	1.514148
15265	H	0.969699	-2.061394	-0.827234
15266	O	0.853238	-2.671701	-0.059815
15267	H	-0.017388	-3.089297	-0.172707
15268	H	2.239475	-1.257166	-2.420106
15269	O	1.302136	-1.093237	-2.207947
15270	H	1.228392	-0.125609	-2.039992
15271	H	1.003046	1.945662	-0.979870
15272	O	1.062281	1.601109	-1.903509
15273	H	0.221092	1.829170	-2.334130
15274	H	1.944396	2.975548	0.695117
15275	O	1.026954	2.664217	0.581746
15276	H	0.861103	2.047810	1.331854
15277	O	0.525725	1.081140	2.735073
15278	H	0.578203	0.109630	2.575759
15279	H	-0.390938	1.267118	2.998731
15280	H	-1.137207	-1.736090	2.629478
15281	O	-1.975860	-1.491611	2.204029
15282	H	-2.017463	-0.505421	2.213957
15283	H	-1.965262	-2.211466	0.628803
15284	O	-1.932136	-2.697317	-0.227736
15285	H	-2.838156	-3.016554	-0.389854
15286	H	-0.550195	-1.362505	-2.722364
15287	O	-1.464332	-1.198543	-2.435410
15288	H	-1.587542	-1.703195	-1.596943
15289	H	-1.637825	0.516087	-2.281298
15290	O	-1.699050	1.499585	-2.278177
15291	H	-2.582987	1.714535	-2.626852
15292	O	-1.723204	2.697142	0.150197
15293	H	-0.850337	3.098530	0.297933
15294	H	-1.666065	2.215396	-0.708550
15295	O	-2.234912	1.193613	2.352745
15296	H	-3.181948	1.310136	2.549333

15297	H	-2.064168	1.693831	1.521355
15298	H	-3.876750	-1.752692	2.146759
15299	O	-4.758293	-1.511277	1.815641
15300	H	-4.838766	-1.908516	0.927407
15301	H	-5.328728	-3.390248	-0.957917
15302	O	-4.685097	-2.717627	-0.714628
15303	H	-4.602340	-2.090644	-1.489648
15304	O	-5.016682	1.072715	2.152878
15305	H	-5.752263	1.256960	2.745128
15306	H	-5.000358	0.085365	1.995256
15307	H	-4.795945	2.114059	0.651950
15308	O	-4.520342	2.667695	-0.103321
15309	H	-3.620219	2.977923	0.093469
15310	O	-4.474608	1.676381	-2.526708
15311	H	-5.081060	2.162957	-3.093591
15312	H	-4.575802	2.039878	-1.600756
15313	H	-3.306880	-1.192907	-2.954488
15314	O	-4.251899	-1.115730	-2.738864
15315	H	-4.440806	-0.161339	-2.659110
15316	H	4.952308	-3.527333	-0.680024
15317	O	5.451316	-3.547157	-1.514659
15318	H	6.216347	-4.113957	-1.387550
15319	O	5.502308	3.703441	-1.123260
15320	H	5.963659	4.311388	-1.706310
15321	H	5.082719	3.019992	-1.673545

15322

15323 Cartesian coordinates of : W26_12

15324

15325	O	-1.000316	2.177342	4.162019
15326	H	-1.328753	2.312562	5.054575
15327	H	-0.701936	1.249329	4.093041
15328	O	-2.536209	-0.637391	1.833681
15329	H	-2.557803	0.159885	1.262964
15330	H	-1.894204	-0.459068	2.547510
15331	O	3.718843	-2.628304	-2.030887
15332	H	3.397540	-1.790612	-2.410902
15333	H	4.157936	-2.349260	-1.213113
15334	O	1.850350	-4.360019	-1.302533
15335	H	2.531142	-3.753952	-1.698078
15336	H	2.135471	-5.261043	-1.484545
15337	O	0.701058	-3.022870	3.235263
15338	H	1.398549	-3.029785	2.526556
15339	H	0.928794	-3.721865	3.855753
15340	O	-0.995378	5.177260	-0.369055
15341	H	-1.188392	4.754846	0.489419
15342	H	-1.584066	5.931318	-0.459022
15343	O	-2.834971	1.590096	0.234819
15344	H	-3.776151	1.507157	-0.009752
15345	H	-2.332309	1.484688	-0.608468
15346	O	0.204477	-0.742135	-1.188109
15347	H	-0.127879	-1.668118	-1.253931
15348	H	0.429636	-0.579158	-0.245278
15349	O	-0.720014	-3.278478	-1.177194
15350	H	-0.895207	-3.320659	-0.192113
15351	H	0.069262	-3.818414	-1.364316
15352	O	3.716671	-0.827928	0.287382
15353	H	3.428477	-0.395997	-0.548310
15354	H	4.449299	-0.276353	0.645863
15355	O	0.133136	3.287957	-2.013860
15356	H	-0.548341	2.610778	-2.222438
15357	H	-0.320150	4.070918	-1.641634
15358	O	1.214311	0.076434	1.205836
15359	H	2.138011	-0.224901	1.111943
15360	H	1.199083	1.038633	0.966013
15361	O	-5.281467	0.635903	-0.702594
15362	H	-5.146098	-0.259815	-0.280123
15363	H	-6.208241	0.875009	-0.609497
15364	O	-1.373257	-3.091488	1.325672
15365	H	-1.779866	-2.207160	1.427077
15366	H	-0.725842	-3.176030	2.048458
15367	O	2.674237	2.714418	-2.653848
15368	H	1.749512	3.037915	-2.543230
15369	H	3.029433	3.128126	-3.446663
15370	O	2.662848	-0.054931	-2.109889
15371	H	1.719865	-0.260569	-1.924608

15372	H	2.710947	0.864836	-2.428671
15373	O	-3.263274	-2.801547	-1.955357
15374	H	-2.325995	-3.062786	-1.800422
15375	H	-3.700792	-3.564641	-2.346550
15376	O	-3.701666	-0.135706	-2.940890
15377	H	-4.394858	0.190046	-2.340960
15378	H	-3.575953	-1.074778	-2.720582
15379	O	1.004761	2.634959	0.534094
15380	H	0.246763	2.975334	1.058406
15381	H	0.741941	2.780981	-0.399247
15382	O	-1.368393	3.387239	1.703521
15383	H	-1.321428	3.114815	2.641419
15384	H	-2.007487	2.786224	1.265176
15385	O	-1.503594	1.157796	-2.086303
15386	H	-0.898938	0.427819	-1.819851
15387	H	-2.253528	0.738675	-2.572920
15388	O	2.414751	-3.129917	1.226002
15389	H	2.922941	-2.358486	0.915224
15390	H	2.139680	-3.630121	0.438395
15391	O	-4.621578	-1.687261	0.293822
15392	H	-4.112572	-2.177505	-0.377009
15393	H	-4.022411	-1.530632	1.043790
15394	O	3.755490	2.901424	0.013017
15395	H	3.579020	2.904977	-0.942095
15396	H	2.876916	2.953793	0.427076
15397	O	-0.261886	-0.380018	3.421668
15398	H	0.008182	-1.265459	3.718845
15399	H	0.331026	-0.204106	2.653285
15400	O	5.483039	1.080062	0.963228
15401	H	4.924634	1.832443	0.655783
15402	H	5.909373	1.347002	1.781712

15403

15404

15405

15406 Cartesian coordinates of the water 27-mer

15407

15408 Cartesian coordinates of : W27_ 1

15409

15410	O	2.577312	-0.700763	3.796855
15411	H	2.935772	-1.044347	4.621990
15412	H	1.810618	-1.275691	3.548896
15413	O	0.774982	1.491636	4.257917
15414	H	1.541377	0.919012	4.081401
15415	H	0.851661	2.275266	3.693590
15416	O	4.304295	0.082961	1.664728
15417	H	3.842989	-0.386750	2.382113
15418	H	3.718352	0.832918	1.454299
15419	O	0.410686	-1.918169	2.776814
15420	H	0.721709	-1.595073	1.896581
15421	H	-0.331919	-1.319890	2.994964
15422	O	-1.405212	0.166984	3.269735
15423	H	-1.528015	0.768717	2.514222
15424	H	-0.747542	0.626403	3.836533
15425	O	4.980919	-0.886887	-0.677169
15426	H	4.771052	-0.572979	0.248349
15427	H	5.927472	-1.055085	-0.715596
15428	O	0.303101	3.236784	1.986773
15429	H	-0.576537	2.883896	1.759916
15430	H	0.476833	3.969598	1.371761
15431	O	2.183850	1.623526	0.813578
15432	H	1.537743	2.149883	1.328957
15433	H	2.156547	1.985988	-0.101221
15434	O	-0.617031	-4.079882	1.220548
15435	H	-0.266841	-3.499371	1.918395
15436	H	-1.552487	-3.836970	1.108192
15437	O	1.248038	-0.872907	0.481974
15438	H	1.676895	0.002674	0.634906
15439	H	1.824516	-1.405774	-0.122428
15440	O	-3.718929	-1.138094	2.300943
15441	H	-3.010655	-0.800800	2.875482
15442	H	-4.086901	-0.374136	1.819247
15443	O	2.680712	-2.263718	-1.267865
15444	H	3.615352	-2.010268	-1.150022
15445	H	2.334837	-1.819596	-2.074623
15446	O	-1.961545	1.867112	1.018223

15447	H	-1.658849	1.129483	0.416497
15448	H	-2.935818	1.781056	1.068036
15449	O	0.940684	4.660163	-0.428836
15450	H	1.489875	4.042319	-0.962577
15451	H	1.279177	5.548485	-0.580065
15452	O	0.691506	-4.220227	-1.142573
15453	H	0.250402	-4.202733	-0.259780
15454	H	1.546399	-3.766429	-1.054289
15455	O	-3.281059	-3.209134	0.767090
15456	H	-3.978500	-3.850573	0.936272
15457	H	-3.449212	-2.431788	1.374210
15458	O	-1.046995	-0.052711	-0.514799
15459	H	-0.219639	-0.460666	-0.144460
15460	H	-1.636894	-0.783583	-0.827785
15461	O	3.711705	0.663262	-2.710736
15462	H	3.185552	0.012742	-3.198477
15463	H	4.220051	0.173805	-2.038666
15464	O	2.002417	2.559203	-1.740176
15465	H	1.201576	2.132798	-2.127000
15466	H	2.752171	2.065670	-2.140719
15467	O	-4.550709	1.036028	0.722814
15468	H	-4.420290	0.814497	-0.247866
15469	H	-5.419420	1.438235	0.820328
15470	O	-1.735460	3.866794	-0.960332
15471	H	-0.841006	4.245102	-0.897535
15472	H	-1.828904	3.250829	-0.209532
15473	O	1.400011	-1.099270	-3.374913
15474	H	0.738657	-1.806774	-3.500605
15475	H	0.875593	-0.285540	-3.237573
15476	O	-2.600441	-1.941734	-1.578492
15477	H	-1.986149	-2.424150	-2.173552
15478	H	-2.902697	-2.547519	-0.871221
15479	O	-0.092236	1.152678	-2.693364
15480	H	-0.494884	0.744513	-1.886132
15481	H	-0.828155	1.601088	-3.146122
15482	O	-0.582268	-3.106579	-3.053850
15483	H	-0.092404	-3.593262	-2.305921
15484	H	-0.779958	-3.760207	-3.732923
15485	O	-4.029839	0.460380	-1.755262
15486	H	-3.505085	1.114333	-2.254317
15487	H	-3.620701	-0.415804	-1.877441
15488	O	-2.508637	2.466255	-3.036542
15489	H	-2.239748	3.093223	-2.308746
15490	H	-2.982832	2.973714	-3.702612
15491				
15492	Cartesian coordinates of : W27_ 2			
15493				
15494	O	-0.369173	-3.849394	0.117780
15495	H	-0.212063	-4.134344	1.035117
15496	H	0.472504	-3.422704	-0.152717
15497	O	-0.659110	3.063310	-3.029001
15498	H	-1.069619	2.162924	-3.053232
15499	H	-0.700250	3.436568	-3.914806
15500	O	4.226217	-0.694860	1.907340
15501	H	4.312946	0.259464	1.735318
15502	H	4.524879	-1.164474	1.106338
15503	O	-2.797436	2.594761	2.590485
15504	H	-2.534268	1.878963	3.192502
15505	H	-1.996409	3.097438	2.366824
15506	O	-1.510691	0.318814	0.049187
15507	H	-1.881460	-0.576402	0.232720
15508	H	-2.280461	0.946117	0.105044
15509	O	-2.197230	4.074983	-0.861645
15510	H	-1.604453	4.228861	-0.106348
15511	H	-1.638941	3.875705	-1.631578
15512	O	-3.613548	1.969121	0.068612
15513	H	-3.601778	2.179002	1.027085
15514	H	-3.245160	2.775996	-0.363879
15515	O	-4.220285	-2.435414	-1.383578
15516	H	-5.085229	-2.842986	-1.490595
15517	H	-4.314525	-1.454200	-1.589319
15518	O	-4.293911	0.104059	-1.887542
15519	H	-4.340583	0.724265	-1.135491
15520	H	-3.465643	0.337707	-2.346073
15521	O	4.379892	2.100329	-1.461697

15522	H	4.508795	2.150539	-0.500524
15523	H	3.445944	2.328675	-1.610902
15524	O	0.253046	-3.610617	2.888166
15525	H	0.628556	-4.216702	3.534783
15526	H	0.904103	-2.876819	2.761518
15527	O	-0.635279	4.206020	1.525230
15528	H	-0.478492	5.063491	1.933771
15529	H	0.241860	3.781571	1.384246
15530	O	1.887249	-2.356934	-0.266650
15531	H	1.809430	-1.975319	0.641813
15532	H	2.838490	-2.556303	-0.380602
15533	O	1.528134	-0.559704	-2.275032
15534	H	0.898579	-0.964500	-2.899102
15535	H	1.573840	-1.172248	-1.506108
15536	O	-0.555314	-1.713444	-3.755801
15537	H	-1.008361	-2.437105	-3.233625
15538	H	-0.496530	-2.013112	-4.668275
15539	O	1.720698	-1.471318	2.266100
15540	H	1.148075	-0.669861	2.278073
15541	H	2.666524	-1.167805	2.296859
15542	O	-2.435495	-2.151108	0.675953
15543	H	-1.701322	-2.756870	0.428322
15544	H	-3.199200	-2.368454	0.106348
15545	O	4.346875	-0.467988	-2.380665
15546	H	3.398703	-0.506265	-2.600963
15547	H	4.504609	0.460179	-2.094092
15548	O	1.547002	2.106936	-1.592676
15549	H	0.896371	2.587277	-2.137262
15550	H	1.450238	1.156269	-1.825052
15551	O	4.632547	-2.160805	-0.472566
15552	H	5.357699	-2.773285	-0.628598
15553	H	4.608555	-1.506320	-1.244593
15554	O	0.107343	0.689349	2.132081
15555	H	-0.425832	0.754360	2.949170
15556	H	-0.528358	0.560952	1.377722
15557	O	4.189621	2.110943	1.407342
15558	H	4.671216	2.715500	1.980599
15559	H	3.245892	2.402446	1.392652
15560	O	-2.054260	-2.006966	3.421035
15561	H	-1.278333	-2.594844	3.410271
15562	H	-2.403415	-2.047833	2.510364
15563	O	-1.814620	-3.518395	-2.344364
15564	H	-1.377595	-3.881908	-1.556909
15565	H	-2.704846	-3.219652	-2.076015
15566	O	1.567462	2.666176	1.066341
15567	H	1.096337	1.928459	1.523376
15568	H	1.504718	2.466648	0.100509
15569	O	-1.719639	0.474557	4.165922
15570	H	-1.885232	-0.489265	3.951716
15571	H	-1.712118	0.566172	5.123335
15572	O	-1.620520	0.602685	-2.673184
15573	H	-1.274618	-0.155111	-3.185037
15574	H	-1.380381	0.438334	-1.732068
15575				
15576	Cartesian coordinates of : W27_ 3			
15577				
15578	O	3.284267	0.560099	2.203966
15579	O	3.745006	2.111110	0.024540
15580	O	2.974394	-1.982738	-1.355781
15581	O	3.175001	-2.014931	1.343658
15582	O	0.523472	0.810322	2.236928
15583	O	0.980886	2.480859	0.120227
15584	O	0.232998	-1.570879	-1.478760
15585	O	0.404541	-1.732875	1.239609
15586	H	3.388551	1.146088	1.417728
15587	H	1.906818	2.772120	0.158179
15588	H	2.989165	-2.001309	-0.369005
15589	H	0.365534	-1.692819	0.255062
15590	H	2.415544	0.768045	2.589995
15591	H	0.844101	1.885622	0.893182
15592	H	2.057337	-2.171103	-1.622134
15593	H	1.246455	-2.163010	1.464525
15594	H	4.036712	-2.429476	1.526681
15595	H	-0.353595	1.050833	2.584487
15596	H	4.692814	2.322072	0.080603

15597	H	-0.693743	-1.765428	-1.706992
15598	H	3.237082	-1.087209	1.671146
15599	H	0.440145	-0.107991	1.890367
15600	H	3.651744	1.549058	-0.780729
15601	H	0.393623	-0.637504	-1.750727
15602	H	4.474749	0.526675	-2.507354
15603	O	3.560946	0.525655	-2.177723
15604	H	3.366516	-0.398807	-1.890305
15605	H	1.701994	1.003947	-2.556364
15606	O	0.804433	1.005251	-2.184307
15607	H	0.860225	1.547455	-1.364213
15608	O	-1.984208	1.247018	-2.214354
15609	H	-2.151214	0.317463	-1.932817
15610	H	-1.097350	1.258888	-2.609710
15611	H	-3.462376	-1.405824	-1.612989
15612	O	-2.516847	-1.298171	-1.388381
15613	H	-2.480618	-1.304036	-0.406360
15614	O	-2.343360	-1.298312	1.356843
15615	H	-2.244936	-0.364940	1.664434
15616	H	-1.508746	-1.748712	1.568433
15617	O	-2.209342	1.273664	2.178851
15618	H	-2.099668	1.852153	1.384009
15619	H	-3.100917	1.448785	2.529499
15620	H	-1.882802	2.256089	-0.813378
15621	O	-1.796904	2.804796	0.002814
15622	H	-0.871696	3.100664	0.022937
15623	H	6.400801	1.105501	0.946631
15624	O	6.540341	1.748098	0.181878
15625	H	7.259042	2.337644	0.432125
15626	H	7.100763	0.519376	-2.764264
15627	O	6.378279	0.356888	-2.149558
15628	H	6.545444	0.898865	-1.343484
15629	O	5.752298	-2.289069	-1.318574
15630	H	6.035250	-1.418840	-1.651832
15631	H	4.820569	-2.397865	-1.577403
15632	O	5.917128	-2.540261	1.284562
15633	H	5.932399	-2.496522	0.286353
15634	H	6.506216	-3.249069	1.560581
15635	O	6.039805	0.116855	2.123271
15636	H	5.144781	0.279497	2.469100
15637	H	6.091012	-0.834776	1.906398
15638	H	-4.226459	-1.381527	1.421067
15639	O	-5.105338	-1.008499	1.225053
15640	H	-5.139365	-0.905195	0.230125
15641	O	-5.220735	-0.868669	-1.407220
15642	H	-6.078007	-1.266551	-1.662851
15643	H	-5.171844	0.069038	-1.742660
15644	O	-4.809030	1.619567	-2.162867
15645	H	-4.842154	2.223077	-1.389847
15646	H	-3.899621	1.675050	-2.495672
15647	H	-3.662260	3.380691	0.167266
15648	O	-4.606742	3.164833	0.118421
15649	H	-4.812171	2.651367	0.917578
15650	H	-5.683187	1.582501	3.008009
15651	O	-4.985187	1.422098	2.365482
15652	H	-5.137249	0.525866	1.972694
15653	H	-8.484440	-1.695295	-1.784424
15654	O	-7.664590	-2.120305	-1.517132
15655	H	-7.733680	-2.300640	-0.557214
15656	H	-6.598564	-2.018572	1.384862
15657	O	-7.456349	-2.456866	1.209947
15658	H	-7.410023	-3.335729	1.597529
15659				
15660	Cartesian coordinates of : W27_ 4			
15661				
15662	O	-2.308789	0.454315	1.874263
15663	O	-2.473580	1.838786	-0.500211
15664	O	-5.090177	0.449195	1.913007
15665	O	-5.383964	-1.816571	0.403794
15666	O	-5.152689	-0.307273	-1.868758
15667	O	-5.236863	1.976078	-0.357435
15668	O	-2.378888	-0.536665	-1.881274
15669	O	-2.616331	-1.906288	0.495653
15670	O	-8.151657	-1.736684	0.616768
15671	O	-7.887364	0.576100	1.837665

15672	H	-5.138762	-0.430692	1.475522
15673	H	-4.199165	0.520965	2.295209
15674	H	-3.352647	2.251671	-0.561009
15675	H	-2.488264	1.059974	-1.100051
15676	H	-5.123059	0.574182	-1.432936
15677	H	-4.276649	-0.451985	-2.264758
15678	H	-2.556546	-1.129542	1.095169
15679	H	-3.525453	-2.244881	0.571287
15680	H	-2.320298	1.056041	1.097243
15681	H	-1.408886	0.491475	2.241426
15682	H	-5.220651	1.539825	0.523766
15683	H	-5.348447	-1.381479	-0.477494
15684	H	-2.422210	-1.135994	-1.103540
15685	H	-1.491888	-0.643854	-2.265758
15686	H	-8.014567	1.267726	1.162774
15687	H	-6.976543	0.671016	2.164344
15688	H	-8.131248	-0.901845	1.163428
15689	H	-6.307105	-2.101224	0.532618
15690	H	-6.137146	2.331717	-0.470821
15691	H	-8.864979	-2.292768	0.944076
15692	H	0.414871	0.350303	-1.500428
15693	O	0.404635	-0.531513	-1.934337
15694	H	1.290630	-0.666961	-2.312216
15695	H	0.313255	1.319694	0.477975
15696	O	0.292563	1.752838	-0.404368
15697	H	-0.589748	2.152583	-0.498212
15698	H	0.182902	-1.604847	-0.529584
15699	O	0.144035	-2.032835	0.354407
15700	H	-0.763799	-2.365477	0.464196
15701	H	0.397457	-0.649040	1.441660
15702	O	0.466782	0.229970	1.876782
15703	H	1.366533	0.292356	2.240736
15704	H	4.165902	0.278961	2.170536
15705	O	3.258791	0.239697	1.822810
15706	H	3.232248	0.839603	1.044849
15707	H	1.996946	-2.447204	0.514470
15708	O	2.907951	-2.116198	0.432441
15709	H	2.985739	-1.348722	1.040306
15710	H	2.159131	2.022418	-0.607139
15711	O	3.046448	1.627526	-0.544473
15712	H	3.056036	0.852792	-1.149985
15713	H	3.137903	-1.342930	-1.154682
15714	O	3.189169	-0.740746	-1.930434
15715	H	4.081232	-0.836484	-2.305560
15716	O	-7.950323	-0.215062	-1.744599
15717	H	-7.055097	-0.384267	-2.084092
15718	H	-8.125735	-0.894989	-1.068631
15719	O	5.795079	1.719657	-0.425149
15720	H	4.885142	2.054699	-0.512162
15721	H	5.816090	1.178644	0.399303
15722	H	5.966497	0.301862	-1.579821
15723	O	5.996603	-0.584036	-1.993831
15724	H	6.922994	-0.873503	-1.892438
15725	H	5.972801	-0.836796	1.286286
15726	O	6.054332	0.050067	1.708617
15727	H	6.999935	0.179249	1.900658
15728	H	5.606969	-1.737875	-0.601714
15729	O	5.667503	-2.208456	0.254186
15730	H	4.788134	-2.587741	0.416643
15731	H	-8.065230	1.278265	-1.069738
15732	O	-8.005569	2.110697	-0.522280
15733	H	-8.683399	2.721133	-0.827712
15734	H	8.750002	1.337388	0.794461
15735	O	8.803232	0.502616	1.321322
15736	H	9.564879	0.577906	1.904441
15737	H	7.377439	2.532673	-0.391252
15738	O	8.329932	2.661093	-0.197308
15739	H	8.775555	2.798266	-1.038752
15740	H	8.605597	-0.888623	0.009699
15741	O	8.281208	-1.516875	-0.657506
15742	H	7.758141	-2.169115	-0.170625
15743				
15744	Cartesian coordinates of : W27_ 5			
15745				
15746	O	3.171731	-2.097365	0.943967

15747	O	3.496023	0.279234	2.221361
15748	O	3.099574	1.076171	-2.068167
15749	O	3.289127	-1.600855	-1.723358
15750	O	0.400301	-2.125456	0.967454
15751	O	0.713692	0.193363	2.373796
15752	O	0.336310	1.227259	-1.913960
15753	O	0.502668	-1.489750	-1.689516
15754	H	3.222736	-1.237346	1.422985
15755	H	1.613178	0.207455	2.740517
15756	H	3.114169	0.095773	-1.952113
15757	H	0.470964	-0.509726	-1.788693
15758	H	2.288759	-2.463085	1.127706
15759	H	0.628302	-0.654357	1.877954
15760	H	2.203238	1.304497	-2.370911
15761	H	1.374338	-1.769758	-2.015115
15762	H	4.181502	-1.833770	-2.034827
15763	H	-0.495490	-2.445407	1.176902
15764	H	4.421455	0.258064	2.520083
15765	H	-0.571854	1.411688	-2.213549
15766	H	3.269660	-1.800240	-0.758045
15767	H	0.395241	-1.907492	0.006971
15768	H	3.458207	0.998705	1.547507
15769	H	0.413592	1.616891	-1.012698
15770	H	4.370392	2.578515	0.379289
15771	O	3.459331	2.243270	0.341982
15772	H	3.348779	1.829093	-0.547593
15773	H	1.568838	2.649555	0.613514
15774	O	0.673042	2.273461	0.589653
15775	H	0.679700	1.534354	1.240883
15776	O	-2.118067	2.329918	0.579440
15777	H	-2.197799	1.919329	-0.312862
15778	H	-1.231694	2.725564	0.620346
15779	H	-3.341990	1.361749	-2.126922
15780	O	-2.427361	1.151305	-1.860870
15781	H	-2.405725	0.174987	-1.728337
15782	O	-2.279934	-1.541569	-1.478915
15783	H	-2.272197	-1.732206	-0.509561
15784	H	-1.413697	-1.818781	-1.821028
15785	O	-2.355775	-2.018552	1.185939
15786	H	-2.292064	-1.158288	1.664219
15787	H	-3.263997	-2.343019	1.339699
15788	H	-2.102168	1.080152	1.804682
15789	O	-2.076345	0.357042	2.472903
15790	H	-1.175141	0.370542	2.836198
15791	H	6.228547	-0.748060	1.581734
15792	O	6.312614	0.098166	2.124879
15793	H	6.974803	-0.064884	2.804419
15794	H	6.987764	2.853709	0.558601
15795	O	6.279179	2.217019	0.421203
15796	H	6.396974	1.493408	1.080052
15797	O	5.892361	1.023670	-2.131460
15798	H	6.100095	1.474524	-1.293586
15799	H	4.973251	1.255080	-2.352144
15800	O	6.069326	-1.589279	-2.006041
15801	H	6.084558	-0.594642	-2.099074
15802	H	6.721221	-1.954826	-2.612090
15803	O	5.958043	-2.052852	0.739694
15804	H	5.051839	-2.382828	0.870241
15805	H	6.091624	-1.967543	-0.224930
15806	H	-4.160183	-1.662320	-1.786669
15807	O	-5.076063	-1.483687	-1.510147
15808	H	-5.249163	-0.540206	-1.711473
15809	O	-5.185505	1.255349	-1.734879
15810	H	-5.902188	1.842620	-2.021934
15811	H	-5.070120	1.509378	-0.787687
15812	O	-4.917880	2.226845	0.793179
15813	H	-4.996985	1.548539	1.509991
15814	H	-4.017639	2.586608	0.863912
15815	H	-3.972798	0.244060	2.945117
15816	O	-4.899509	0.287982	2.659514
15817	H	-5.111479	-0.585991	2.283407
15818	H	-5.779195	-2.808146	1.143989
15819	O	-5.108730	-2.109128	1.192889
15820	H	-5.097439	-1.761100	0.274985
15821	H	-6.310274	3.179753	-0.096573

15822	O	-6.812164	3.347072	-0.913695
15823	H	-7.643677	3.757658	-0.663203
15824	H	-6.323747	-2.901032	-1.182694
15825	O	-6.730967	-3.527080	-0.559616
15826	H	-7.555195	-3.829633	-0.949391
15827				
15828	Cartesian coordinates of : W27_ 6			
15829				
15830	O	-3.646406	-1.145681	-2.729198
15831	H	-3.988581	-1.527536	-3.542910
15832	H	-2.742798	-1.540437	-2.547938
15833	O	1.451135	2.970421	0.927649
15834	H	0.758572	3.592322	0.588778
15835	H	1.377935	2.884527	1.899113
15836	O	2.582651	-3.119735	-2.582178
15837	H	2.023322	-3.668818	-2.011029
15838	H	3.268694	-2.730615	-2.017766
15839	O	0.928880	-2.320773	2.686028
15840	H	1.231802	-2.074409	1.784510
15841	H	0.497921	-3.187391	2.589561
15842	O	-1.720726	-0.284992	0.338093
15843	H	-2.670570	-0.508732	0.191464
15844	H	-1.526599	-0.528177	1.278982
15845	O	1.326126	2.179603	3.564565
15846	H	1.689320	2.636460	4.329842
15847	H	1.783458	1.293284	3.516081
15848	O	-1.480905	1.845068	3.346896
15849	H	-1.549081	0.873792	3.406478
15850	H	-0.539190	2.043955	3.493867
15851	O	-4.883450	1.801988	0.099123
15852	H	-5.658283	2.338255	0.292490
15853	H	-4.119262	2.165174	0.612996
15854	O	-2.457480	2.412706	0.960875
15855	H	-2.132313	2.304478	1.898402
15856	H	-2.162824	1.591077	0.525609
15857	O	4.617557	0.065749	1.420067
15858	H	5.455262	0.189707	1.878681
15859	H	4.395628	0.937078	0.974583
15860	O	-0.815052	-4.332469	1.622278
15861	H	-0.393095	-4.266799	0.728522
15862	H	-0.891856	-5.268580	1.833593
15863	O	2.590458	-0.120856	3.388312
15864	H	3.262431	-0.175826	2.682294
15865	H	2.110193	-0.963965	3.407312
15866	O	-1.290046	-1.896624	-1.947099
15867	H	-1.228527	-1.350943	-1.139667
15868	H	-0.537045	-1.627551	-2.561617
15869	O	1.207370	1.359468	-2.946105
15870	H	0.596951	2.054770	-3.246488
15871	H	0.940022	1.205544	-2.002955
15872	O	-1.005239	3.102592	-2.874273
15873	H	-1.732703	2.494535	-2.596784
15874	H	-1.389826	3.711370	-3.513279
15875	O	0.372431	-3.756797	-0.710608
15876	H	0.812812	-2.927325	-0.409386
15877	H	-0.343336	-3.422489	-1.282842
15878	O	-4.314182	-0.958937	-0.048678
15879	H	-4.766596	-0.107914	0.098801
15880	H	-4.355981	-1.134716	-1.007848
15881	O	3.821323	1.155438	-2.514820
15882	H	2.896890	1.320463	-2.826781
15883	H	4.417010	1.354284	-3.244080
15884	O	0.582075	0.885075	-0.425740
15885	H	0.880206	1.629960	0.164660
15886	H	-0.362255	0.704199	-0.256323
15887	O	0.683744	-1.343120	-3.514466
15888	H	0.957634	-0.409463	-3.488080
15889	H	1.452349	-1.905196	-3.279433
15890	O	1.624785	-1.528727	0.175234
15891	H	1.225056	-0.646931	-0.005797
15892	H	2.523018	-1.475525	-0.221669
15893	O	4.066715	-1.230697	-0.984994
15894	H	4.519642	-0.933874	-0.172770
15895	H	4.031281	-0.455316	-1.577007
15896	O	-3.189395	-2.747101	2.037950

15897	H	-2.534157	-3.371057	1.682699
15898	H	-3.692852	-2.369465	1.300241
15899	O	-2.927600	1.448811	-1.947812
15900	H	-3.184401	0.617590	-2.388720
15901	H	-3.710156	1.740582	-1.450660
15902	O	3.992016	2.219854	0.102240
15903	H	3.141150	2.632477	0.348530
15904	H	3.955074	2.014572	-0.848046
15905	O	-1.410800	-0.900727	2.936354
15906	H	-2.115546	-1.582266	2.875518
15907	H	-0.556258	-1.377138	3.003764
15908	O	-0.620010	4.185001	-0.224304
15909	H	-0.637493	3.947445	-1.167045
15910	H	-1.369860	3.704234	0.176438

15911

15912 Cartesian coordinates of : W27_ 7

15913

15914	O	-0.021806	-3.734285	-0.087693
15915	H	-0.693956	-4.167958	-0.639965
15916	H	-0.499909	-2.944290	0.265059
15917	O	2.177868	2.949914	2.183938
15918	H	2.591672	2.066467	2.152879
15919	H	2.413170	3.382648	1.347302
15920	O	-3.866044	0.624184	-2.404522
15921	H	-4.670066	0.813621	-2.899991
15922	H	-3.857782	1.268730	-1.647092
15923	O	1.083731	2.048104	-3.249805
15924	H	0.326656	1.502822	-3.520052
15925	H	0.725054	2.853480	-2.842777
15926	O	1.742997	-0.165693	-0.474903
15927	H	1.793871	-1.035286	-0.942110
15928	H	2.342596	0.457611	-0.951228
15929	O	2.804486	4.015154	-0.430237
15930	H	3.388932	4.778219	-0.483291
15931	H	1.956478	4.260110	-0.868507
15932	O	3.348643	1.580329	-1.750160
15933	H	2.718153	1.682364	-2.494377
15934	H	3.316912	2.435782	-1.281613
15935	O	4.183932	-2.789544	-0.447282
15936	H	4.974628	-3.332720	-0.525317
15937	H	4.491323	-1.839453	-0.381558
15938	O	4.912889	-0.279518	-0.176955
15939	H	4.610705	0.330827	-0.870195
15940	H	4.470387	0.006839	0.644908
15941	O	-3.225761	1.740920	2.359598
15942	H	-3.324374	1.328158	3.233889
15943	H	-2.349986	2.165614	2.385201
15944	O	-2.211673	-3.782758	-1.835902
15945	H	-2.761107	-4.440963	-2.273432
15946	H	-2.833528	-3.081528	-1.509546
15947	O	0.385999	4.297115	-1.604651
15948	H	-0.037204	5.106337	-1.908076
15949	H	-0.247534	3.837229	-0.972250
15950	O	-1.273715	-1.528162	0.752229
15951	H	-1.172301	-0.818574	0.064027
15952	H	-2.226250	-1.537675	0.968623
15953	O	-0.442322	-0.439584	3.076297
15954	H	0.383499	-0.856634	3.389855
15955	H	-0.648671	-0.870036	2.212625
15956	O	2.008925	-1.737495	3.513612
15957	H	2.092580	-2.429780	2.798588
15958	H	2.321790	-2.136388	4.331339
15959	O	-3.934758	-1.878561	-1.112455
15960	H	-3.902353	-1.039608	-1.610555
15961	H	-4.147418	-1.641990	-0.195442
15962	O	1.750966	-2.548851	-1.737857
15963	H	1.161982	-3.081233	-1.152985
15964	H	2.664928	-2.840749	-1.570707
15965	O	-2.940899	-0.387576	4.182491
15966	H	-1.988223	-0.462527	3.943806
15967	H	-3.022881	-0.596277	5.117704
15968	O	-0.440957	2.304217	2.486452
15969	H	0.477053	2.665653	2.489993
15970	H	-0.344433	1.350195	2.681618
15971	O	-3.831835	-0.878317	1.546966

15972	H	-3.879986	-1.103258	2.490040
15973	H	-3.593817	0.069955	1.563801
15974	O	-0.745983	0.462824	-0.892676
15975	H	-0.924307	0.381586	-1.866238
15976	H	0.234035	0.315433	-0.772226
15977	O	-3.846160	2.374166	-0.386846
15978	H	-4.107075	2.159020	0.520756
15979	H	-2.944755	2.741491	-0.285794
15980	O	-0.474004	-2.259923	-3.499860
15981	H	-1.043681	-2.842684	-2.965574
15982	H	0.421978	-2.342071	-3.132623
15983	O	2.283220	-3.449408	1.544868
15984	H	1.500997	-3.766654	1.062632
15985	H	2.970279	-3.233780	0.885396
15986	O	-1.153788	2.897410	-0.073438
15987	H	-1.005182	1.972930	-0.428177
15988	H	-0.883176	2.809546	0.869534
15989	O	-1.234632	0.307952	-3.487388
15990	H	-1.031820	-0.649461	-3.632993
15991	H	-2.199321	0.416123	-3.430022
15992	O	3.046500	0.287052	1.864003
15993	H	2.880333	-0.310774	2.613915
15994	H	2.424543	0.006217	1.158624
15995				
15996	Cartesian coordinates of : W27_ 8			
15997				
15998	O	-1.990313	2.205149	0.633468
15999	O	-2.232157	0.188762	2.416053
16000	O	-2.178673	-1.528860	-1.594981
16001	O	-2.355940	1.154985	-1.852575
16002	O	0.790746	2.232472	0.521019
16003	O	0.570505	0.238664	2.366221
16004	O	0.612610	-1.614767	-1.627344
16005	O	0.423868	1.090900	-1.928236
16006	H	-1.980011	1.467804	1.289783
16007	H	-0.299860	0.333257	2.787227
16008	H	-2.161284	-0.547445	-1.704184
16009	H	0.491268	1.517729	-1.042500
16010	H	-1.101594	2.601612	0.646717
16011	H	0.525465	-0.625945	1.893295
16012	H	-1.305212	-1.850584	-1.878177
16013	H	-0.468665	1.284306	-2.259949
16014	H	-3.262912	1.336244	-2.158395
16015	H	1.687276	2.611459	0.513051
16016	H	-3.114768	0.292947	2.810522
16017	H	1.500091	-1.922328	-1.883149
16018	H	-2.280881	1.556955	-0.956462
16019	H	0.798690	1.516776	1.198755
16020	H	-2.271344	-0.667443	1.925123
16021	H	0.616835	-0.637564	-1.754001
16022	H	-3.338481	-2.425639	1.223841
16023	O	-2.427051	-2.140457	1.040831
16024	H	-2.388577	-1.936568	0.076546
16025	H	-0.514227	-2.493624	1.228165
16026	O	0.368494	-2.136049	1.037167
16027	H	0.395385	-1.963518	0.066906
16028	O	3.174684	-2.097177	1.020672
16029	H	3.196444	-1.954034	0.045066
16030	H	2.297540	-2.459957	1.225872
16031	H	4.291908	-1.950389	-1.891689
16032	O	3.394453	-1.657984	-1.647967
16033	H	3.386482	-0.681448	-1.785894
16034	O	3.212513	1.027582	-1.997105
16035	H	3.275066	1.477672	-1.119757
16036	H	2.324744	1.217386	-2.342369
16037	O	3.568900	2.223240	0.394554
16038	H	3.565171	1.523458	1.091264
16039	H	4.483668	2.559502	0.355504
16040	H	3.333993	-0.581646	1.837566
16041	O	3.372059	0.297434	2.285594
16042	H	2.507500	0.391684	2.718033
16043	H	-5.675705	0.342850	3.405076
16044	O	-5.052685	0.291193	2.673365
16045	H	-5.236701	-0.548737	2.184012
16046	H	-5.939259	-2.567684	1.084046

16047	O	-5.223451	-1.914292	1.149964
16048	H	-5.119779	-1.626130	0.212755
16049	O	-4.978821	-1.483511	-1.535827
16050	H	-5.148744	-0.556841	-1.805367
16051	H	-4.065565	-1.691855	-1.803100
16052	O	-5.132964	1.241707	-1.833260
16053	H	-5.033177	1.501256	-0.891017
16054	H	-5.801972	1.866056	-2.154343
16055	O	-4.776520	2.280666	0.699865
16056	H	-4.946000	1.674976	1.446730
16057	H	-3.837684	2.537420	0.755500
16058	H	5.312454	0.524427	2.519402
16059	O	6.187706	0.483768	2.101138
16060	H	6.241569	-0.426774	1.726693
16061	H	6.366446	1.592594	0.999141
16062	O	6.341317	2.282565	0.262398
16063	H	7.055729	2.907212	0.419774
16064	H	6.229869	1.381416	-1.326815
16065	O	6.023557	0.848178	-2.119867
16066	H	5.106795	1.063167	-2.359955
16067	O	6.163766	-1.751930	-1.825713
16068	H	6.210290	-0.762868	-1.960837
16069	H	6.843474	-2.155758	-2.373437
16070	O	6.022558	-1.996453	0.997831
16071	H	5.124551	-2.322808	1.165206
16072	H	6.141671	-2.003343	0.031262
16073	H	-7.030142	4.306656	-1.063744
16074	O	-6.632476	3.432163	-1.065172
16075	H	-6.104459	3.344176	-0.254701
16076	H	-6.369355	-2.801712	-1.231281
16077	O	-6.882308	-3.277855	-0.556855
16078	H	-7.429025	-3.929102	-1.003615
16079				
16080	Cartesian coordinates of : W27_ 9			
16081				
16082	O	-3.100039	1.810750	1.428300
16083	O	-3.488157	-0.781283	2.119861
16084	O	-3.221702	-0.528671	-2.239783
16085	O	-3.383649	1.980529	-1.265305
16086	O	-0.310790	1.779862	1.460783
16087	O	-0.691919	-0.813490	2.208000
16088	O	-0.440536	-0.685398	-2.188164
16089	O	-0.597196	1.870210	-1.243931
16090	H	-3.145567	0.864835	1.702896
16091	H	-1.579038	-0.884296	2.597528
16092	H	-3.194564	0.398028	-1.899388
16093	H	-0.564556	1.856799	-0.258602
16094	H	-2.210149	2.127543	1.660101
16095	H	-0.731791	-1.367374	1.392414
16096	H	-2.338790	-0.716827	-2.602232
16097	H	-1.468139	2.223936	-1.489305
16098	H	-4.275182	2.301799	-1.486768
16099	H	0.590000	2.082882	1.670320
16100	H	-4.394967	-0.839090	2.462853
16101	H	0.456712	-0.870853	-2.517485
16102	H	-3.340701	1.933801	-0.281333
16103	H	-0.364150	0.839515	1.750606
16104	H	-3.510688	-1.309505	1.285416
16105	H	-0.424299	0.242979	-1.859205
16106	H	-4.572686	-2.530823	-0.209255
16107	O	-3.654608	-2.213225	-0.172393
16108	H	-3.542493	-1.602045	-0.940190
16109	H	-1.760791	-2.690996	-0.085653
16110	O	-0.862910	-2.321465	-0.055094
16111	H	-0.772629	-1.739508	-0.846213
16112	O	1.941364	-2.406784	0.061995
16113	H	2.026155	-1.848971	-0.745049
16114	H	1.042813	-2.775501	0.046914
16115	H	3.221389	-1.012195	-2.475669
16116	O	2.335569	-0.815092	-2.124106
16117	H	2.368402	0.118344	-1.812313
16118	O	2.192201	1.769818	-1.232902
16119	H	2.228117	1.775076	-0.248250
16120	H	1.311841	2.099982	-1.478368
16121	O	2.478552	1.736473	1.480199

16122	H	2.428051	0.798308	1.784210
16123	H	3.370057	2.050568	1.707171
16124	H	2.082128	-1.407548	1.476097
16125	O	2.102285	-0.825960	2.272931
16126	H	1.209729	-0.895296	2.650834
16127	H	-7.033299	-0.985785	2.691740
16128	O	-6.322520	-0.785466	2.074452
16129	H	-6.476328	-1.323988	1.263648
16130	H	-7.147785	-2.782714	-0.534060
16131	O	-6.471417	-2.147812	-0.277662
16132	H	-6.372157	-1.489044	-1.034313
16133	O	-6.026991	-0.463706	-2.184369
16134	H	-6.158575	0.479704	-1.963919
16135	H	-5.114003	-0.550572	-2.509220
16136	O	-6.171769	2.182658	-1.318068
16137	H	-6.168182	2.118415	-0.321279
16138	H	-6.832575	2.833688	-1.573101
16139	O	-5.903950	1.902921	1.269592
16140	H	-6.088182	1.002705	1.594341
16141	H	-4.989940	2.111334	1.528749
16142	H	4.003717	-0.880117	2.794118
16143	O	4.912220	-0.804948	2.460676
16144	H	4.928549	-1.380798	1.665951
16145	H	5.213183	0.704710	1.952177
16146	O	5.267853	1.624264	1.563942
16147	H	6.204906	1.858984	1.516002
16148	H	4.904426	1.633861	-0.143866
16149	O	4.973118	1.711536	-1.124829
16150	H	4.121788	2.062882	-1.433357
16151	O	5.106171	-0.814456	-2.197343
16152	H	5.114303	0.109377	-1.866622
16153	H	6.029116	-1.111835	-2.103919
16154	O	4.769520	-2.295235	0.160097
16155	H	3.914342	-2.751373	0.204068
16156	H	4.749470	-1.774105	-0.668055
16157	O	7.555846	1.553275	-0.218872
16158	H	8.381445	1.944004	-0.522237
16159	H	6.857273	1.838430	-0.834764
16160	H	7.540730	-0.414611	-0.357639
16161	O	7.424680	-1.298004	-0.744727
16162	H	6.983749	-1.847125	-0.082744
16163				
16164	Cartesian coordinates of : W27_10			
16165				
16166	O	3.567016	-1.234364	-2.412561
16167	H	3.541027	-1.714134	-1.543613
16168	H	4.378538	-1.508304	-2.854055
16169	H	3.379305	0.500246	-2.242607
16170	O	3.325371	1.479795	-2.207370
16171	H	2.448704	1.717278	-2.554463
16172	O	3.565510	2.714816	0.136387
16173	H	3.540938	2.202095	-0.713603
16174	H	4.377627	3.233264	0.122298
16175	O	3.323096	1.173997	2.378622
16176	H	3.377302	1.696771	1.549426
16177	H	2.446294	1.354219	2.758255
16178	O	3.325293	-2.652724	-0.174940
16179	H	3.378084	-2.194497	0.691628
16180	H	2.448708	-3.072090	-0.208971
16181	H	3.542365	-0.480137	2.254773
16182	O	3.568412	-1.472427	2.276631
16183	H	4.380749	-1.716776	2.733678
16184	H	1.661784	-1.303785	-2.796572
16185	O	0.768621	-1.124866	-2.458524
16186	H	0.712236	-0.150376	-2.323970
16187	H	0.576343	1.932693	-1.300944
16188	O	0.533582	1.578770	-2.218952
16189	H	-0.356823	1.788453	-2.549379
16190	H	1.659184	3.080253	0.271459
16191	O	0.766781	2.696227	0.257811
16192	H	0.711930	2.092651	1.034816
16193	H	0.575825	0.162004	2.320943
16194	O	0.532946	1.133424	2.476951
16195	H	-0.358268	1.313663	2.822334
16196	H	1.661800	-1.772301	2.527282

16197	O	0.768913	-1.568894	2.202618
16198	H	0.711924	-1.943332	1.292977
16199	O	0.534325	-2.717168	-0.257503
16200	H	0.575861	-2.096421	-1.020933
16201	H	-0.356273	-3.107685	-0.273752
16202	H	-1.136956	-1.408569	-2.768246
16203	O	-2.016147	-1.236491	-2.392140
16204	H	-2.055806	-1.728872	-1.537810
16205	H	-2.186199	0.476426	-2.257422
16206	O	-2.249684	1.459937	-2.266703
16207	H	-3.167797	1.668002	-2.518743
16208	H	-1.138058	3.104643	0.167235
16209	O	-2.017072	2.692493	0.127151
16210	H	-2.055290	2.198417	-0.726257
16211	H	-2.185703	1.714229	1.539713
16212	O	-2.249642	1.229035	2.395295
16213	H	-3.167318	1.345085	2.702155
16214	O	-2.017143	-1.461067	2.269226
16215	H	-1.138286	-1.700886	2.606971
16216	H	-2.055498	-0.475002	2.265321
16217	O	-2.249600	-2.698585	-0.130658
16218	H	-3.167543	-3.021008	-0.186391
16219	H	-2.187045	-2.201130	0.717851
16220	H	-3.912424	-1.243708	-2.712862
16221	O	-4.825826	-1.161993	-2.390617
16222	H	-5.007463	-0.206165	-2.311223
16223	H	-5.696487	2.108769	-2.717919
16224	O	-5.032930	1.631531	-2.209961
16225	H	-5.038420	2.008625	-1.283837
16226	O	-5.033487	-2.735157	-0.308449
16227	H	-5.697331	-3.412796	-0.470267
16228	H	-5.038840	-2.118553	-1.095752
16229	H	-5.008779	-1.901120	1.332093
16230	O	-4.827520	-1.486888	2.197327
16231	H	-3.916572	-1.729269	2.434111
16232	O	-5.033433	1.103670	2.518522
16233	H	-5.694036	1.302712	3.189429
16234	H	-5.040337	0.113885	2.376934
16235	H	-3.913089	2.976996	0.279731
16236	O	-4.827028	2.658533	0.189512
16237	H	-5.010395	2.115369	0.979604
16238	H	5.366671	1.412243	-1.858037
16239	O	5.999505	1.096885	-1.200181
16240	H	5.979250	0.123497	-1.237120
16241	O	5.997827	0.490583	1.552601
16242	H	5.985785	1.007995	0.727165
16243	H	5.362257	0.906460	2.149159
16244	H	5.365529	-2.317023	-0.290652
16245	O	5.997263	-1.588966	-0.350447
16246	H	5.981424	-1.133862	0.510854
16247				
16248				
16249	Cartesian coordinates of the water 28-mer			
16250				
16251	Cartesian coordinates of : W28_1			
16252				
16253	O	2.717192	-3.301221	-2.292039
16254	H	2.388608	-3.672728	-1.417090
16255	H	3.102708	-4.021187	-2.799595
16256	O	1.630516	-4.059791	-0.070326
16257	H	1.932904	-3.627895	0.751169
16258	H	0.693192	-3.803634	-0.160381
16259	O	3.389629	-0.822753	-1.372673
16260	H	3.360120	-1.654028	-1.883700
16261	H	3.643608	-0.076301	-1.948706
16262	O	0.469631	-1.661611	-2.523708
16263	H	1.201257	-2.294893	-2.645181
16264	H	-0.028788	-1.971011	-1.735261
16265	O	4.408148	-0.875602	1.214004
16266	H	3.742078	-1.406255	1.690427
16267	H	4.168459	-0.937082	0.268793
16268	O	3.647905	1.617572	-2.618097
16269	H	3.600905	2.201774	-1.802973
16270	H	4.319731	1.991970	-3.196153
16271	O	2.102804	-2.280997	2.045443

16272	H	1.589521	-1.634595	1.515447
16273	H	1.679988	-2.309758	2.922061
16274	O	-0.849458	-2.777125	-0.398367
16275	H	-1.733145	-3.084925	-0.677144
16276	H	-0.975455	-2.322613	0.460918
16277	O	-1.353099	-0.469022	-4.236246
16278	H	-0.864128	0.357490	-4.348736
16279	H	-0.696338	-1.072405	-3.840633
16280	O	1.000386	0.967717	-3.206834
16281	H	0.941865	0.063954	-2.835447
16282	H	1.941108	1.225284	-3.176478
16283	O	1.226706	-0.436677	0.268639
16284	H	1.849464	-0.561313	-0.478150
16285	H	0.322247	-0.278244	-0.079195
16286	O	-3.547347	-3.116366	-1.046568
16287	H	-3.852005	-2.786130	-0.149965
16288	H	-4.070509	-3.889682	-1.277760
16289	O	4.518381	1.645046	1.772736
16290	H	4.575087	0.656996	1.595633
16291	H	5.284239	1.905413	2.293113
16292	O	3.547324	3.063805	-0.460004
16293	H	3.940287	2.637867	0.325801
16294	H	2.714319	3.479375	-0.179160
16295	O	-3.076999	-0.629407	-2.147004
16296	H	-2.586301	-0.564265	-2.998526
16297	H	-3.330497	-1.559784	-1.996696
16298	O	0.385178	-1.929796	4.248809
16299	H	0.337978	-2.278770	5.143689
16300	H	0.261536	-0.939241	4.289040
16301	O	-1.369328	-1.739809	2.119055
16302	H	-0.851524	-2.064300	2.880248
16303	H	-1.447460	-0.775646	2.239096
16304	O	-1.282248	0.363158	-0.373665
16305	H	-1.037390	1.200232	-0.842205
16306	H	-1.924991	-0.105970	-0.956250
16307	O	1.794723	1.464156	2.097977
16308	H	2.752859	1.600116	2.226645
16309	H	1.695589	0.759476	1.415126
16310	O	-0.392001	2.569253	-1.590626
16311	H	0.149088	2.085592	-2.262400
16312	H	0.212199	2.919610	-0.891015
16313	O	-4.026323	-2.152314	1.310364
16314	H	-4.393918	-1.249858	1.381600
16315	H	-3.163407	-2.131491	1.762441
16316	O	0.932934	3.529080	0.548071
16317	H	1.179700	2.817549	1.179595
16318	H	0.103083	3.907896	0.906719
16319	O	-0.005401	0.639902	3.986414
16320	H	0.715409	1.003775	3.430883
16321	H	-0.826138	0.909460	3.541955
16322	O	-2.099038	1.038844	2.074116
16323	H	-3.072245	0.943649	2.097624
16324	H	-1.845997	0.849831	1.134340
16325	O	-4.534389	1.398585	-0.930167
16326	H	-4.143634	0.695210	-1.484394
16327	H	-3.985631	2.194339	-1.060369
16328	O	-2.817726	3.606516	-1.252902
16329	H	-1.928596	3.313233	-1.563618
16330	H	-3.095196	4.342220	-1.807973
16331	O	-4.757748	0.535808	1.487549
16332	H	-5.587565	0.812710	1.888423
16333	H	-4.728054	0.909990	0.551426
16334	O	-1.676963	3.861260	1.375633
16335	H	-2.232279	3.902035	0.579833
16336	H	-1.865048	3.001255	1.786407
16337				
16338	Cartesian coordinates of : W28_2			
16339				
16340	O	-2.679762	0.006882	1.942234
16341	O	-2.866485	1.939345	-0.009447
16342	O	-5.455058	-0.111179	1.928471
16343	O	-5.637651	-1.928863	-0.110784
16344	O	-5.455115	0.111135	-1.928477
16345	O	-5.637686	1.928826	0.110805
16346	O	-2.679793	-0.006866	-1.942258

16347	O	-2.866488	-1.939303	0.009433
16348	O	-8.408630	-2.006034	0.069418
16349	O	-8.252990	-0.065763	1.835356
16350	H	-5.461079	-0.853706	1.283089
16351	H	-4.570588	-0.101896	2.332106
16352	H	-3.761531	2.319947	0.019476
16353	H	-2.846023	1.336412	-0.785891
16354	H	-5.461144	0.853667	-1.283104
16355	H	-4.570648	0.101878	-2.332121
16356	H	-2.846037	-1.336332	0.785851
16357	H	-3.761515	-2.319951	-0.019497
16358	H	-2.704250	0.783257	1.339870
16359	H	-1.784451	-0.019091	2.321881
16360	H	-5.614812	1.284392	0.853521
16361	H	-5.614771	-1.284527	-0.853576
16362	H	-2.704260	-0.783242	-1.339897
16363	H	-1.784500	0.019108	-2.321952
16364	H	-8.401295	0.766193	1.349833
16365	H	-7.348823	-0.022937	2.190510
16366	H	-8.429269	-1.336926	0.809994
16367	H	-6.549035	-2.271818	-0.073284
16368	H	-6.549090	2.271747	0.073355
16369	H	-9.103571	-2.651869	0.228688
16370	H	0.071995	0.856106	-1.292681
16371	O	0.094179	0.112983	-1.936090
16372	H	0.989144	0.104733	-2.317767
16373	H	-0.071998	1.292736	0.855991
16374	O	-0.094205	1.936157	0.112873
16375	H	-0.989150	2.317878	0.104688
16376	H	-0.072162	-1.292437	-0.855954
16377	O	-0.094237	-1.935952	-0.112911
16378	H	-0.989167	-2.317713	-0.104690
16379	H	0.072132	-0.855851	1.292460
16380	O	0.094266	-0.112815	1.935987
16381	H	0.989205	-0.104667	2.317725
16382	H	3.761544	-0.019392	2.319958
16383	O	2.866521	0.009484	1.939294
16384	H	2.846063	0.785893	1.336320
16385	H	1.784473	-2.321852	-0.019157
16386	O	2.679799	-1.942244	0.006854
16387	H	2.704313	-1.339907	0.783248
16388	H	1.784465	2.321998	0.019055
16389	O	2.679764	1.942317	-0.006933
16390	H	2.704223	1.339986	-0.783330
16391	H	2.846017	-0.785813	-1.336291
16392	O	2.866438	-0.009427	-1.939312
16393	H	3.761463	0.019512	-2.319959
16394	O	-8.253087	0.065661	-1.835327
16395	H	-7.348934	0.022828	-2.190517
16396	H	-8.401376	-0.766292	-1.349799
16397	O	5.455073	1.928613	0.111220
16398	H	4.570582	2.332207	0.101901
16399	H	5.461127	1.283326	0.853811
16400	H	5.614796	0.853575	-1.284330
16401	O	5.637627	0.110854	-1.928752
16402	H	6.549037	0.073310	-2.271653
16403	H	5.614778	-0.853434	1.284619
16404	O	5.637708	-0.110661	1.928972
16405	H	6.549096	-0.073252	2.271929
16406	H	5.460993	-1.282877	-0.853489
16407	O	5.455101	-1.928349	-0.111030
16408	H	4.570687	-2.332105	-0.101786
16409	H	-8.429187	1.336724	-0.809886
16410	O	-8.408615	2.005860	-0.069322
16411	H	-9.103603	2.651635	-0.228649
16412	H	7.348904	2.190389	0.022808
16413	O	8.253060	1.835212	0.065637
16414	H	8.401374	1.349717	-0.766329
16415	H	8.429181	0.809715	1.336709
16416	O	8.408674	0.069200	2.005893
16417	H	9.103687	0.228641	2.651614
16418	H	8.401542	-1.350034	0.766165
16419	O	8.253082	-1.835532	-0.065776
16420	H	7.348828	-2.190466	-0.022871
16421	H	8.429146	-0.810073	-1.336843

16422	O	8.408530	-0.069543	-2.006018
16423	H	9.103317	-0.229048	-2.651965
16424				
16425	Cartesian coordinates of : W28_3			
16426				
16427	O	3.161911	-3.877290	0.759572
16428	H	3.233698	-3.078700	1.311653
16429	H	2.276009	-4.242950	0.912828
16430	O	5.189594	0.235207	0.570211
16431	H	5.212193	-0.131680	-0.330569
16432	H	4.608171	-0.363143	1.074558
16433	O	-1.874487	-2.492621	-1.668575
16434	H	-2.813041	-2.600100	-1.902905
16435	H	-1.718403	-1.520012	-1.685804
16436	O	0.937514	2.978271	-2.477614
16437	H	1.303079	3.703326	-1.920180
16438	H	1.619819	2.278646	-2.493800
16439	O	-3.563224	3.098331	-1.401851
16440	H	-4.055703	2.267716	-1.294444
16441	H	-2.938493	2.949529	-2.132260
16442	O	1.404934	-0.044572	3.682611
16443	H	1.398074	-0.027751	4.644315
16444	H	1.407521	0.886379	3.353634
16445	O	-4.671461	-2.169689	-1.686780
16446	H	-4.669136	-1.203200	-1.472672
16447	H	-5.394863	-2.337567	-2.298411
16448	O	3.570864	2.376994	0.523607
16449	H	4.322829	1.742675	0.615936
16450	H	3.010667	2.272146	1.313523
16451	O	0.108962	4.651163	1.729097
16452	H	-0.033818	5.501786	2.155925
16453	H	-0.772150	4.317585	1.436653
16454	O	-4.308739	0.344532	-0.796704
16455	H	-3.327996	0.309010	-0.803460
16456	H	-4.598023	0.276914	0.134155
16457	O	0.476085	-4.880827	0.707319
16458	H	-0.317386	-4.348733	0.958376
16459	H	0.288515	-5.804234	0.901616
16460	O	-1.667476	0.185793	-1.482059
16461	H	-1.643098	0.794667	-2.246937
16462	H	-0.989251	0.541218	-0.867361
16463	O	2.553163	0.971342	-1.585667
16464	H	3.313193	0.445626	-1.915179
16465	H	2.903853	1.491920	-0.822897
16466	O	-2.577730	1.096910	2.139394
16467	H	-1.865465	0.440666	2.007761
16468	H	-3.414406	0.606751	2.207542
16469	O	-1.512954	2.338687	-3.244809
16470	H	-1.614405	2.402997	-4.199772
16471	H	-0.605486	2.673534	-3.026563
16472	O	-1.583460	-3.173645	0.973720
16473	H	-1.241422	-2.368555	1.420298
16474	H	-1.653637	-2.930460	0.021777
16475	O	-0.551714	-0.770880	1.819501
16476	H	0.032091	-0.681990	1.031866
16477	H	0.028823	-0.668153	2.597099
16478	O	4.645130	-0.742644	-2.061302
16479	H	4.249489	-1.664962	-1.984063
16480	H	5.292267	-0.769661	-2.772742
16481	O	3.564566	-3.080784	-1.818634
16482	H	2.652767	-3.166013	-2.137242
16483	H	3.528027	-3.423532	-0.895900
16484	O	-4.942937	-0.376829	1.824462
16485	H	-5.756267	-0.308081	2.333173
16486	H	-4.770258	-1.343679	1.641820
16487	O	-4.389864	-2.820739	1.070972
16488	H	-3.454641	-3.072665	1.190131
16489	H	-4.557472	-2.824320	0.112601
16490	O	1.959901	4.476566	-0.480412
16491	H	2.711985	3.959103	-0.144830
16492	H	1.361013	4.621057	0.272144
16493	O	0.765827	-3.354863	-1.624856
16494	H	0.738251	-4.064065	-0.955460
16495	H	-0.150731	-3.241051	-1.932563
16496	O	1.389625	2.202949	2.256971

16497	H	1.048591	3.098725	2.428860
16498	H	0.908985	1.930750	1.438786
16499	O	-2.021367	3.310464	0.814325
16500	H	-2.635931	3.388373	0.046701
16501	H	-2.364436	2.572630	1.380090
16502	O	1.168338	-0.978541	-0.255421
16503	H	1.100403	-1.814503	-0.765084
16504	H	1.561735	-0.282883	-0.829341
16505	O	-0.000622	1.784742	-0.030775
16506	H	-0.746023	2.398873	0.201093
16507	H	0.445011	2.192018	-0.797970
16508	O	3.077900	-1.253909	1.731537
16509	H	2.671978	-0.929766	2.553335
16510	H	2.406655	-1.125170	1.027450
16511				
16512	Cartesian coordinates of : W28_4			
16513				
16514	O	3.489305	-2.271644	0.316909
16515	O	3.780787	-0.362283	2.227636
16516	O	3.446704	1.619314	-1.687467
16517	O	3.624187	-1.047268	-2.107141
16518	O	0.728813	-2.277227	0.296004
16519	O	0.984821	-0.473664	2.330452
16520	O	0.674736	1.740655	-1.513139
16521	O	0.837528	-0.923353	-2.076509
16522	H	3.528627	-1.585385	1.023536
16523	H	1.877812	-0.573846	2.699874
16524	H	3.451448	0.646729	-1.856730
16525	H	0.808968	0.045020	-1.894569
16526	H	2.602558	-2.669304	0.372626
16527	H	0.915246	-1.133667	1.601554
16528	H	2.556276	1.936331	-1.918418
16529	H	1.712066	-1.106665	-2.458565
16530	H	4.520088	-1.187793	-2.461541
16531	H	-0.171218	-2.636425	0.398490
16532	H	4.702582	-0.475729	2.516595
16533	H	-0.230162	2.015927	-1.745126
16534	H	3.598109	-1.503080	-1.233406
16535	H	0.733171	-1.795969	-0.563476
16536	H	3.762082	0.515023	1.777599
16537	H	0.760606	1.854389	-0.538841
16538	H	4.733468	2.342329	1.089955
16539	O	3.818700	2.043486	0.956315
16540	H	3.706157	1.900704	-0.014265
16541	H	1.940912	2.359196	1.324477
16542	O	1.043639	2.012943	1.186069
16543	H	1.026812	1.125082	1.613099
16544	O	-1.728146	2.060466	1.177909
16545	H	-1.834890	1.944083	0.205441
16546	H	-0.832768	2.408770	1.322985
16547	H	-3.018098	1.977024	-1.679673
16548	O	-2.103437	1.687728	-1.502606
16549	H	-2.092710	0.717729	-1.666544
16550	O	-1.949733	-1.018977	-1.914514
16551	H	-1.944463	-1.471865	-1.040636
16552	H	-1.076520	-1.181851	-2.308855
16553	O	-2.010774	-2.266589	0.530104
16554	H	-1.997190	-1.581370	1.241207
16555	H	-2.883967	-2.693157	0.577837
16556	H	-1.820198	0.522700	1.993126
16557	O	-1.833164	-0.352861	2.446692
16558	H	-0.940085	-0.452762	2.817159
16559	H	6.524762	-1.175138	1.333289
16560	O	6.601418	-0.519687	2.097101
16561	H	7.260381	-0.869930	2.705454
16562	H	7.341853	2.547852	1.360556
16563	O	6.632925	1.981654	1.039703
16564	H	6.728148	1.103742	1.478450
16565	O	6.242682	1.556787	-1.742716
16566	H	6.451598	1.758017	-0.812981
16567	H	5.327833	1.851150	-1.894849
16568	O	6.407418	-0.986484	-2.354130
16569	H	6.428703	-0.005981	-2.163911
16570	H	7.052021	-1.170506	-3.044364
16571	O	6.270355	-2.190282	0.156506

16572	H	5.360096	-2.534523	0.177650
16573	H	6.421000	-1.846312	-0.745824
16574	H	-3.891104	-1.010707	-2.178395
16575	O	-4.739450	-0.856416	-1.730755
16576	H	-4.797975	0.125027	-1.558081
16577	O	-4.850514	1.746774	-1.264970
16578	H	-5.768978	2.029921	-1.443087
16579	H	-4.748543	1.874740	-0.281812
16580	O	-4.516413	2.042603	1.339728
16581	H	-4.608709	1.164524	1.758162
16582	H	-3.609347	2.333538	1.525124
16583	H	-3.806197	-0.535201	2.882138
16584	O	-4.680513	-0.514060	2.460852
16585	H	-4.685791	-1.259898	1.827396
16586	H	-5.578454	-2.910676	0.345261
16587	O	-4.759111	-2.411761	0.462978
16588	H	-4.723466	-1.809408	-0.322409
16589	H	-7.477669	1.408945	-0.217150
16590	O	-7.557150	2.022794	-0.977823
16591	H	-8.021908	2.801577	-0.659210
16592	H	-6.439825	-1.638317	-1.642705
16593	O	-7.100966	-2.044531	-1.050900
16594	H	-7.932180	-2.097354	-1.532357
16595	O	-7.159905	0.051919	0.886745
16596	H	-6.534874	-0.023054	1.620594
16597	H	-7.124033	-0.774468	0.375898
16598				
16599	Cartesian coordinates of : W28_ 5			
16600				
16601	O	3.609400	-1.911651	0.663571
16602	H	3.560552	-1.109550	1.231081
16603	H	4.518404	-2.257092	0.741807
16604	H	3.285637	-1.616496	-0.982664
16605	O	3.163006	-1.513680	-1.957870
16606	H	2.300892	-1.910913	-2.170793
16607	O	3.234388	0.972421	-2.879475
16608	H	3.250960	0.045467	-2.520614
16609	H	4.020752	1.072972	-3.427550
16610	O	2.707348	3.040288	-1.089680
16611	H	2.972887	2.385267	-1.763280
16612	H	1.756528	3.201962	-1.216259
16613	O	3.241047	0.182589	2.395463
16614	H	3.221554	1.102877	2.061293
16615	H	2.368955	0.012300	2.791334
16616	H	3.059645	2.947845	0.508676
16617	O	3.133875	2.807838	1.491317
16618	H	3.881979	3.332577	1.796197
16619	H	1.794984	-2.509403	0.827021
16620	O	0.851673	-2.286563	0.738785
16621	H	0.709986	-2.064029	-0.209464
16622	H	0.353863	-0.867613	-2.182163
16623	O	0.410861	-1.814592	-1.916752
16624	H	-0.453368	-2.212775	-2.116706
16625	H	1.273235	0.939476	-3.158037
16626	O	0.401882	0.768704	-2.763783
16627	H	0.272882	1.450699	-2.064529
16628	H	0.062337	2.514210	0.008504
16629	O	-0.052949	2.733816	-0.945630
16630	H	-0.977117	3.013912	-1.057711
16631	H	1.244831	2.698150	1.882531
16632	O	0.384439	2.287061	1.692125
16633	H	0.457155	1.341555	1.959784
16634	O	0.488203	-0.291992	2.547112
16635	H	0.570863	-0.986073	1.851856
16636	H	-0.365026	-0.447953	2.986681
16637	H	-0.990666	-2.840724	1.083919
16638	O	-1.911939	-2.545112	0.994644
16639	H	-2.008014	-1.752002	1.574492
16640	H	-2.201835	-2.259472	-0.682878
16641	O	-2.328862	-2.175801	-1.656866
16642	H	-3.227780	-2.503999	-1.841094
16643	H	-1.530662	0.512552	-3.093001
16644	O	-2.374559	0.337879	-2.645252
16645	H	-2.304979	-0.560837	-2.243336
16646	H	-2.670300	1.614721	-1.518470

16647	O	-2.807822	2.402690	-0.942965
16648	H	-3.758772	2.610397	-0.986069
16649	O	-2.394367	2.045381	1.705433
16650	H	-1.542815	2.451363	1.938293
16651	H	-2.492412	2.136558	0.727968
16652	O	-2.288442	-0.477296	2.691715
16653	H	-3.173702	-0.665561	3.053037
16654	H	-2.346314	0.416825	2.281262
16655	H	-3.759800	-3.069286	1.063715
16656	O	-4.706131	-2.846630	1.065809
16657	H	-4.956817	-2.691212	0.135363
16658	H	-5.740154	-2.938370	-2.176765
16659	O	-5.104712	-2.411984	-1.681715
16660	H	-5.217540	-1.460509	-1.967907
16661	O	-5.029852	-0.970070	2.864594
16662	H	-5.622495	-1.270794	3.560525
16663	H	-4.995334	-1.688351	2.170069
16664	H	-5.234772	0.736188	2.201269
16665	O	-5.170976	1.649052	1.861536
16666	H	-4.277097	1.963020	2.079015
16667	O	-5.572904	2.185962	-0.668518
16668	H	-6.323080	2.781323	-0.761619
16669	H	-5.498974	1.948390	0.300089
16670	H	-4.298871	0.301955	-2.827028
16671	O	-5.178240	0.080775	-2.477573
16672	H	-5.413324	0.786271	-1.844668
16673	H	5.144787	-1.497180	-2.109876
16674	O	5.907228	-1.009044	-1.765753
16675	H	6.263068	-1.546987	-1.036227
16676	O	6.039067	-0.032946	2.114998
16677	H	5.755550	0.520487	1.354532
16678	H	5.246515	-0.086755	2.670107
16679	H	7.033105	-2.877560	1.055708
16680	O	6.384169	-2.239223	0.744989
16681	H	6.403948	-1.448299	1.353442
16682	H	4.152545	1.249498	-0.302411
16683	O	5.100752	1.109325	-0.196256
16684	H	5.358964	0.433404	-0.860480

16685

16686 Cartesian coordinates of : W28_6

16687

16688	O	-3.561686	2.020459	-0.947423
16689	O	-3.860942	1.417205	1.679599
16690	O	-3.360993	-2.308395	-0.545633
16691	O	-3.632305	-0.310332	-2.339831
16692	O	-0.794135	2.247529	-0.919734
16693	O	-1.075240	1.692048	1.734703
16694	O	-0.604074	-2.124672	-0.412694
16695	O	-0.835108	-0.127299	-2.265871
16696	H	-3.579753	1.820911	0.018027
16697	H	-1.982617	1.935483	1.982322
16698	H	-3.379632	-1.581441	-1.213997
16699	H	-0.882451	0.735953	-1.793091
16700	H	-2.701108	2.436131	-1.129169
16701	H	-1.036817	0.712770	1.854229
16702	H	-2.451557	-2.654642	-0.546401
16703	H	-1.702220	-0.255103	-2.685449
16704	H	-4.520322	-0.432962	-2.718994
16705	H	0.078049	2.639948	-1.099767
16706	H	-4.785403	1.628297	1.890603
16707	H	0.319673	-2.434504	-0.393656
16708	H	-3.660428	0.542755	-1.846248
16709	H	-0.819711	2.063809	0.048350
16710	H	-3.807718	0.435101	1.774499
16711	H	-0.628173	-1.408911	-1.089080
16712	H	-4.719705	-1.521926	2.185514
16713	O	-3.819562	-1.279597	1.909830
16714	H	-3.694463	-1.667850	1.010204
16715	H	-1.904148	-1.276147	2.360398
16716	O	-1.028021	-1.013380	2.033153
16717	H	-0.928367	-1.434226	1.146203
16718	O	1.782733	-0.739929	2.145263
16719	H	1.869638	-1.181613	1.267048
16720	H	0.908762	-0.994354	2.484684
16721	H	3.047613	-2.232927	-0.279980

16722	O	2.127777	-1.903884	-0.287051
16723	H	2.117425	-1.195853	-0.970919
16724	O	1.976572	0.066350	-2.184931
16725	H	1.909926	0.935982	-1.724071
16726	H	1.116285	-0.078168	-2.613126
16727	O	1.969027	2.445605	-0.881009
16728	H	1.936620	2.263953	0.089590
16729	H	2.839903	2.846076	-1.053025
16730	H	1.759264	0.957755	1.914815
16731	O	1.708257	1.933618	1.761127
16732	H	0.803185	2.179837	2.015379
16733	H	-7.423280	1.582420	2.148845
16734	O	-6.687357	1.179447	1.677152
16735	H	-6.765067	0.203200	1.790078
16736	H	-7.266142	-2.098735	2.270481
16737	O	-6.628735	-1.534910	1.820928
16738	H	-6.513226	-1.896540	0.886235
16739	O	-6.154176	-2.437904	-0.549361
16740	H	-6.332028	-1.827306	-1.291894
16741	H	-5.219412	-2.698978	-0.623894
16742	O	-6.423939	-0.479737	-2.516537
16743	H	-6.491917	0.375177	-2.004303
16744	H	-7.088500	-0.462989	-3.212040
16745	O	-6.344807	1.715507	-1.091090
16746	H	-6.515598	1.581280	-0.141096
16747	H	-5.455121	2.103099	-1.160364
16748	H	3.569275	2.451730	1.906149
16749	O	4.484956	2.284418	1.626054
16750	H	4.625945	1.326156	1.796362
16751	H	4.710399	2.645520	0.127085
16752	O	4.719861	2.802727	-0.872301
16753	H	5.372703	3.482393	-1.065241
16754	H	4.754486	1.207301	-1.646797
16755	O	4.790428	0.306898	-2.036356
16756	H	3.925397	0.149666	-2.452364
16757	O	4.836166	-1.846183	-0.236388
16758	H	4.914735	-1.119306	-0.884543
16759	H	5.682511	-2.355913	-0.257407
16760	O	4.627986	-0.418636	2.063546
16761	H	3.793962	-0.636981	2.508854
16762	H	4.658328	-0.985919	1.258210
16763	O	7.436753	-0.288172	-1.497370
16764	H	8.126780	0.197831	-1.959648
16765	H	6.596571	-0.087129	-1.949584
16766	H	7.676801	-2.320996	-0.920402
16767	O	7.335047	-2.875383	-0.203769
16768	H	7.558266	-2.360991	0.594594
16769	O	7.465269	-0.620683	1.440838
16770	H	6.664093	-0.482541	1.967883
16771	H	7.320264	-0.177311	0.591149
16772	Cartesian coordinates of : W28_7			
16774	O	-3.502947	-2.173463	-0.758927
16776	O	-3.685055	0.060722	-2.296845
16777	O	-3.494231	1.299896	1.910430
16778	O	-3.718791	-1.391109	1.835856
16779	O	-0.746465	-2.236636	-0.641951
16780	O	-0.888774	-0.083036	-2.309692
16781	O	-0.715381	1.389123	1.879309
16782	O	-0.928083	-1.329461	1.930300
16783	H	-3.505616	-1.368956	-1.328192
16784	H	-1.768418	-0.092101	-2.722578
16785	H	-3.519643	0.312469	1.898404
16786	H	-0.884805	-0.344905	1.930348
16787	H	-2.620476	-2.572562	-0.855694
16788	H	-0.859541	-0.870054	-1.716021
16789	H	-2.613718	1.549561	2.239780
16790	H	-1.816063	-1.564544	2.247057
16791	H	-4.630028	-1.576271	2.124943
16792	H	0.151838	-2.590025	-0.775508
16793	H	-4.593718	0.017268	-2.641530
16794	H	0.183364	1.596398	2.191266
16795	H	-3.660124	-1.690341	0.898443
16796	H	-0.776124	-1.919359	0.290022

16797	H	-3.676685	0.841795	-1.695150
16798	H	-0.761189	1.683482	0.941155
16799	H	-4.644612	2.538069	-0.742665
16800	O	-3.738941	2.207149	-0.623107
16801	H	-3.673029	1.890651	0.309882
16802	H	-1.846350	2.539755	-0.849460
16803	O	-0.959901	2.156563	-0.739553
16804	H	-0.936866	1.356781	-1.315012
16805	O	1.800490	2.178573	-0.615940
16806	H	1.867933	1.877628	0.319468
16807	H	0.908098	2.548201	-0.727454
16808	H	2.948737	1.547100	2.275288
16809	O	2.064556	1.294697	1.957421
16810	H	2.046605	0.308694	1.940541
16811	O	1.870131	-1.415564	1.863171
16812	H	1.898635	-1.716293	0.926669
16813	H	0.982136	-1.639455	2.188939
16814	O	1.993428	-2.222255	-0.763853
16815	H	2.018491	-1.419961	-1.335158
16816	H	2.867112	-2.642904	-0.853770
16817	H	1.901659	0.803819	-1.707348
16818	O	1.933287	0.030178	-2.315881
16819	H	1.052559	0.003903	-2.726838
16820	H	-6.478862	-0.864429	-1.695177
16821	O	-6.508106	-0.082689	-2.332858
16822	H	-7.135949	-0.306087	-3.027557
16823	H	-7.235008	2.823063	-1.088230
16824	O	-6.544817	2.195485	-0.851590
16825	H	-6.638230	1.411088	-1.441455
16826	O	-6.290440	1.282831	1.828445
16827	H	-6.450164	1.639554	0.936388
16828	H	-5.381502	1.530251	2.071713
16829	O	-6.509207	-1.323765	1.982485
16830	H	-6.512044	-0.324891	1.968569
16831	H	-7.188806	-1.614853	2.598216
16832	O	-6.288194	-2.068622	-0.696487
16833	H	-5.382994	-2.423457	-0.742056
16834	H	-6.468948	-1.879195	0.245091
16835	H	3.837837	-1.533212	2.241525
16836	O	4.699374	-1.315281	1.850936
16837	H	4.781064	-0.335516	1.896799
16838	O	4.842023	1.410009	1.858884
16839	H	5.741994	1.739751	2.016920
16840	H	4.693283	1.677450	0.920051
16841	O	4.562095	2.202149	-0.717990
16842	H	4.645031	1.385893	-1.252901
16843	H	3.657384	2.525970	-0.865466
16844	H	3.930596	-0.106003	-2.673549
16845	O	4.758363	-0.159001	-2.168523
16846	H	4.698424	-0.989486	-1.633655
16847	H	5.604220	-2.729909	-0.618267
16848	O	4.708983	-2.350102	-0.618138
16849	H	4.659477	-1.947802	0.287090
16850	H	6.459940	2.832357	0.018002
16851	O	7.136795	2.414282	0.569580
16852	H	7.408351	1.646223	0.043316
16853	H	6.786702	-1.985345	1.274533
16854	O	7.252252	-2.185835	0.450671
16855	H	7.398060	-1.334375	0.007488
16856	H	6.565689	0.122630	-1.818509
16857	O	7.378221	0.153682	-1.279250
16858	H	8.118960	0.124326	-1.893958
16859				
16860	Cartesian coordinates of : W28_ 8			
16861				
16862	O	3.107275	-2.773685	1.691724
16863	H	3.175205	-1.811960	1.880690
16864	H	3.695687	-3.161104	2.359648
16865	H	3.088938	-3.093364	-0.074944
16866	O	2.891717	-3.118302	-1.034325
16867	H	1.934557	-3.277338	-1.118318
16868	O	3.377893	-0.923183	-2.640767
16869	H	3.230298	-1.578269	-1.924056
16870	H	3.962759	-1.405781	-3.247472
16871	O	3.494997	1.644208	-1.664644

16872	H	3.572477	0.742657	-2.043677
16873	H	2.579130	1.935380	-1.831502
16874	O	3.230124	-0.210141	2.712943
16875	H	3.520690	0.566696	2.188799
16876	H	2.317577	-0.029158	2.999374
16877	H	3.716547	1.759377	0.161153
16878	O	3.695704	1.982637	1.113878
16879	H	4.387940	2.667094	1.240946
16880	H	1.225959	-2.848325	1.793424
16881	O	0.350585	-2.479922	1.572133
16882	H	0.293013	-2.494248	0.589711
16883	H	0.263532	-1.859158	-1.666215
16884	O	0.125630	-2.680697	-1.137768
16885	H	-0.793826	-2.954415	-1.294583
16886	H	1.530080	-0.675687	-3.009959
16887	O	0.626828	-0.511368	-2.683230
16888	H	0.668528	0.351789	-2.211154
16889	H	0.753649	1.976656	-0.530247
16890	O	0.725124	1.947753	-1.518710
16891	H	-0.105590	2.379429	-1.780531
16892	H	1.899632	2.329638	1.270083
16893	O	0.947120	2.142182	1.152073
16894	H	0.767743	1.321892	1.665145
16895	O	0.429712	-0.028310	2.718597
16896	H	0.356448	-0.900737	2.264012
16897	H	-0.439822	0.146900	3.115979
16898	H	-1.569061	-2.489388	1.889099
16899	O	-2.394334	-2.038660	1.643514
16900	H	-2.313432	-1.111984	1.972242
16901	H	-2.567758	-2.201239	-0.072338
16902	O	-2.649425	-2.384511	-1.037009
16903	H	-3.595586	-2.549664	-1.200146
16904	H	-1.271037	-0.438511	-3.088918
16905	O	-2.141123	-0.295108	-2.680198
16906	H	-2.274921	-1.036518	-2.043063
16907	H	-2.101632	1.281957	-1.964527
16908	O	-2.051067	2.211138	-1.640780
16909	H	-2.925522	2.603477	-1.816377
16910	O	-1.797384	2.556470	1.030757
16911	H	-0.876079	2.809062	1.210907
16912	H	-1.849653	2.372287	0.062812
16913	O	-2.317883	0.462103	2.675993
16914	H	-3.230926	0.586051	2.992268
16915	H	-2.149655	1.194120	2.038040
16916	H	-4.308081	-2.097069	1.690834
16917	O	-5.177326	-1.686436	1.545039
16918	H	-5.362198	-1.760198	0.589278
16919	H	-6.146730	-2.483454	-1.611920
16920	O	-5.410070	-1.993211	-1.233875
16921	H	-5.301401	-1.156965	-1.771212
16922	O	-5.105301	0.655537	2.715546
16923	H	-5.773617	0.694716	3.406703
16924	H	-5.213773	-0.221271	2.247332
16925	H	-4.876586	2.109860	1.611239
16926	O	-4.588387	2.855890	1.051380
16927	H	-3.648326	3.004004	1.250544
16928	O	-4.796650	2.714348	-1.554250
16929	H	-5.367615	3.417840	-1.878177
16930	H	-4.802239	2.761835	-0.555240
16931	H	-3.999004	0.049965	-2.990857
16932	O	-4.913009	0.139391	-2.671463
16933	H	-4.981063	1.027812	-2.272977
16934	H	4.056831	-3.610421	-2.471939
16935	O	4.510639	-3.341017	-3.289237
16936	H	5.152062	-4.020878	-3.510435
16937	O	5.644865	3.893511	0.979674
16938	H	5.502706	4.809396	1.235280
16939	H	5.723756	3.876460	0.002602
16940	H	4.333737	-1.373277	3.754008
16941	O	4.678828	-2.272156	3.894023
16942	H	5.151804	-2.282754	4.729740
16943	H	4.798232	2.859067	-1.846040
16944	O	5.499871	3.530632	-1.720982
16945	H	6.225992	3.294962	-2.305343
16946				

16947 Cartesian coordinates of : W28_ 9

16948				
16949	0	-1.638514	2.431363	0.418502
16950	0	-1.966773	0.577644	2.389861
16951	0	-1.943430	-1.352012	-1.608339
16952	0	-1.997166	1.296252	-2.037103
16953	0	1.152272	2.358623	0.370503
16954	0	0.817521	0.495463	2.332148
16955	0	0.819624	-1.578266	-1.563882
16956	0	0.782073	1.105206	-2.019020
16957	H	-1.660820	1.761501	1.140138
16958	H	-0.045726	0.660555	2.746282
16959	H	-1.884737	-0.380497	-1.787044
16960	H	0.852002	1.577377	-1.156292
16961	H	-0.741709	2.808630	0.422498
16962	H	0.716024	-0.385516	1.902215
16963	H	-1.073668	-1.726224	-1.835405
16964	H	-0.089559	1.326914	-2.385979
16965	H	-2.892626	1.465827	-2.381475
16966	H	2.066315	2.693059	0.360648
16967	H	-2.823023	0.747131	2.814026
16968	H	1.695571	-1.948273	-1.773664
16969	H	-1.940396	1.732669	-1.156225
16970	H	1.113510	1.686511	1.090592
16971	H	-2.094383	-0.282723	1.927376
16972	H	0.881713	-0.610873	-1.744267
16973	H	-3.286263	-2.115449	1.128792
16974	O	-2.391454	-1.751873	1.026463
16975	H	-2.269793	-1.596538	0.058539
16976	H	-0.478106	-2.211912	1.286622
16977	O	0.431463	-1.921076	1.111190
16978	H	0.509411	-1.809993	0.134905
16979	O	3.249740	-2.039448	1.175298
16980	H	3.306443	-1.958124	0.194051
16981	H	2.350164	-2.342558	1.377963
16982	H	4.469663	-2.133627	-1.699381
16983	O	3.583666	-1.777062	-1.502803
16984	H	3.636689	-0.811342	-1.697652
16985	O	3.565038	0.884337	-2.017244
16986	H	3.635700	1.381779	-1.166248
16987	H	2.697693	1.104702	-2.394452
16988	O	3.934038	2.195988	0.309762
16989	H	3.883103	1.540367	1.046518
16990	H	4.864705	2.485698	0.274665
16991	H	3.518772	-0.493453	1.914881
16992	O	3.609163	0.404702	2.312903
16993	H	2.743211	0.578315	2.717373
16994	H	-5.661472	0.436258	2.699730
16995	O	-4.754909	0.448372	2.345881
16996	H	-4.698656	-0.414199	1.900588
16997	H	-5.559890	-2.878629	0.630958
16998	O	-5.249130	-1.972084	0.797911
16999	H	-5.107203	-1.636327	-0.119136
17000	O	-4.717688	-1.434982	-1.822323
17001	H	-4.888710	-0.512734	-2.104544
17002	H	-3.760419	-1.578388	-1.947305
17003	O	-4.779355	1.301547	-2.149839
17004	H	-4.682824	1.572583	-1.209870
17005	H	-5.450634	1.920337	-2.477449
17006	O	-4.443019	2.371074	0.364509
17007	H	-4.584673	1.748923	1.108766
17008	H	-3.530198	2.699152	0.442695
17009	H	5.550554	0.542658	2.583822
17010	O	6.430192	0.424314	2.189964
17011	H	6.431658	-0.507857	1.870387
17012	H	6.685080	1.454446	1.027328
17013	O	6.707356	2.098796	0.250186
17014	H	7.454629	2.690526	0.379326
17015	H	6.576536	1.106099	-1.278356
17016	O	6.364201	0.536757	-2.044465
17017	H	5.471406	0.790402	-2.331569
17018	O	6.342535	-2.044425	-1.598141
17019	H	6.450985	-1.068846	-1.786394
17020	H	7.003729	-2.518443	-2.111149
17021	O	6.105485	-2.104199	1.228505

17022	H	5.183804	-2.362554	1.384681
17023	H	6.256214	-2.185856	0.269915
17024	H	-6.764417	4.311250	-1.389250
17025	O	-6.355055	3.442109	-1.385038
17026	H	-5.821851	3.369288	-0.576026
17027	H	-5.720140	-3.100553	-1.714490
17028	O	-6.057821	-3.771850	-1.098131
17029	H	-6.215816	-4.578897	-1.594846
17030	O	-7.257342	-0.662359	2.369729
17031	H	-6.843340	-1.215991	1.686862
17032	H	-8.175920	-0.529871	2.119427
17033				
17034				
17035				
17036	Cartesian coordinates of the water 29-mer			
17037				
17038	Cartesian coordinates of : W29_1			
17039				
17040	O	-0.078918	-0.050572	-0.169516
17041	H	-0.625202	0.516086	-0.775381
17042	H	0.515725	-0.562957	-0.763256
17043	O	-2.748250	0.899423	2.258688
17044	H	-2.287209	0.031299	2.228996
17045	H	-3.720222	0.718314	2.272071
17046	O	-1.454566	1.401540	-1.898446
17047	H	-2.018227	1.976360	-1.337421
17048	H	-0.747811	1.938358	-2.337528
17049	O	1.589151	-1.289031	-1.910347
17050	H	2.105673	-0.472165	-2.110572
17051	H	2.113433	-1.821073	-1.264887
17052	O	-1.331557	-1.359894	1.802750
17053	H	-0.805379	-0.947472	1.079531
17054	H	-0.691572	-1.892988	2.335118
17055	O	2.804409	2.611717	0.091388
17056	H	2.351640	3.436196	-0.173304
17057	H	2.242435	2.208415	0.790675
17058	O	-2.634592	-1.020175	-2.304337
17059	H	-2.234420	-0.124308	-2.272768
17060	H	-1.991904	-1.576785	-2.780307
17061	O	2.725952	-0.978636	2.291463
17062	H	3.663629	-0.722108	2.391680
17063	H	2.207928	-0.148560	2.233466
17064	O	2.805442	-2.594756	0.097199
17065	H	2.700966	-2.005201	0.880491
17066	H	2.313638	-3.416674	0.296067
17067	O	1.186883	1.250848	1.788661
17068	H	0.553055	1.694002	2.383320
17069	H	0.661261	0.834928	1.061907
17070	O	-2.984724	-2.473149	0.008005
17071	H	-2.828552	-1.863307	-0.748831
17072	H	-2.440451	-2.128325	0.757178
17073	O	-2.994614	2.530047	0.016309
17074	H	-2.870619	1.891064	0.750920
17075	H	-3.941476	2.484669	-0.225569
17076	O	2.904762	1.054535	-2.169700
17077	H	3.852296	0.874232	-2.319244
17078	H	2.861155	1.543104	-1.316597
17079	O	1.030329	-4.598264	0.769325
17080	H	0.254516	-4.478498	0.147579
17081	H	1.183311	-5.544447	0.853712
17082	O	1.073224	4.593953	-0.762849
17083	H	1.215685	5.537119	-0.889235
17084	H	0.281753	4.493429	-0.159216
17085	O	5.405922	-0.253809	2.045009
17086	H	6.069409	-0.189094	2.738850
17087	H	5.435703	0.596728	1.513570
17088	O	-5.604720	1.888868	-0.612594
17089	H	-6.307077	2.426087	-0.991053
17090	H	-5.519485	1.062508	-1.168394
17091	O	5.588073	0.336016	-1.928918
17092	H	6.311171	0.258885	-2.558672
17093	H	5.542509	-0.517997	-1.409717
17094	O	-0.964798	-4.233111	-0.880501
17095	H	-1.753955	-3.783027	-0.523924
17096	H	-0.750925	-3.771094	-1.710783

17097	O	-0.982385	4.275987	0.820306
17098	H	-0.857476	3.846648	1.684801
17099	H	-1.786166	3.865880	0.450464
17100	O	-0.906887	2.596647	3.114001
17101	H	-1.690948	2.013604	2.951161
17102	H	-0.939551	2.874577	4.034789
17103	O	-0.413274	-2.566679	-3.115817
17104	H	-0.201574	-2.901816	-3.992769
17105	H	0.379452	-2.071494	-2.790617
17106	O	5.432949	1.820269	0.468806
17107	H	4.567878	2.268708	0.401426
17108	H	5.630891	1.480558	-0.422428
17109	O	5.430773	-1.744704	-0.346509
17110	H	5.562280	-1.395313	0.553977
17111	H	4.587186	-2.231828	-0.312432
17112	O	-5.549027	-2.040056	0.462612
17113	H	-6.087345	-2.815191	0.649153
17114	H	-4.603996	-2.334959	0.371722
17115	O	-5.365733	-0.416088	-1.831162
17116	H	-4.498446	-0.668393	-2.195001
17117	H	-5.581307	-1.076558	-1.147974
17118	O	-5.362814	0.449782	1.831188
17119	H	-5.525619	-0.451252	1.500379
17120	H	-5.631745	1.043128	1.108942
17121	O	0.663427	2.730129	-2.854143
17122	H	0.861007	3.457307	-2.236580
17123	H	1.460465	2.175676	-2.889742
17124	O	0.636327	-2.799988	2.935271
17125	H	1.450615	-2.269873	2.959310
17126	H	0.795867	-3.531915	2.313822
17127				
17128	Cartesian coordinates of : W29_2			
17129				
17130	O	-1.017876	2.341518	-0.229489
17131	O	-1.398882	1.014089	2.129804
17132	O	-0.912476	-2.010819	-1.032919
17133	O	-1.108044	0.454880	-2.197226
17134	O	1.775390	2.375047	-0.197502
17135	O	1.366449	1.163019	2.220702
17136	O	1.841900	-2.016738	-0.792886
17137	O	1.667630	0.390182	-2.070341
17138	H	-1.106125	1.879298	0.635657
17139	H	0.455239	1.338844	2.508596
17140	H	-0.943512	-1.123962	-1.460284
17141	H	1.703375	-0.485479	-1.619393
17142	H	-0.125532	2.729974	-0.248693
17143	H	1.485513	1.616352	1.354852
17144	H	-0.000048	-2.332991	-1.144669
17145	H	0.796436	0.443952	-2.497774
17146	H	-1.975693	0.498489	-2.632587
17147	H	2.676565	2.742505	-0.175290
17148	H	-2.308568	1.190347	2.422862
17149	H	2.748042	-2.331346	-0.963737
17150	H	-1.107869	1.150747	-1.499190
17151	H	1.784000	1.668611	-0.883720
17152	H	-1.349114	0.042890	1.971101
17153	H	1.781348	-1.858073	0.178579
17154	H	-2.149546	-1.998390	1.884611
17155	O	-1.260708	-1.680736	1.655100
17156	H	-1.159406	-1.819592	0.684499
17157	H	0.654933	-1.868572	2.103412
17158	O	1.541708	-1.543594	1.874657
17159	H	1.497921	-0.568426	2.011389
17160	O	4.367288	-1.558923	1.830550
17161	H	4.414364	-1.732954	0.863644
17162	H	3.501310	-1.885312	2.123703
17163	H	5.501434	-2.296428	-1.000353
17164	O	4.598008	-1.957792	-0.869138
17165	H	4.584555	-1.053839	-1.265100
17166	O	4.437540	0.535390	-1.911456
17167	H	4.438431	1.186434	-1.163999
17168	H	3.566104	0.601027	-2.336495
17169	O	4.554390	2.312789	0.102020
17170	H	4.415646	1.885351	0.991121
17171	H	5.501907	2.533764	0.083039

17172	H	4.212658	0.161995	2.258359
17173	O	4.147214	1.125244	2.421877
17174	H	3.237202	1.279198	2.721868
17175	H	-4.055081	1.521832	1.036820
17176	O	-4.171914	1.081798	1.913091
17177	H	-5.095453	1.227025	2.177814
17178	H	-4.972810	-1.903881	1.752606
17179	O	-4.058056	-1.616513	1.589591
17180	H	-4.071976	-0.638659	1.717981
17181	O	-3.683095	-2.092424	-1.058120
17182	H	-3.752307	-1.933753	-0.087544
17183	H	-2.783934	-2.427554	-1.220256
17184	O	-3.882905	0.291153	-2.347260
17185	H	-3.831596	-0.581612	-1.891708
17186	H	-4.774515	0.347623	-2.734414
17187	O	-3.789496	2.252453	-0.490219
17188	H	-2.910960	2.670415	-0.487807
17189	H	-3.765360	1.547300	-1.181082
17190	H	6.278797	0.472941	-2.375866
17191	O	7.218587	0.420442	-2.127904
17192	H	7.381320	-0.506852	-1.877402
17193	O	7.373803	-2.070512	-0.826132
17194	H	8.081723	-2.720835	-0.800024
17195	H	7.335571	-1.615890	0.060888
17196	O	7.055163	-0.684350	1.383356
17197	H	7.042712	0.266581	1.168366
17198	H	6.239227	-0.906249	1.857881
17199	H	8.115933	2.338890	0.226996
17200	O	7.306091	1.834945	0.101859
17201	H	7.374195	1.365444	-0.774203
17202	H	-7.699374	1.171699	2.488338
17203	O	-6.979900	0.906432	1.906798
17204	H	-7.051452	-0.066600	1.765003
17205	H	-6.636095	-1.217500	-1.731629
17206	O	-6.471869	-2.010562	-1.184504
17207	H	-5.551750	-2.281334	-1.349594
17208	H	-7.307093	0.626217	-3.244459
17209	O	-6.665003	0.403631	-2.563436
17210	H	-6.715885	1.102420	-1.851396
17211	H	-6.797533	1.788156	0.258389
17212	O	-6.582940	2.157510	-0.616776
17213	H	-5.677660	2.509314	-0.558769
17214	H	-7.521270	-2.404247	1.642484
17215	O	-6.872860	-1.753403	1.354648
17216	H	-6.770040	-1.858570	0.356652
17217				
17218	Cartesian coordinates of : W29_3			
17219				
17220	O	-0.910775	1.540391	-1.779110
17221	O	-1.337562	2.238511	0.822710
17222	O	-0.942471	-2.142023	0.639173
17223	O	-1.129800	-1.171016	-1.904935
17224	O	1.888231	1.642749	-1.746710
17225	O	1.439684	2.383524	0.830176
17226	O	1.820782	-1.995104	0.758050
17227	O	1.656026	-1.064365	-1.799514
17228	H	-0.973550	1.816949	-0.835706
17229	H	0.534729	2.728005	0.909457
17230	H	-0.940848	-1.801564	-0.285336
17231	H	1.671117	-0.078223	-1.798519
17232	H	-0.019002	1.783543	-2.082784
17233	H	1.460067	1.582088	1.404779
17234	H	-0.033435	-2.443501	0.815927
17235	H	0.788269	-1.330562	-2.145941
17236	H	-1.994983	-1.435372	-2.258957
17237	H	2.787874	1.858344	-2.047100
17238	H	-2.237466	2.595056	0.903980
17239	H	2.721150	-2.321303	0.936790
17240	H	-1.122495	-0.185677	-1.879502
17241	H	1.823526	1.937426	-0.807827
17242	H	-1.339784	1.416736	1.368952
17243	H	1.832090	-1.663665	-0.169986
17244	H	-2.281359	-0.105848	2.687860
17245	O	-1.388385	-0.042585	2.310585
17246	H	-1.283523	-0.821266	1.713928

17247	H	0.530734	0.103456	2.770887
17248	O	1.426290	0.151838	2.397484
17249	H	1.523388	-0.639351	1.818134
17250	O	4.270456	0.300102	2.363301
17251	H	4.316768	-0.536341	1.847369
17252	H	3.404631	0.302176	2.801471
17253	H	5.461843	-2.323592	1.022324
17254	O	4.575234	-1.956054	0.858214
17255	H	4.592266	-1.615759	-0.068451
17256	O	4.443562	-0.992278	-1.664536
17257	H	4.474830	-0.000829	-1.642692
17258	H	3.573378	-1.238388	-2.019720
17259	O	4.690505	1.677021	-1.616327
17260	H	4.546830	2.042179	-0.698637
17261	H	5.644856	1.779384	-1.768465
17262	H	4.267113	1.789031	1.391826
17263	O	4.224257	2.573997	0.806503
17264	H	3.316551	2.904728	0.896873
17265	H	-5.039470	2.376335	0.871277
17266	O	-4.121621	2.065302	0.806621
17267	H	-4.109684	1.226767	1.328847
17268	H	-5.099405	-0.310715	2.541184
17269	O	-4.184588	-0.243186	2.219433
17270	H	-4.055578	-0.998590	1.596030
17271	O	-3.716972	-2.275292	0.501868
17272	H	-3.704307	-1.923512	-0.420923
17273	H	-2.822422	-2.613559	0.680348
17274	O	-3.915165	-1.277661	-1.996062
17275	H	-3.898993	-0.293610	-1.937758
17276	H	-4.801775	-1.520201	-2.315604
17277	O	-3.702838	1.420722	-1.793041
17278	H	-3.756240	1.681320	-0.843733
17279	H	-2.821673	1.684369	-2.109140
17280	H	7.246811	1.144013	-0.092132
17281	O	7.425231	1.338514	-1.047772
17282	H	8.184177	1.929096	-1.077508
17283	H	7.433615	-0.448801	-1.626611
17284	O	7.211928	-1.397985	-1.658129
17285	H	6.272729	-1.431961	-1.913410
17286	O	7.338412	-2.242506	0.818443
17287	H	7.390583	-2.017011	-0.153527
17288	H	8.031184	-2.877595	1.021376
17289	O	7.002078	0.486152	1.453834
17290	H	6.202645	0.625326	1.983790
17291	H	7.173070	-0.472733	1.447721
17292	H	-5.596528	1.469310	-2.085345
17293	O	-6.502130	1.180714	-1.879119
17294	H	-6.696609	1.491565	-0.976186
17295	H	-7.676680	2.538004	1.025369
17296	O	-6.949295	1.943584	0.815816
17297	H	-7.073529	1.123981	1.349008
17298	H	-7.669202	-0.702568	2.794733
17299	O	-7.002927	-0.420362	2.159993
17300	H	-6.887094	-1.166289	1.491343
17301	O	-6.521531	-2.295300	0.452114
17302	H	-6.665634	-2.070292	-0.488391
17303	H	-5.599239	-2.595381	0.530140
17304	H	-6.724278	-0.413751	-2.110431
17305	O	-6.702254	-1.409557	-2.185617
17306	H	-7.356936	-1.674153	-2.838995
17307				
17308	Cartesian coordinates of : W29_ 4			
17309				
17310	O	2.990659	1.240410	-1.502355
17311	O	3.165207	1.492675	1.234139
17312	O	5.769059	1.243417	-1.548015
17313	O	6.041190	-1.451344	-1.150512
17314	O	5.837262	-1.057378	1.550569
17315	O	5.936847	1.649806	1.154868
17316	O	3.069454	-1.242809	1.481064
17317	O	3.270036	-1.482668	-1.251726
17318	O	8.810145	-1.313058	-1.331352
17319	O	8.566555	1.302159	-1.433959
17320	H	5.808069	0.260455	-1.528045
17321	H	4.879118	1.478697	-1.860510

17322	H	4.047674	1.833412	1.461609
17323	H	3.175174	0.532495	1.446155
17324	H	5.813053	-0.073944	1.531374
17325	H	4.960335	-1.350351	1.851439
17326	H	3.214778	-0.524739	-1.467224
17327	H	4.175623	-1.762565	-1.471898
17328	H	3.007728	1.456811	-0.543691
17329	H	2.088111	1.430028	-1.812099
17330	H	5.915706	1.633013	0.171691
17331	H	6.015170	-1.432404	-0.167394
17332	H	3.103881	-1.456290	0.521960
17333	H	2.182484	-1.496071	1.790032
17334	H	8.705653	1.634053	-0.528240
17335	H	7.655862	1.536913	-1.680972
17336	H	8.798996	-0.324469	-1.468762
17337	H	6.960269	-1.662082	-1.396562
17338	H	6.840594	1.914323	1.405763
17339	H	9.517254	-1.683436	-1.867994
17340	H	0.281695	-0.259834	1.535292
17341	O	0.294587	-1.242643	1.558365
17342	H	-0.591128	-1.523525	1.846799
17343	H	0.371247	1.447668	0.153532
17344	O	0.391227	1.472942	1.136331
17345	H	1.275606	1.792687	1.386006
17346	H	0.480825	-1.634863	-0.169499
17347	O	0.501974	-1.659187	-1.152061
17348	H	1.405557	-1.918245	-1.403013
17349	H	0.277961	0.061975	-1.548702
17350	O	0.221669	1.043251	-1.573000
17351	H	-0.679739	1.259672	-1.868508
17352	H	-3.452099	1.226115	-1.823373
17353	O	-2.550371	1.036866	-1.509352
17354	H	-2.539074	1.257962	-0.551714
17355	H	-1.371454	-1.967926	-1.465381
17356	O	-2.275936	-1.687660	-1.242310
17357	H	-2.333989	-0.731629	-1.464581
17358	H	-1.498213	1.647451	1.448124
17359	O	-2.381443	1.305904	1.225210
17360	H	-2.372034	0.346973	1.441742
17361	H	-2.441578	-1.650142	0.524441
17362	O	-2.470503	-1.431930	1.483241
17363	H	-3.355485	-1.684914	1.798097
17364	O	8.631793	-0.953466	1.458958
17365	H	7.733400	-1.239311	1.696976
17366	H	8.796686	-1.275966	0.554210
17367	O	-5.154606	1.287272	1.127041
17368	H	-4.274907	1.616032	1.380428
17369	H	-5.170873	1.260946	0.142709
17370	H	-5.247639	-0.438379	1.530314
17371	O	-5.243828	-1.420982	1.561204
17372	H	-6.147856	-1.689157	1.806561
17373	H	-5.263078	-0.120117	-1.544593
17374	O	-5.311640	0.861975	-1.571485
17375	H	-6.219307	1.082315	-1.851281
17376	H	-5.054940	-1.805571	-0.159730
17377	O	-5.052925	-1.830589	-1.142731
17378	H	-4.162690	-2.114551	-1.410645
17379	H	8.759416	0.685059	1.493569
17380	O	8.707976	1.672385	1.355961
17381	H	9.386355	2.086885	1.897492
17382	H	-7.012470	1.387019	1.459472
17383	O	-7.926489	1.134158	1.238084
17384	H	-8.048313	0.213117	1.539196
17385	H	-7.996789	1.026942	-0.547120
17386	O	-8.069790	0.919963	-1.520907
17387	H	-8.822428	1.487854	-1.741538
17388	H	-8.065578	-0.953973	-1.452936
17389	O	-7.861453	-1.831846	-1.079117
17390	H	-6.952964	-2.045835	-1.351067
17391	H	-8.028932	-1.799770	0.539686
17392	O	-8.014037	-1.643615	1.528323
17393	H	-8.695821	-2.193051	1.926888
17394	H	-9.382280	2.264605	0.591395
17395	O	-9.887932	2.549539	-0.186972
17396	H	-10.490125	3.243255	0.094077

17397
17398 Cartesian coordinates of : W29_ 5
17399
17400 O 3.196672 -1.570044 1.948448
17401 H 3.078024 -0.612531 2.136778
17402 H 4.128650 -1.778117 2.146936
17403 H 3.033247 -2.008018 0.297293
17404 O 3.013630 -2.318497 -0.639547
17405 H 2.141058 -2.725084 -0.778238
17406 O 3.222237 -0.298311 -2.417981
17407 H 3.170903 -1.007910 -1.733423
17408 H 4.139359 -0.311999 -2.746069
17409 O 2.802739 2.231477 -1.597121
17410 H 2.923515 1.278383 -1.833018
17411 H 1.933200 2.489371 -1.948163
17412 O 2.757866 1.030166 2.672639
17413 H 2.717582 1.755958 2.015634
17414 H 1.892550 1.015144 3.113518
17415 H 2.848732 2.762058 -0.041555
17416 O 2.803919 3.106611 0.890292
17417 H 3.541371 3.712224 1.020735
17418 H 1.333512 -2.068648 2.143112
17419 O 0.423347 -1.861197 1.870327
17420 H 0.389191 -2.004346 0.897214
17421 H 0.276538 -1.644762 -1.418438
17422 O 0.250639 -2.414372 -0.804510
17423 H -0.613535 -2.841284 -0.933642
17424 H 1.355308 -0.404492 -2.930564
17425 O 0.440120 -0.370937 -2.603198
17426 H 0.310408 0.536904 -2.245683
17427 H -0.010641 2.310766 -0.759637
17428 O 0.007120 2.186544 -1.735994
17429 H -0.886969 2.405996 -2.048960
17430 H 0.890486 3.184314 1.076210
17431 O 0.050339 2.714529 0.945103
17432 H 0.056572 1.949304 1.567272
17433 O -0.029492 0.684427 2.749925
17434 H 0.104881 -0.220627 2.385504
17435 H -0.936555 0.704031 3.099648
17436 H -1.474657 -2.218055 2.165767
17437 O -2.366895 -1.970498 1.870800
17438 H -2.483066 -1.017320 2.098624
17439 H -2.490441 -2.333029 0.188237
17440 O -2.516047 -2.621884 -0.753758
17441 H -3.407675 -2.984924 -0.904954
17442 H -1.434607 -0.715843 -3.017690
17443 O -2.330181 -0.692286 -2.641226
17444 H -2.348943 -1.358850 -1.914187
17445 H -2.627195 0.931632 -2.130625
17446 O -2.767546 1.881990 -1.910999
17447 H -3.695079 2.075965 -2.138109
17448 O -2.702953 2.531267 0.712967
17449 H -1.857699 2.980605 0.882323
17450 H -2.677472 2.244272 -0.230726
17451 O -2.822004 0.590783 2.604358
17452 H -3.749423 0.561398 2.901776
17453 H -2.794213 1.253603 1.875444
17454 H -4.238596 -2.414025 1.910486
17455 O -5.167030 -2.200452 1.717190
17456 H -5.311895 -2.408632 0.774660
17457 H -5.888254 -3.491006 -1.350350
17458 O -5.281665 -2.820826 -1.020398
17459 H -5.314986 -2.047929 -1.654123
17460 O -5.592222 0.228963 2.597574
17461 H -6.280912 0.221967 3.269598
17462 H -5.512628 -0.702619 2.243633
17463 H -5.637034 1.549708 1.312918
17464 O -5.490947 2.276127 0.677353
17465 H -4.604880 2.629723 0.865522
17466 O -5.562107 1.837650 -1.901946
17467 H -6.253304 2.370729 -2.306891
17468 H -5.616769 1.981087 -0.913438
17469 H -4.216787 -0.764478 -3.003157
17470 O -5.138593 -0.817645 -2.699332
17471 H -5.390261 0.082791 -2.417928

17472	H	5.994409	-2.010363	0.845636
17473	O	5.969916	-1.723811	1.804729
17474	H	6.675378	-2.185440	2.268106
17475	O	5.591840	1.899451	-0.904463
17476	H	5.493283	1.650596	0.041646
17477	H	4.760570	2.298249	-1.199079
17478	H	4.731273	1.118059	2.320647
17479	O	5.479415	1.047754	1.710848
17480	H	5.798971	0.129879	1.787384
17481	H	5.949730	0.630639	-1.852713
17482	O	6.010024	-0.187532	-2.424983
17483	H	6.739405	-0.064706	-3.040089
17484	H	5.987004	-1.669277	-1.338022
17485	O	5.807810	-2.397937	-0.713212
17486	H	4.879740	-2.653099	-0.853859
17487				
17488	Cartesian coordinates of : W29_6			
17489				
17490	O	-0.592852	2.757587	0.920047
17491	H	-0.904487	2.678961	-0.012958
17492	H	-0.011334	3.553577	0.926042
17493	O	-4.956823	-0.247788	-2.628164
17494	H	-5.222337	-0.573988	-1.723720
17495	H	-5.690800	-0.403143	-3.230112
17496	O	-0.630185	1.189611	4.491754
17497	H	-0.595204	1.743158	5.278285
17498	H	-1.421113	1.461204	3.972734
17499	O	0.198034	-1.375425	0.483488
17500	H	-0.056511	-2.247206	0.087272
17501	H	0.725787	-1.613460	1.270107
17502	O	1.991172	-4.455192	0.620545
17503	H	2.442413	-3.736563	0.104841
17504	H	2.542161	-5.242342	0.567251
17505	O	-2.516039	-1.566895	-2.308381
17506	H	-3.318524	-1.129443	-2.649199
17507	H	-2.770806	-1.969928	-1.447663
17508	O	-4.795600	1.489448	1.093717
17509	H	-4.043523	1.647071	1.712942
17510	H	-5.576317	1.893210	1.486503
17511	O	-0.755717	-1.650606	4.124213
17512	H	0.075242	-2.050580	3.811570
17513	H	-0.544197	-0.780407	4.497442
17514	O	-0.521931	-3.802179	-0.464566
17515	H	0.214338	-4.343047	-0.130816
17516	H	-0.418341	-3.732276	-1.448974
17517	O	-4.002189	2.196380	-1.573759
17518	H	-4.308216	2.039646	-0.663502
17519	H	-4.350750	1.457078	-2.102115
17520	O	-0.354582	-3.235700	-3.061786
17521	H	0.416468	-2.660815	-3.208695
17522	H	-1.144338	-2.672146	-3.127497
17523	O	3.682777	0.638749	-3.220793
17524	H	3.119326	1.263450	-2.680690
17525	H	4.023572	1.120362	-3.980203
17526	O	3.083355	-0.669993	1.690877
17527	H	3.919265	-0.171020	1.634837
17528	H	2.363742	-0.020892	1.841421
17529	O	-1.360510	2.565628	-1.660749
17530	H	-2.348024	2.488932	-1.696245
17531	H	-0.994828	1.665483	-1.833442
17532	O	1.099092	1.122122	2.244891
17533	H	0.691378	1.158744	3.128603
17534	H	0.452831	1.556004	1.640586
17535	O	-3.041357	-2.702352	0.140146
17536	H	-2.734868	-2.122647	0.870223
17537	H	-2.379187	-3.412856	0.073273
17538	O	5.258521	0.876363	0.921458
17539	H	6.154582	0.972673	1.257719
17540	H	5.307056	0.359244	0.061227
17541	O	1.490302	-2.616532	2.691790
17542	H	2.325516	-2.120417	2.627588
17543	H	1.634511	-3.455420	2.217680
17544	O	5.194101	-0.582141	-1.228824
17545	H	4.797980	-0.137392	-2.003333
17546	H	4.620894	-1.350912	-1.053513

17547	O	1.234140	4.732883	0.522223
17548	H	2.085268	4.278401	0.629573
17549	H	1.096860	4.844159	-0.433769
17550	O	2.107348	2.023522	-1.666653
17551	H	2.430243	2.202163	-0.760103
17552	H	1.640314	2.825387	-1.961071
17553	O	-0.428161	0.053167	-1.794452
17554	H	-0.121487	-0.179544	-0.897539
17555	H	-1.210998	-0.523116	-1.972669
17556	O	-2.025334	-0.876636	1.915205
17557	H	-1.218765	-0.886449	1.348160
17558	H	-1.695890	-1.252298	2.773465
17559	O	3.070281	2.610928	0.883967
17560	H	3.949177	2.189901	0.935166
17561	H	2.511226	2.185940	1.559648
17562	O	1.708674	-1.304201	-2.785727
17563	H	1.017877	-0.656197	-2.523852
17564	H	2.414984	-0.785391	-3.208451
17565	O	-5.323980	-1.015646	-0.151839
17566	H	-5.068588	-0.282708	0.437243
17567	H	-4.759498	-1.777873	0.055668
17568	O	-2.501225	1.656474	2.539509
17569	H	-1.904875	2.210498	1.989446
17570	H	-2.331540	0.716986	2.260540
17571	O	0.525600	4.307340	-2.194784
17572	H	-0.308802	3.777290	-2.111406
17573	H	0.442326	4.872875	-2.968065
17574	O	3.002883	-2.277606	-0.554820
17575	H	2.444994	-1.972896	-1.306681
17576	H	2.875432	-1.629513	0.170961
17577				
17578	Cartesian coordinates of : W29_7			
17579				
17580	O	3.642175	-2.061608	-0.673471
17581	H	3.618672	-1.791971	0.272366
17582	H	4.516811	-2.465667	-0.827770
17583	H	3.455800	-0.764734	-1.767676
17584	O	3.406726	-0.067553	-2.466266
17585	H	2.535741	-0.164552	-2.888958
17586	O	3.686887	2.431922	-1.623933
17587	H	3.626326	1.487829	-1.929410
17588	H	4.503029	2.791888	-1.988808
17589	O	3.188667	2.914339	1.071868
17590	H	3.455448	2.829629	0.136688
17591	H	2.257767	3.196494	1.073922
17592	O	3.322916	-1.507951	1.993397
17593	H	3.389740	-0.589034	2.324809
17594	H	2.418898	-1.809768	2.188022
17595	H	3.456728	1.818130	2.272553
17596	O	3.457396	1.096945	2.956861
17597	H	4.217792	1.249918	3.527890
17598	H	1.786824	-2.459638	-0.936708
17599	O	0.867687	-2.145147	-0.873897
17600	H	0.806001	-1.365678	-1.471686
17601	H	0.661956	0.825160	-2.254915
17602	O	0.646080	-0.077890	-2.648929
17603	H	-0.225615	-0.186154	-3.065695
17604	H	1.745077	2.750009	-1.853466
17605	O	0.842895	2.444810	-1.661791
17606	H	0.717218	2.533890	-0.688489
17607	H	0.457458	2.058167	1.597548
17608	O	0.408967	2.833443	0.989847
17609	H	-0.486148	3.202113	1.079544
17610	H	1.545127	0.935516	3.177319
17611	O	0.671134	0.810288	2.769836
17612	H	0.664299	-0.095276	2.381557
17613	O	0.544680	-1.725092	1.795730
17614	H	0.618749	-1.822575	0.817940
17615	H	-0.341439	-2.047991	2.033055
17616	H	-1.022757	-2.616307	-0.966304
17617	O	-1.917684	-2.253832	-0.853540
17618	H	-1.996134	-2.003034	0.099424
17619	H	-2.074680	-0.961709	-1.999788
17620	O	-2.119044	-0.285929	-2.715372
17621	H	-3.015572	-0.345156	-3.091955

17622	H	-1.080731	2.631501	-2.084867
17623	O	-1.956228	2.277441	-1.858380
17624	H	-1.960553	1.330683	-2.133635
17625	H	-2.234533	2.559442	-0.167732
17626	O	-2.357333	2.816848	0.774491
17627	H	-3.291951	3.077802	0.866571
17628	O	-2.115753	0.853738	2.623404
17629	H	-1.254547	0.950295	3.062924
17630	H	-2.150051	1.540914	1.916791
17631	O	-2.237835	-1.715633	1.768330
17632	H	-3.153492	-2.007315	1.936661
17633	H	-2.208899	-0.766492	2.032961
17634	H	-3.749549	-2.556160	-1.216278
17635	O	-4.694448	-2.332393	-1.140869
17636	H	-4.870668	-1.627074	-1.794913
17637	H	-5.529470	-0.221986	-3.680395
17638	O	-4.897213	-0.228503	-2.955068
17639	H	-4.933017	0.673050	-2.521321
17640	O	-4.998984	-1.868219	1.582979
17641	H	-5.629980	-2.592042	1.724554
17642	H	-4.912521	-1.849377	0.606573
17643	H	-5.105530	-0.171347	2.262276
17644	O	-4.930735	0.745758	2.550201
17645	H	-4.024105	0.755786	2.900189
17646	O	-5.138892	2.706692	0.843027
17647	H	-5.835423	3.309347	1.121914
17648	H	-5.137484	1.936197	1.484232
17649	H	-3.871806	2.488208	-2.001137
17650	O	-4.773334	2.147734	-1.876525
17651	H	-5.007702	2.307683	-0.941701
17652	H	5.387969	-0.168559	-2.573129
17653	O	6.158576	-0.081410	-1.992891
17654	H	6.425709	-0.988769	-1.762309
17655	O	6.106578	-1.748790	1.640897
17656	H	5.898000	-0.822160	1.390318
17657	H	5.286204	-2.068500	2.045577
17658	H	6.942065	-3.410202	-0.952655
17659	O	6.371539	-2.650450	-0.804034
17660	H	6.411414	-2.412459	0.164591
17661	H	4.454138	0.933817	0.538228
17662	O	5.378435	0.658444	0.545770
17663	H	5.640265	0.526372	-0.391639
17664	H	-5.946007	-3.585002	-0.397429
17665	O	-6.447005	-3.887647	0.379028
17666	H	-6.785670	-4.765987	0.188172
17667				
17668				
17669	Cartesian coordinates of the water 30-mer			
17670				
17671	Cartesian coordinates of : W30_ 1			
17672				
17673	O	3.092930	-3.357369	0.060148
17674	H	2.630196	-3.399738	0.914442
17675	H	3.542931	-2.488272	0.044616
17676	O	4.428656	1.120731	1.969274
17677	H	5.143280	1.400744	2.549176
17678	H	4.146541	1.916320	1.432359
17679	O	3.991621	-0.730681	-0.072696
17680	H	4.411439	-0.247310	0.660980
17681	H	3.097555	-0.336105	-0.171917
17682	O	1.597100	-2.748587	2.367902
17683	H	0.963632	-3.020052	3.055136
17684	H	1.904728	-1.844028	2.608272
17685	O	4.272518	0.108240	-2.739740
17686	H	4.412696	-0.271159	-1.851196
17687	H	3.542950	-0.404262	-3.129922
17688	O	1.868679	-3.954405	-2.154407
17689	H	2.321202	-4.714193	-2.534394
17690	H	2.324148	-3.756926	-1.280523
17691	O	2.065377	-0.117742	2.763732
17692	H	2.928513	0.316930	2.619922
17693	H	1.416366	0.330977	2.177917
17694	O	-0.673112	-2.866486	4.030140
17695	H	-1.342185	-2.520359	3.394889
17696	H	-1.091336	-3.561712	4.547266

17697	O	3.611302	3.096512	0.472618
17698	H	3.684428	2.950120	-0.489701
17699	H	2.728963	3.467340	0.648564
17700	O	3.681261	2.609452	-2.313090
17701	H	4.239516	3.171821	-2.859455
17702	H	3.926379	1.658110	-2.521165
17703	O	0.200082	-0.271085	4.901816
17704	H	-0.017213	-1.214712	4.832047
17705	H	0.991976	-0.141413	4.350559
17706	O	1.910616	-1.393624	-3.228319
17707	H	1.010669	-1.195744	-3.545736
17708	H	1.929931	-2.346119	-3.001479
17709	O	1.505750	-0.023217	-0.880385
17710	H	1.243635	0.888978	-1.134418
17711	H	1.638041	-0.504818	-1.727450
17712	O	-0.067410	-1.818954	0.443375
17713	H	0.427565	-1.078402	0.024561
17714	H	0.557543	-2.229717	1.085602
17715	O	-0.808625	-3.305272	-1.662635
17716	H	-0.022978	-3.812123	-1.936273
17717	H	-0.542824	-2.866730	-0.818926
17718	O	0.034861	1.186610	1.467455
17719	H	-0.415463	0.859515	0.657334
17720	H	-0.643882	1.146654	2.183801
17721	O	-2.174144	-1.593814	2.154103
17722	H	-3.022061	-1.840281	1.732160
17723	H	-1.498521	-1.557832	1.439035
17724	O	0.972790	2.567173	-1.751941
17725	H	0.989246	3.060181	-0.898085
17726	H	1.841493	2.714372	-2.171637
17727	O	0.849144	3.629757	0.723881
17728	H	0.550208	2.777578	1.123724
17729	H	0.074692	4.217958	0.778223
17730	O	-0.807095	-0.956072	-3.007612
17731	H	-0.868057	-1.863666	-2.630239
17732	H	-1.653730	-0.790333	-3.463914
17733	O	-1.798575	0.850311	3.427833
17734	H	-2.128628	0.006230	3.060439
17735	H	-1.167977	0.585729	4.135498
17736	O	-1.438779	0.575582	-0.762326
17737	H	-1.132646	0.010292	-1.504505
17738	H	-1.536759	1.477825	-1.141001
17739	O	-3.550765	-2.648354	-1.676527
17740	H	-3.576750	-1.943478	-2.352209
17741	H	-2.675874	-3.072037	-1.724410
17742	O	-4.471388	-2.026818	0.674234
17743	H	-5.240250	-2.561000	0.895403
17744	H	-4.154014	-2.312743	-0.232342
17745	O	-1.737886	3.102676	-1.803379
17746	H	-0.819835	3.115983	-2.130562
17747	H	-1.782182	3.734505	-1.055368
17748	O	-3.150536	2.760811	1.905453
17749	H	-3.574858	2.073729	1.354734
17750	H	-2.720195	2.277721	2.633323
17751	O	-1.801890	4.528276	0.567425
17752	H	-2.315211	3.864129	1.121969
17753	H	-2.231987	5.380875	0.688353
17754	O	-3.486260	-0.577188	-3.586283
17755	H	-4.005614	-0.678415	-4.390170
17756	H	-3.736973	0.307855	-3.181110
17757	O	-3.962087	0.691431	0.209934
17758	H	-4.406811	-0.130809	0.480016
17759	H	-3.060452	0.425156	-0.074179
17760	O	-4.102152	1.667001	-2.424108
17761	H	-3.363371	2.300144	-2.388893
17762	H	-4.287682	1.427564	-1.496129
17763				
17764	Cartesian coordinates of : W30_2			
17765				
17766	O	4.008837	-1.349479	-1.880473
17767	O	4.273317	-2.166358	0.698583
17768	O	3.997691	2.209903	0.671707
17769	O	4.212943	1.358479	-1.886351
17770	O	1.230099	-1.295565	-1.937111
17771	O	1.491269	-2.245903	0.606081

17772	O	1.224951	2.173094	0.805124
17773	O	1.431298	1.424301	-1.812183
17774	H	4.038986	-1.663896	-0.946851
17775	H	2.378175	-2.631412	0.700183
17776	H	4.017071	1.910021	-0.268632
17777	H	1.387880	1.714441	-0.871343
17778	H	3.125325	-1.574329	-2.220117
17779	H	1.426038	-1.917578	-0.321034
17780	H	3.110916	2.579282	0.826567
17781	H	2.315413	1.665882	-2.135392
17782	H	5.117935	1.594908	-2.156715
17783	H	0.332662	-1.530226	-2.232354
17784	H	5.188619	-2.491203	0.751652
17785	H	0.326018	2.528770	0.920876
17786	H	4.165073	0.373977	-1.900838
17787	H	1.262104	-0.311336	-1.905621
17788	H	4.247908	-1.367864	1.276959
17789	H	1.276034	1.361280	1.360388
17790	H	5.185037	0.050165	2.622898
17791	O	4.278534	0.051690	2.273427
17792	H	4.199465	0.851404	1.699405
17793	H	2.380654	-0.072651	2.697820
17794	O	1.490826	-0.096495	2.307532
17795	H	1.487963	-0.876094	1.705493
17796	O	-1.295567	0.008154	2.340140
17797	H	-1.360092	0.806913	1.767446
17798	H	-0.404980	0.020344	2.729004
17799	H	-2.449315	2.535691	0.866429
17800	O	-1.549045	2.195487	0.717558
17801	H	-1.522571	1.889980	-0.218548
17802	O	-1.349614	1.317862	-1.860753
17803	H	-1.391551	0.333293	-1.870187
17804	H	-0.462760	1.559014	-2.176554
17805	O	-1.546026	-1.405537	-1.843698
17806	H	-1.498988	-1.716205	-0.909665
17807	H	-2.445940	-1.610673	-2.154119
17808	H	-1.307741	-1.427496	1.333140
17809	O	-1.294414	-2.221526	0.750118
17810	H	-0.401530	-2.595369	0.840073
17811	H	7.035071	-1.814924	-0.382090
17812	O	7.090738	-2.193819	0.550778
17813	H	7.737503	-2.906545	0.530636
17814	H	7.790229	-0.143201	2.964678
17815	O	7.091863	-0.115316	2.302966
17816	H	7.197481	-0.905470	1.723145
17817	O	6.793877	2.177515	0.649843
17818	H	6.967300	1.430878	1.250640
17819	H	5.880608	2.466509	0.820252
17820	O	6.997812	1.563827	-1.890582
17821	H	7.006825	1.842570	-0.931445
17822	H	7.662817	2.079489	-2.356979
17823	O	6.802494	-1.216596	-1.824758
17824	H	5.897944	-1.379822	-2.143879
17825	H	6.969734	-0.258802	-1.924010
17826	H	-3.252217	1.638989	-2.099489
17827	O	-4.131628	1.399240	-1.763587
17828	H	-4.157583	1.679389	-0.817471
17829	O	-4.316054	2.128053	0.840609
17830	H	-5.228461	2.465899	0.910498
17831	H	-4.277082	1.312722	1.395662
17832	O	-4.093768	-0.116722	2.338563
17833	H	-4.105062	-0.904802	1.746705
17834	H	-3.210150	-0.106794	2.742278
17835	H	-3.197947	-2.657144	0.764031
17836	O	-4.080316	-2.265059	0.657534
17837	H	-4.125867	-1.927991	-0.267599
17838	H	-5.237223	-1.533402	-2.117719
17839	O	-4.317949	-1.308176	-1.880270
17840	H	-4.282304	-0.323733	-1.845628
17841	H	-7.077035	-1.778809	-0.844629
17842	O	-7.080018	-1.478399	-1.809839
17843	H	-7.773946	-1.963567	-2.266564
17844	H	-6.007690	-2.516815	0.829237
17845	O	-6.901164	-2.175195	0.662079
17846	H	-7.012047	-1.412788	1.276447

17847	O	-6.926341	0.003706	2.303697
17848	H	-7.076724	0.837144	1.823776
17849	H	-6.023230	0.047963	2.655235
17850	H	-7.107556	1.955030	-0.255987
17851	O	-7.074596	2.322937	0.673022
17852	H	-7.751020	3.003300	0.742388
17853	H	-6.034073	1.465465	-2.059866
17854	O	-6.939698	1.312279	-1.742868
17855	H	-7.094892	0.349174	-1.807709
17856				
17857	Cartesian coordinates of : W30_ 3			
17858				
17859	O	0.218510	-0.506955	-1.417100
17860	O	-1.770431	3.701325	-1.394864
17861	O	-1.503273	3.611199	1.502561
17862	O	0.030975	-0.676584	1.345567
17863	O	0.785527	1.963196	1.519150
17864	O	-2.526527	-0.801804	-1.327600
17865	O	-3.595771	1.701641	-1.446871
17866	O	-3.495780	1.791445	1.353491
17867	O	-2.733462	-0.812629	1.421447
17868	H	-2.542359	-0.898307	-0.348917
17869	H	-1.590090	-0.868003	-1.592467
17870	H	-0.881772	-0.889610	1.615165
17871	H	0.041092	-0.714605	0.364823
17872	H	-2.822556	2.465766	1.606087
17873	H	-3.555146	1.856001	0.378874
17874	H	-2.501944	3.058589	-1.536389
17875	H	-1.944009	4.464485	-1.954836
17876	H	0.340602	0.466164	-1.488435
17877	H	1.058884	-0.916804	-1.688708
17878	H	-2.996865	0.130302	1.544061
17879	H	-3.498694	-1.354346	1.681631
17880	H	-3.185532	0.811056	-1.544581
17881	H	-4.540871	1.602164	-1.664825
17882	H	-0.647106	3.184745	1.679671
17883	H	-1.492934	3.878132	0.569719
17884	H	1.722661	1.992517	1.780990
17885	H	0.489610	1.032454	1.625031
17886	H	0.640848	2.210780	-0.211247
17887	O	0.584148	2.196298	-1.194139
17888	H	-0.157757	2.779177	-1.439014
17889	H	-4.216061	-1.658975	-1.662495
17890	O	-5.153948	-1.687477	-1.405089
17891	H	-5.486965	-0.765999	-1.485158
17892	H	-7.138080	0.738408	-1.591425
17893	O	-6.213483	0.842202	-1.300832
17894	H	-6.238833	0.925529	-0.318999
17895	H	-6.113698	-2.338368	1.593178
17896	O	-5.318760	-1.841626	1.326822
17897	H	-5.254708	-1.925459	0.349340
17898	H	-5.314657	1.363378	1.680117
17899	O	-6.061260	0.795006	1.416512
17900	H	-5.745879	-0.131998	1.508526
17901	H	4.442840	1.524301	1.712320
17902	O	3.515479	1.467136	1.424054
17903	H	3.514150	1.618939	0.452483
17904	H	3.118701	0.614850	-1.453831
17905	O	3.287179	1.572547	-1.310334
17906	H	2.454078	2.029678	-1.522706
17907	H	1.819795	-1.268386	1.626802
17908	O	2.755125	-1.176278	1.371551
17909	H	2.989039	-0.232923	1.517788
17910	H	2.871671	-1.293531	-0.391596
17911	O	2.909764	-1.152317	-1.364838
17912	H	3.730254	-1.574370	-1.673718
17913	H	6.058314	1.116350	-0.275371
17914	O	6.022013	1.078647	-1.258152
17915	H	5.209403	1.540688	-1.525630
17916	H	5.977543	-0.144979	1.505025
17917	O	6.208494	0.810027	1.457780
17918	H	7.158496	0.873514	1.665544
17919	H	5.436988	-1.853258	0.256314
17920	O	5.455546	-1.812885	1.239136
17921	H	4.535594	-1.912429	1.537954

17922	H	5.811534	-0.656025	-1.531026
17923	O	5.636689	-1.622965	-1.487057
17924	H	6.472953	-2.063580	-1.724487
17925	H	7.894348	0.805934	-1.535325
17926	O	8.738795	0.399414	-1.276249
17927	H	8.692633	-0.535640	-1.547313
17928	O	8.955594	0.414159	1.342675
17929	H	9.755881	0.821410	1.687467
17930	H	8.971145	0.489145	0.347421
17931	O	8.213718	-2.298587	1.156883
17932	H	8.558543	-1.426456	1.422182
17933	H	7.287950	-2.333779	1.452392
17934	H	8.329734	-2.462454	-0.472785
17935	O	8.309133	-2.379848	-1.467501
17936	H	8.857389	-3.077485	-1.838806
17937	H	-8.880158	0.004019	0.346563
17938	O	-8.683144	-0.160356	1.286560
17939	H	-7.925568	0.405704	1.514025
17940	H	-8.513542	-3.223930	2.055878
17941	O	-7.966486	-2.681684	1.479552
17942	H	-8.318500	-1.747909	1.503722
17943	O	-8.794743	-0.152011	-1.532477
17944	H	-8.491499	-1.103065	-1.552417
17945	H	-9.551945	-0.065354	-2.119332
17946	H	-7.881680	-2.838935	-0.394658
17947	O	-7.804481	-2.577001	-1.330435
17948	H	-6.854387	-2.553091	-1.536214
17949				
17950	Cartesian coordinates of : W30_ 4			
17951				
17952	O	-3.914282	-1.994916	1.154386
17953	O	-4.230777	-1.701118	-1.520323
17954	O	-4.051829	2.263486	0.302348
17955	O	-4.238366	0.449374	2.287284
17956	O	-1.127574	-1.986508	1.174042
17957	O	-1.432220	-1.741166	-1.523265
17958	O	-1.261603	2.306763	0.217384
17959	O	-1.450452	0.495710	2.246197
17960	H	-3.936065	-1.902086	0.172752
17961	H	-2.310690	-2.088858	-1.749559
17962	H	-4.037690	1.611187	1.044202
17963	H	-1.404073	-0.415265	1.872298
17964	H	-3.026963	-2.319759	1.384942
17965	H	-1.481475	-0.780305	-1.740742
17966	H	-3.173870	2.681634	0.285291
17967	H	-2.332665	0.589012	2.642525
17968	H	-5.140014	0.531703	2.644420
17969	H	-0.228978	-2.282774	1.401771
17970	H	-5.128678	-2.015399	-1.716840
17971	H	-0.368666	2.692654	0.186787
17972	H	-4.178854	-0.450275	1.888170
17973	H	-1.155079	-1.910445	0.191841
17974	H	-4.264252	-0.733421	-1.715629
17975	H	-1.256884	1.663150	0.963750
17976	H	-5.331617	1.089509	-2.335271
17977	O	-4.418464	0.952919	-2.031213
17978	H	-4.333268	1.444047	-1.178568
17979	H	-2.517351	1.073954	-2.449328
17980	O	-1.625737	0.919683	-2.095647
17981	H	-1.560242	1.440845	-1.261007
17982	O	1.171292	0.876243	-2.150669
17983	H	1.238214	1.413249	-1.327038
17984	H	0.275885	1.018811	-2.500234
17985	H	2.419776	2.695712	0.095025
17986	O	1.525008	2.314743	0.139351
17987	H	1.532582	1.686830	0.899184
17988	O	1.339549	0.548957	2.205938
17989	H	1.390949	-0.368260	1.848775
17990	H	0.452268	0.646062	2.590083
17991	O	1.657515	-1.957313	1.184326
17992	H	1.636402	-1.900726	0.199943
17993	H	2.555355	-2.246841	1.423501
17994	H	1.323190	-0.813407	-1.755367
17995	O	1.365847	-1.768932	-1.513930
17996	H	0.484817	-2.115230	-1.733179

17997	H	-7.752397	-2.229161	-1.998623
17998	O	-7.063349	-1.711179	-1.570351
17999	H	-7.226376	-0.764380	-1.789191
18000	H	-7.909889	1.430696	-2.514608
18001	O	-7.238261	0.970929	-2.000848
18002	H	-7.165944	1.437831	-1.110738
18003	O	-6.859248	2.148646	0.267481
18004	H	-7.002362	1.606724	1.068694
18005	H	-5.953595	2.499095	0.325647
18006	O	-7.030666	0.395322	2.426968
18007	H	-7.011104	-0.511005	2.007476
18008	H	-7.707536	0.393345	3.110637
18009	O	-6.718475	-1.915389	1.239548
18010	H	-6.883722	-1.898265	0.279276
18011	H	-5.801565	-2.217403	1.358793
18012	H	3.289093	-2.148587	-1.717812
18013	O	4.165204	-1.795366	-1.491610
18014	H	4.129474	-0.846052	-1.760865
18015	H	4.404737	-1.875044	0.209024
18016	O	4.437500	-1.912865	1.195509
18017	H	5.354964	-2.151198	1.424912
18018	H	4.174582	-0.335873	1.811056
18019	O	4.135538	0.591608	2.149338
18020	H	3.259260	0.704419	2.552643
18021	O	4.302436	2.310553	0.057347
18022	H	4.301298	1.690417	0.824404
18023	H	5.206828	2.671426	0.011566
18024	O	3.978013	0.820517	-2.188508
18025	H	3.090977	0.959754	-2.558616
18026	H	4.035023	1.379334	-1.378130
18027	H	7.774018	3.101109	0.152975
18028	O	7.075589	2.448285	0.047100
18029	H	7.129404	1.814240	0.817501
18030	H	7.134347	-0.189528	1.805600
18031	O	6.952831	0.743723	2.034099
18032	H	6.047545	0.767583	2.385818
18033	H	7.210571	-1.924264	0.236582
18034	O	7.212888	-1.926460	1.246558
18035	H	7.923487	-2.504248	1.540509
18036	H	7.042570	-0.935462	-1.664501
18037	O	6.983757	-1.856340	-1.317652
18038	H	6.093813	-2.154130	-1.566845
18039	H	6.983100	1.374268	-1.486913
18040	O	6.829058	0.717662	-2.189586
18041	H	5.921549	0.858479	-2.501612
18042				
18043	Cartesian coordinates of : W30_5			
18044				
18045	O	-2.300262	-0.800783	-1.421803
18046	O	-4.800684	3.151446	-1.389791
18047	O	-4.547026	3.092990	1.515260
18048	O	-2.475977	-0.995956	1.338614
18049	O	-2.076176	1.723447	1.511434
18050	O	-4.996203	-1.407611	-1.339028
18051	O	-6.351208	0.938600	-1.441041
18052	O	-6.281052	1.013057	1.343983
18053	O	-5.199575	-1.465454	1.393435
18054	H	-4.984659	-1.499351	-0.358758
18055	H	-4.063686	-1.382129	-1.621440
18056	H	-3.355596	-1.324929	1.601789
18057	H	-2.456238	-1.030808	0.357789
18058	H	-5.725542	1.774364	1.627062
18059	H	-6.315355	1.083331	0.367873
18060	H	-5.444611	2.419967	-1.528869
18061	H	-5.076490	3.887778	-1.944523
18062	H	-2.305872	0.179436	-1.495064
18063	H	-1.413299	-1.101228	-1.687292
18064	H	-5.572005	-0.561859	1.527252
18065	H	-5.917352	-2.094960	1.590717
18066	H	-5.831182	0.108068	-1.549414
18067	H	-7.285368	0.711085	-1.614433
18068	H	-3.646589	2.768391	1.687650
18069	H	-4.570356	3.356179	0.581609
18070	H	-1.149420	1.869532	1.771149
18071	H	-2.252751	0.763045	1.616723

18072	H	-2.240191	1.953127	-0.217064
18073	O	-2.282941	1.932899	-1.200831
18074	H	-3.086113	2.424647	-1.451904
18075	H	-6.610979	-2.381126	-1.588044
18076	O	-7.517294	-2.616109	-1.322652
18077	H	-8.072420	-1.843695	-1.533260
18078	H	-9.754320	0.083534	-1.673906
18079	O	-8.885880	-0.151703	-1.333766
18080	H	-8.933250	-0.165160	-0.331923
18081	H	-7.920472	-3.725634	1.617264
18082	O	-7.592496	-2.881822	1.292167
18083	H	-7.593405	-2.908633	0.294442
18084	H	-7.999114	0.283170	1.553922
18085	O	-8.723690	-0.300779	1.263326
18086	H	-8.449759	-1.209707	1.482834
18087	H	1.603752	1.763365	1.709274
18088	O	0.693499	1.582331	1.417557
18089	H	0.678029	1.723652	0.444564
18090	H	0.425879	0.656644	-1.454127
18091	O	0.472449	1.629029	-1.318526
18092	H	-0.411186	1.978742	-1.532082
18093	H	-0.630934	-1.347238	1.632537
18094	O	0.288417	-1.137172	1.388068
18095	H	0.395338	-0.169731	1.525237
18096	H	0.432677	-1.258550	-0.375045
18097	O	0.454748	-1.121213	-1.349079
18098	H	1.322150	-1.438812	-1.654180
18099	H	3.283793	1.546774	-0.289551
18100	O	3.244641	1.492255	-1.270469
18101	H	2.371217	1.832529	-1.530105
18102	H	3.349232	0.307225	1.525418
18103	O	3.447338	1.283598	1.465095
18104	H	4.363487	1.485743	1.723414
18105	H	3.056504	-1.493674	0.300468
18106	O	3.046974	-1.432499	1.281337
18107	H	2.137207	-1.633574	1.561385
18108	H	3.278527	-0.274362	-1.521261
18109	O	3.225975	-1.254117	-1.461621
18110	H	4.096685	-1.594050	-1.732031
18111	H	5.141327	1.560565	-1.629645
18112	O	6.003119	1.186683	-1.378733
18113	H	5.935148	0.213567	-1.506262
18114	O	6.213975	1.168102	1.351150
18115	H	7.140383	1.301669	1.623040
18116	H	6.189831	1.299553	0.376754
18117	O	5.824129	-1.542065	1.340681
18118	H	5.907336	-0.569964	1.467516
18119	H	4.920691	-1.782058	1.608275
18120	H	5.959498	-1.679692	-0.417147
18121	O	5.984895	-1.552503	-1.392120
18122	H	6.878103	-1.816046	-1.678971
18123	H	8.912817	-0.106959	1.496362
18124	O	8.969513	0.889808	1.506799
18125	H	9.682121	1.144416	2.100568
18126	H	7.694011	-1.927848	1.438313
18127	O	8.615893	-1.698769	1.230284
18128	H	8.746985	-1.903289	0.286488
18129	O	8.791931	0.944853	-1.305792
18130	H	8.969180	1.130399	-0.365652
18131	H	7.907451	1.300393	-1.497883
18132	H	8.850595	-0.674652	-1.575429
18133	O	8.754827	-1.668290	-1.584915
18134	H	9.423690	-2.029219	-2.174603
18135				
18136	Cartesian coordinates of : W30_ 6			
18137				
18138	O	-5.739293	-1.414523	2.346755
18139	H	-5.735437	-1.872861	1.458305
18140	H	-6.413160	-1.838352	2.887203
18141	H	-5.651236	0.416724	2.285682
18142	O	-5.464570	1.375084	2.264841
18143	H	-4.549629	1.484040	2.574303
18144	O	-5.738747	2.742300	0.053557
18145	H	-5.733901	2.201450	0.894502
18146	H	-6.414067	3.420874	0.150097

18147	O	-5.470032	1.274001	-2.319197
18148	H	-5.653804	1.771615	-1.499007
18149	H	-4.556034	1.487891	-2.571665
18150	O	-5.467300	-2.653216	0.059930
18151	H	-5.654137	-2.192207	-0.780637
18152	H	-4.551411	-2.973248	-0.000181
18153	H	-5.737340	-0.325980	-2.345365
18154	O	-5.742239	-1.324672	-2.395356
18155	H	-6.418873	-1.578533	-3.030608
18156	H	-3.857679	-1.519725	2.604226
18157	O	-2.943628	-1.383885	2.296969
18158	H	-2.889322	-1.810403	1.409317
18159	H	-2.674550	0.305873	2.281031
18160	O	-2.644547	1.290712	2.348063
18161	H	-1.765961	1.516845	2.696028
18162	H	-3.857243	3.019856	0.014216
18163	O	-2.943103	2.685929	0.049540
18164	H	-2.889030	2.129367	0.861965
18165	H	-2.677353	1.826967	-1.407303
18166	O	-2.648249	1.391167	-2.292936
18167	H	-1.769515	1.578750	-2.662799
18168	H	-3.861107	-1.495437	-2.619075
18169	O	-2.946916	-1.297247	-2.348170
18170	H	-2.892630	-0.315326	-2.273331
18171	O	-2.646907	-2.680736	-0.058915
18172	H	-2.676499	-2.130616	-0.878659
18173	H	-1.768658	-3.095981	-0.036747
18174	H	-1.041534	-1.573738	2.666117
18175	O	-0.150126	-1.401812	2.318832
18176	H	-0.111599	-1.833254	1.434165
18177	H	0.114392	0.325301	2.301405
18178	O	0.153017	1.307115	2.371598
18179	H	1.043796	1.521800	2.695845
18180	H	-1.040980	3.099561	0.029932
18181	O	-0.150140	2.711438	0.053923
18182	H	-0.111774	2.159781	0.869160
18183	H	0.111419	1.833491	-1.434413
18184	O	0.150115	1.401906	-2.319007
18185	H	1.041589	1.573808	-2.666158
18186	O	-0.153046	-1.307032	-2.371734
18187	H	-1.043838	-1.521727	-2.695926
18188	H	-0.114423	-0.325224	-2.301586
18189	O	0.149988	-2.711326	-0.054109
18190	H	1.040790	-3.099528	-0.030081
18191	H	0.111755	-2.159632	-0.869323
18192	H	1.769537	-1.578825	2.662314
18193	O	2.648248	-1.391105	2.292464
18194	H	2.677276	-1.826555	1.406654
18195	H	3.861129	1.495412	2.619489
18196	O	2.946970	1.297279	2.348383
18197	H	2.892645	0.315359	2.273460
18198	O	2.942995	-2.685980	-0.049869
18199	H	3.857112	-3.019958	-0.014511
18200	H	2.888889	-2.129685	-0.862475
18201	H	2.674480	-0.305830	-2.281029
18202	O	2.644487	-1.290647	-2.348339
18203	H	1.765895	-1.516680	-2.696354
18204	O	2.943595	1.383945	-2.296755
18205	H	3.857677	1.519858	-2.603883
18206	H	2.889183	1.810265	-1.409021
18207	H	1.768940	3.096155	0.037209
18208	O	2.647153	2.680820	0.059152
18209	H	2.676910	2.130743	0.878917
18210	H	5.737521	0.325825	2.346452
18211	O	5.742278	1.324525	2.396143
18212	H	6.418822	1.578653	3.031378
18213	O	5.470079	-1.274135	2.318732
18214	H	5.653797	-1.771055	1.498098
18215	H	4.556067	-1.488145	2.571069
18216	O	5.738619	-2.742516	-0.054033
18217	H	6.414113	-3.420967	-0.150154
18218	H	5.733933	-2.201972	-0.895178
18219	H	5.651082	-0.416628	-2.285386
18220	O	5.464506	-1.375021	-2.265103
18221	H	4.549541	-1.483808	-2.574574

18222	O	5.739309	1.414644	-2.346294
18223	H	6.413178	1.838421	-2.886779
18224	H	5.735327	1.873045	-1.457878
18225	H	4.551736	2.973308	0.001148
18226	O	5.467492	2.652922	-0.059163
18227	H	5.654101	2.191373	0.781168
18228				
18229	Cartesian coordinates of : W30_7			
18230				
18231	O	3.283687	-1.403623	1.350857
18232	O	3.473028	-1.352829	-1.395990
18233	O	6.061923	-1.484936	1.420128
18234	O	6.414317	1.227848	1.307497
18235	O	6.222801	1.118968	-1.421009
18236	O	6.236184	-1.617797	-1.308617
18237	O	3.462377	1.398314	-1.336172
18238	O	3.646580	1.322015	1.408250
18239	O	9.173960	0.990182	1.484943
18240	O	8.855734	-1.611765	1.323156
18241	H	6.130253	-0.506913	1.502520
18242	H	5.161548	-1.724988	1.697392
18243	H	4.347236	-1.696747	-1.649400
18244	H	3.516995	-0.376409	-1.501099
18245	H	6.166691	0.140445	-1.505229
18246	H	5.357923	1.471627	-1.691391
18247	H	3.560835	0.348175	1.513671
18248	H	4.559492	1.547054	1.659162
18249	H	3.298747	-1.511743	0.374092
18250	H	2.373710	-1.596872	1.635610
18251	H	6.209796	-1.699977	-0.328858
18252	H	6.395037	1.311929	0.327672
18253	H	3.494258	1.500851	-0.358963
18254	H	2.586387	1.713596	-1.617975
18255	H	8.994566	-1.860802	0.391216
18256	H	7.936402	-1.843703	1.539113
18257	H	9.130693	-0.006839	1.518130
18258	H	7.337413	1.385458	1.577666
18259	H	7.132812	-1.884703	-1.581294
18260	H	9.883874	1.280079	2.065660
18261	H	0.645637	0.526995	-1.505277
18262	O	0.690005	1.504881	-1.416341
18263	H	-0.184655	1.845738	-1.672252
18264	H	0.673625	-1.329225	-0.327294
18265	O	0.698002	-1.244854	-1.306789
18266	H	1.572517	-1.564316	-1.589048
18267	H	0.874499	1.693297	0.346261
18268	O	0.889277	1.603858	1.325046
18269	H	1.799693	1.800606	1.606524
18270	H	0.611851	-0.144900	1.520879
18271	O	0.523909	-1.120053	1.431923
18272	H	-0.387347	-1.339186	1.693850
18273	H	-3.155881	-1.214049	1.640678
18274	O	-2.245729	-1.021853	1.353414
18275	H	-2.236640	-1.128328	0.376676
18276	H	-0.973677	1.928635	1.666105
18277	O	-1.885689	1.707592	1.409506
18278	H	-1.976439	0.734691	1.517687
18279	H	-1.191092	-1.313939	-1.648796
18280	O	-2.065805	-0.970757	-1.396431
18281	H	-2.022307	0.005757	-1.499092
18282	H	-2.042310	1.883893	-0.349679
18283	O	-2.068570	1.782601	-1.327869
18284	H	-2.941385	2.101036	-1.615716
18285	O	9.012406	0.910381	-1.326885
18286	H	8.125177	1.247312	-1.538472
18287	H	9.182822	1.141336	-0.395525
18288	O	-4.836489	-0.868496	-1.289926
18289	H	-3.968317	-1.194807	-1.583165
18290	H	-4.848446	-0.942421	-0.305789
18291	H	-4.870071	0.895595	-1.498903
18292	O	-4.840902	1.875017	-1.423156
18293	H	-5.737564	2.187340	-1.640329
18294	H	-4.913531	0.225450	1.514626
18295	O	-4.995163	-0.749341	1.418971
18296	H	-5.922562	-0.968983	1.637094

18297	H	-4.650928	2.065026	0.338481
18298	O	-4.654082	1.973497	1.316757
18299	H	-3.756273	2.191478	1.618758
18300	H	9.092440	-0.719521	-1.525492
18301	O	9.007766	-1.713387	-1.489676
18302	H	9.681460	-2.093700	-2.061349
18303	H	-6.658551	-0.893070	-1.639394
18304	O	-7.589716	-0.674654	-1.447662
18305	H	-7.694083	0.285230	-1.604562
18306	H	-7.742543	-0.838128	0.373029
18307	O	-7.734851	-0.789370	1.350429
18308	H	-8.488143	-1.341830	1.643254
18309	H	-7.656906	1.043641	1.478648
18310	O	-7.461911	1.968861	1.228780
18311	H	-6.559866	2.158265	1.536879
18312	H	-7.621358	2.139428	-0.365979
18313	O	-7.614917	2.104459	-1.368894
18314	H	-8.296967	2.700777	-1.692830
18315	H	-8.981249	-1.838067	-1.484672
18316	O	-9.719073	-2.434516	-1.251790
18317	H	-9.615304	-3.230000	-1.781842
18318	H	-9.992330	-2.529984	0.520952
18319	O	-9.931665	-2.427897	1.492494
18320	H	-10.806819	-2.185367	1.807822
18321				
18322	Cartesian coordinates of : W30_ 8			
18323				
18324	O	3.878080	0.073093	1.471038
18325	H	3.509748	0.566399	2.230182
18326	H	4.237001	0.727067	0.815017
18327	O	-4.660020	-1.409874	-2.744639
18328	H	-3.699829	-1.243066	-2.935978
18329	H	-5.155778	-1.290163	-3.560376
18330	O	-2.008223	-2.338191	1.795260
18331	H	-2.033207	-1.384766	2.074486
18332	H	-2.937878	-2.636610	1.782849
18333	O	-4.485016	-0.190727	-0.182748
18334	H	-4.534472	-0.988077	0.378086
18335	H	-4.806349	-0.475184	-1.057257
18336	O	-0.222755	5.060941	1.068554
18337	H	-1.156409	4.786961	1.134523
18338	H	-0.061528	5.266683	0.131001
18339	O	4.602822	1.645125	-0.537381
18340	H	3.934311	2.287135	-0.831227
18341	H	4.817315	1.086844	-1.306929
18342	O	-0.274529	1.007132	0.609217
18343	H	0.228417	1.804721	0.895123
18344	H	0.424074	0.362184	0.337852
18345	O	0.260917	4.906232	-1.730758
18346	H	0.321591	5.605869	-2.388831
18347	H	-0.648737	4.492138	-1.821091
18348	O	-2.227749	1.168872	-1.213159
18349	H	-2.997422	0.804530	-0.735202
18350	H	-1.485526	1.165752	-0.562700
18351	O	-2.033058	-1.075297	-2.728707
18352	H	-1.991510	-0.187776	-2.304593
18353	H	-1.852126	-1.710100	-1.994637
18354	O	0.239894	-3.049049	3.135307
18355	H	0.074106	-3.632995	3.883172
18356	H	-0.625615	-2.926642	2.679858
18357	O	2.170465	0.507972	-2.619233
18358	H	3.084839	0.339102	-2.913313
18359	H	1.592486	-0.164173	-3.058675
18360	O	4.826630	-0.211235	-2.644692
18361	H	5.524149	-0.314398	-3.299080
18362	H	4.628239	-1.111844	-2.264791
18363	O	0.655646	-1.530527	-3.476407
18364	H	-0.305691	-1.372611	-3.426247
18365	H	0.842661	-2.282461	-2.893425
18366	O	2.385971	1.521357	3.300240
18367	H	2.017852	2.160837	2.637205
18368	H	2.732931	2.042326	4.031822
18369	O	4.560691	-2.486115	1.230225
18370	H	5.403750	-2.740126	1.618364
18371	H	4.408150	-1.533199	1.441291

18372	O	1.390637	2.996665	1.334266
18373	H	0.832080	3.821800	1.355194
18374	H	1.830228	2.985884	0.456653
18375	O	-3.866818	1.896239	1.703429
18376	H	-4.321085	1.326416	1.062469
18377	H	-3.245923	1.319669	2.190596
18378	O	-1.444429	-2.921054	-0.841223
18379	H	-0.494889	-3.132062	-0.953447
18380	H	-1.563547	-2.649031	0.095345
18381	O	-4.106014	-3.724295	-1.226143
18382	H	-3.131837	-3.710386	-1.250091
18383	H	-4.404967	-3.069017	-1.882444
18384	O	2.172139	-4.037067	1.283143
18385	H	1.548266	-3.727593	1.963624
18386	H	3.015228	-3.579662	1.438715
18387	O	-4.641910	-2.722977	1.106726
18388	H	-5.428115	-3.061081	1.545985
18389	H	-4.528600	-3.211471	0.238569
18390	O	-2.946476	4.257020	0.957043
18391	H	-3.271421	3.357124	1.237033
18392	H	-3.581068	4.890619	1.307441
18393	O	1.770685	-0.513280	-0.175774
18394	H	2.036186	-0.088211	-1.029540
18395	H	2.510855	-0.380328	0.456826
18396	O	-2.141049	3.901893	-1.707491
18397	H	-2.217577	2.927732	-1.722718
18398	H	-2.547947	4.156072	-0.858550
18399	O	2.185912	2.938212	-1.301480
18400	H	1.610549	3.672470	-1.595528
18401	H	1.968985	2.161065	-1.851961
18402	O	0.336449	-0.335546	4.127946
18403	H	0.537843	-1.229030	3.805054
18404	H	1.068201	0.248055	3.864508
18405	O	-1.853156	0.196614	2.576607
18406	H	-1.250559	0.107748	3.346491
18407	H	-1.249506	0.514669	1.858540
18408	O	4.161118	-2.511554	-1.562876
18409	H	3.237726	-2.800041	-1.656450
18410	H	4.366928	-2.577281	-0.611599
18411	O	1.331821	-3.025556	-1.071133
18412	H	1.599206	-3.614086	-0.325354
18413	H	1.435808	-2.124587	-0.683094
18414				
18415	Cartesian coordinates of : W30_9			
18416				
18417	O	3.397455	1.008601	1.658572
18418	O	3.600344	-1.657648	1.008996
18419	O	6.171727	1.123479	1.574438
18420	O	6.338292	1.603447	-1.116175
18421	O	6.173521	-1.087689	-1.594873
18422	O	6.370497	-1.565119	1.094385
18423	O	3.396235	-1.013197	-1.654906
18424	O	3.567433	1.656572	-1.006664
18425	O	9.106612	1.781720	-1.014219
18426	O	8.971459	1.058044	1.507731
18427	H	6.171884	1.415254	0.634835
18428	H	5.287998	1.323814	1.926637
18429	H	4.498723	-1.962255	1.225645
18430	H	3.570640	-1.550414	0.031895
18431	H	6.186129	-1.380091	-0.655577
18432	H	5.290067	-1.301183	-1.939895
18433	H	3.548285	1.548343	-0.029377
18434	H	4.459509	1.973575	-1.231346
18435	H	3.433832	0.031812	1.552924
18436	H	2.501811	1.219085	1.974410
18437	H	6.337931	-0.628142	1.391399
18438	H	6.316335	0.666274	-1.413619
18439	H	3.419063	-0.036042	-1.549776
18440	H	2.501465	-1.236954	-1.963992
18441	H	9.127219	0.096218	1.531331
18442	H	8.068114	1.201835	1.837675
18443	H	9.135083	1.602886	-0.032444
18444	H	7.248920	1.916381	-1.267039
18445	H	7.286194	-1.865641	1.239627
18446	H	9.793750	2.421240	-1.224371

18447	H	0.652856	-1.427718	-0.643431
18448	O	0.622995	-1.128526	-1.579398
18449	H	-0.270322	-1.332284	-1.906433
18450	H	0.800327	-0.677468	1.417516
18451	O	0.827576	-1.613861	1.119686
18452	H	1.725021	-1.937788	1.310573
18453	H	0.776583	0.635545	-1.394315
18454	O	0.794659	1.572513	-1.097003
18455	H	1.686562	1.907424	-1.294981
18456	H	0.640519	1.383995	0.667443
18457	O	0.623478	1.085955	1.604136
18458	H	-0.269982	1.276495	1.938453
18459	H	-3.042607	1.183404	1.995391
18460	O	-2.147872	0.967960	1.680298
18461	H	-2.116022	-0.009304	1.572907
18462	H	-1.087008	1.936760	-1.209157
18463	O	-1.978034	1.618066	-0.983162
18464	H	-1.996992	1.510002	-0.005918
18465	H	-1.049901	-2.001022	1.247831
18466	O	-1.946161	-1.690823	1.031104
18467	H	-1.977471	-1.586415	0.053722
18468	H	-2.131309	-0.071682	-1.526295
18469	O	-2.150448	-1.048837	-1.632067
18470	H	-3.045126	-1.275658	-1.940618
18471	O	8.973089	-0.982177	-1.544309
18472	H	8.070468	-1.139865	-1.869712
18473	H	9.113761	-0.018031	-1.568366
18474	O	-4.723482	-1.646493	1.132388
18475	H	-3.827286	-1.970657	1.327047
18476	H	-4.751173	-0.711580	1.431161
18477	H	-4.900306	-1.463574	-0.631866
18478	O	-4.920646	-1.164160	-1.568112
18479	H	-5.804929	-1.380957	-1.910317
18480	H	-4.909593	1.360317	0.682298
18481	O	-4.922409	1.063348	1.619709
18482	H	-5.811905	1.253246	1.961523
18483	H	-4.782161	0.607897	-1.380831
18484	O	-4.752460	1.544557	-1.083739
18485	H	-3.854141	1.864730	-1.277272
18486	H	9.157235	-1.525114	-0.005630
18487	O	9.140025	-1.704265	0.976311
18488	H	9.836695	-2.335537	1.179897
18489	H	-6.646012	-2.011304	1.287328
18490	O	-7.509565	-1.671482	0.999201
18491	H	-7.439248	-1.560314	0.028439
18492	H	-7.720235	-0.062686	1.569814
18493	O	-7.706341	0.917972	1.691235
18494	H	-8.625185	1.216208	1.749165
18495	H	-7.393596	1.430683	0.005043
18496	O	-7.518743	1.619786	-0.950112
18497	H	-6.665124	1.962554	-1.263237
18498	H	-7.686524	-0.081813	-1.614450
18499	O	-7.691376	-1.054544	-1.723353
18500	H	-8.626415	-1.311399	-1.626084
18501	H	-9.668468	-1.692680	0.460240
18502	O	-10.083925	-1.283389	-0.310754
18503	H	-10.217190	-0.347941	-0.084122
18504	H	-10.823793	2.105913	-0.011329
18505	O	-10.041382	1.563424	0.129008
18506	H	-9.363379	1.855757	-0.507161
18507				
18508				
18509				