

## **Supporting information for**

### **Edge-sharing water prisms**

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**Table S1.** The Cartesian coordinates for the lowest-energy configurations of edge-sharing water prisms. Here, the headlines indicate the number of molecules and the numbers of square, pentagonal and hexagonal prisms.

<b>16-210</b>			
O	2.59934703	.77190366	1.39870920
H	2.57401402	1.72795117	1.52447343
H	1.70174066	.48622757	1.61712475
O	1.44543650	3.36320460	1.39422622
H	.49121458	3.19252149	1.46409133
H	1.59593223	4.20512013	1.83045924
O	1.39728996	3.08098320	-1.43415699
H	1.55051410	3.22854033	-.49088969
H	1.97453360	2.34732031	-1.68000702
O	2.82336882	.57166921	-1.35986705
H	2.98483080	-.34062900	-1.63758062
H	2.91445804	.57320506	-.39437580
O	2.86542396	-2.29579169	-1.58976155
H	2.85463249	-2.35974091	-.62211459
H	3.60955620	-2.82115049	-1.89128880
O	2.69120342	-2.26085675	1.14760512
H	2.84393656	-1.36348776	1.46797384
H	1.82108906	-2.53638545	1.46467741
O	.05399821	-.20161661	1.72966684
H	-.85914607	.11703030	1.77684065
H	-.02527156	-1.16600286	1.69194995
O	-2.62250266	.35185463	1.42820800
H	-2.92040722	-.53808962	1.65990845
H	-2.70406735	.40604318	.46401126
O	-1.26436310	2.96844280	1.25353579
H	-1.79242750	2.22406553	1.56620002
H	-1.43546758	3.03736163	.30360555
O	-1.34512419	3.19068888	-1.56629297
H	-.38057466	3.09216305	-1.63262593
H	-1.54740052	4.04569631	-1.95279145
O	-2.48571177	.58567713	-1.34925786
H	-2.59696076	1.50004579	-1.63186800
H	-1.52759835	.45290120	-1.36874554
O	.16240761	.06937821	-1.00532215
H	1.02325181	.39086675	-1.30571570
H	.22213571	.07458049	-.03865733
O	-.03672060	-2.61367141	-1.44575965
H	.82481848	-2.88851781	-1.78006135
H	.02710858	-1.65037603	-1.38126983
O	-2.90742531	-2.25929668	-1.25474131
H	-2.95006611	-1.31647018	-1.46470982
H	-2.02871238	-2.55747202	-1.52436439
O	-3.03890866	-2.49441642	1.44493640
H	-3.09286539	-2.48399290	.47526389
H	-3.76962408	-3.03520132	1.75336281
O	-.20751501	-2.89442210	1.31850370
H	-1.13904548	-2.97124939	1.56611737
H	-.19511675	-2.93414307	.35005256

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O	.16805205	2.69735152	1.35360599
H	1.09762255	2.77210202	1.61028943
H	.16671012	2.73027590	.38496985
O	2.98315597	2.57303540	1.59714131
H	3.32230766	1.66169115	1.61101329
H	3.59762109	3.08993251	2.12413889
O	2.80406027	2.56973249	-1.24359252
H	2.87479554	2.73517711	-.29372999
H	1.87046820	2.69285334	-1.46187262
O	-.04761459	2.47476259	-1.39425775
H	-.95031157	2.76778123	-1.57766531
H	-.07628794	1.51683451	-1.53351887
O	-2.85477331	2.64306831	-1.51058718
H	-3.18460386	1.72956559	-1.55661989
H	-3.48394781	3.17593448	-2.00294147
O	-2.71132543	2.52464157	1.34030108
H	-1.79218844	2.65701794	1.60613691
H	-2.73963578	2.72159293	.39417936
O	-.17481723	-.01268520	1.24933264
H	-.11513229	.91677470	1.51064024
H	-.17332391	.00898542	.28110646
O	1.83974572	-1.85976525	1.50187070
H	1.15385711	-1.17939650	1.56712023
H	1.36331571	-2.69254598	1.64009204
O	3.94334147	.03995539	1.33193136
H	3.36883007	-.70206295	1.56470759
H	4.09329794	-.03301133	.38033649
O	3.97904083	.13464245	-1.53221224
H	3.54890027	1.00721621	-1.53175413
H	4.76157295	.22894522	-2.08115187
O	2.07293951	-1.89517115	-1.22687003
H	2.80198248	-1.31903503	-1.50013794
H	2.10467389	-1.89118043	-.25608765
O	-.14275275	-.27453159	-1.49880710
H	.63318346	-.85306265	-1.53701004
H	-.90237930	-.87227365	-1.55946807
O	-2.08099580	-2.20928759	-1.28830660
H	-1.50230191	-2.94510469	-1.52786902
H	-2.13450217	-2.22512483	-.31992783
O	-3.82100378	.10036022	-1.32947407
H	-3.33532330	-.69682734	-1.57630368
H	-4.00968404	.00924296	-.38519280
O	-4.08124720	.17026494	1.50323722
H	-3.57430723	.99812407	1.55832763
H	-4.90788270	.33617935	1.96281881
O	-2.16201373	-1.90053369	1.44908041
H	-1.47525106	-1.22376794	1.53436598
H	-2.98429013	-1.42352265	1.61932775
O	-.03445974	-3.89050785	1.36367340
H	-.86610273	-3.44117729	1.55757093
H	-.02329635	-4.04618713	.41170999
O	.19171387	-3.92252990	-1.53782041
H	.93230278	-3.29881215	-1.59497152

H .43933747 -4.69087982 -2.05788233

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O -2.71771418 -.16210697 1.29580838  
H -2.96528396 -1.05817159 1.56539467  
H -2.73076285 -.18197799 .32439198  
O -3.04829098 -2.97918134 1.41768062  
H -3.09159862 -3.00489134 .44704607  
H -3.74919033 -3.55256979 1.73663174  
O -2.88256969 -2.79282666 -1.26981527  
H -2.96643202 -1.85395025 -1.48799859  
H -1.98309236 -3.04094367 -1.52116873  
O -2.54428873 .02072473 -1.44464411  
H -2.78573338 .95657255 -1.52167578  
H -1.58479041 .01607494 -1.56935992  
O -2.64403008 2.74438542 -1.19939162  
H -2.68730084 2.83056893 -.23952794  
H -1.76536061 3.05350944 -1.45511717  
O -2.54764544 2.56286702 1.69479904  
H -2.70591156 1.60696175 1.72332362  
H -3.18030647 2.96263902 2.29647313  
O .02192864 -.40278256 1.54293932  
H -.89769418 -.11774298 1.63008297  
H -.02648424 -1.37026991 1.54938887  
O -.19625563 -3.11707532 1.29155102  
H -1.11498709 -3.26124776 1.55580425  
H -.19674778 -3.16547471 .32305183  
O 2.71182142 -2.76582527 1.22919554  
H 1.80827207 -2.96250452 1.50999663  
H 2.88381788 -1.84380007 1.46206285  
O 2.71256467 .14926217 1.36380740  
H 1.76160025 .09638735 1.53508453  
H 2.92947233 1.08154464 1.49791105  
O 2.84819506 -3.00559202 -1.48195026  
H 2.87183681 -3.01215675 -.51127670  
H 3.51658931 -3.62859838 -1.77603018  
O -.01096640 -2.89860495 -1.45951419  
H .88249784 -3.18235893 -1.69297669  
H .03255150 -1.93149894 -1.46816776  
O .20847741 -.17147297 -1.20719677  
H 1.11857784 .01068942 -1.47801068  
H .22729363 -.13712265 -.23956746  
O 2.94733439 -.14083720 -1.38037141  
H 3.04946541 -1.06672712 -1.63908623  
H 2.98705951 -.13505600 -.41157591  
O 2.48663838 2.67052813 -1.47530087  
H 2.73448267 1.76551294 -1.70326560  
H 2.69761945 2.76953549 -.53706934  
O -.00078484 3.77717231 -1.62994432  
H .85332439 3.31714958 -1.68886984  
H .10647456 4.58717026 -2.13483117  
O .04632477 3.71820792 1.19157089  
H -.75832923 3.27694649 1.49348187  
H -.06732655 3.83747700 .23875906

O	2.65330592	2.95712616	1.36878203
H	1.71596529	3.20927990	1.42605501
H	3.14118488	3.64969508	1.82098904

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O	-4.22170471	1.33645913	-1.56881642
H	-4.13830726	.36769367	-1.57994422
H	-4.96658450	1.54653203	-2.13740153
O	-4.02964406	1.43016580	1.28610314
H	-4.18883443	1.55807292	.34149248
H	-3.18382003	1.86083679	1.47301180
O	-1.60348259	2.29460855	-1.32159589
H	-2.51577549	2.09929453	-1.57717204
H	-1.61680920	2.34561256	-.35361612
O	-3.91389628	-1.34345591	-1.30409497
H	-4.00196332	-1.48073374	-.35120756
H	-3.06364372	-1.73587786	-1.54410855
O	-3.99314993	-1.26502624	1.55806357
H	-4.02692391	-.29319184	1.55986853
H	-4.70803542	-1.55521755	2.13007543
O	-1.36675931	2.36069089	1.43344313
H	-.82133779	1.56813104	1.54875498
H	-.75923868	3.09730921	1.58956866
O	.03410043	.09633874	-1.47134505
H	-.56333494	.85158434	-1.58755264
H	-.50767852	-.69994491	-1.58848087
O	.72847053	3.94520425	-1.34283127
H	-.06813653	3.45043975	-1.57682270
H	.64274137	4.14501642	-.40083548
O	-1.25134130	-2.32497170	-1.32876088
H	-.60927817	-2.99630151	-1.59979182
H	-1.25847841	-2.36162316	-.36008305
O	-1.32971468	-2.16417403	1.42536737
H	-2.25467027	-1.94458813	1.60931153
H	-.83816628	-1.33752359	1.54599714
O	.20504272	.11403378	1.28143066
H	1.13698703	.05363803	1.53658464
H	.22190423	.11220537	.31222089
O	.79055728	4.15303846	1.51057207
H	1.60347618	3.62160860	1.56098181
H	.96219497	4.94701042	2.02295562
O	2.78500993	.02841273	-1.36667891
H	1.82763200	.06271263	-1.51369818
H	3.09200823	.92753771	-1.54894909
O	3.18797367	2.80386610	-1.49753293
H	2.30755667	3.21353721	-1.54910533
H	3.76903807	3.35846348	-2.02394723
O	.89800632	-4.11915828	-1.60157697
H	1.74268541	-3.63758698	-1.58073521
H	1.04056660	-4.87730547	-2.17354873
O	.72728160	-4.10433343	1.25183959
H	-.03909929	-3.55256339	1.46004508
H	.68852650	-4.25668663	.29832080
O	2.92704226	-.18281028	1.37623550

H	3.11641827	-1.09547005	1.63502298
H	2.97049873	-.18042941	.40789920
O	3.06314616	2.67357095	1.35734433
H	3.27161357	2.69312898	.41340497
H	3.08558210	1.74068421	1.60905333
O	3.22679452	-2.76746167	-1.25424574
H	3.21081835	-1.81932835	-1.44386414
H	3.38352633	-2.84180959	-.30347055
O	3.17479168	-2.97973579	1.59522465
H	2.29567440	-3.39501644	1.57599639
H	3.72214152	-3.54511461	2.14562340

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O	3.65916705	1.80020518	-1.18759174
H	3.82819864	1.80586549	-.23615885
H	3.35008756	.90777860	-1.39533128
O	3.67678205	1.98128871	1.67389305
H	2.99204120	2.67141384	1.66489219
H	4.38883029	2.32330840	2.22004753
O	2.41661136	-.72112687	-1.37516756
H	1.48280196	-.53307518	-1.55474589
H	2.51589958	-1.66650409	-1.55771278
O	1.92567511	3.86193142	-1.51013727
H	2.52797519	3.09897187	-1.49785210
H	2.36775938	4.53184342	-2.03767322
O	1.82009887	3.93291715	1.32449563
H	1.80783618	4.04676828	.36421972
H	.89259151	3.92887043	1.59367368
O	2.58373181	-.58560030	1.37319019
H	3.02659972	.22758964	1.65328500
H	2.62829487	-.57909141	.40492017
O	-.30731663	-.31546915	-1.54984711
H	-.88057675	.46119835	-1.62834262
H	-.91835611	-1.06424284	-1.61883161
O	2.28441385	-3.52239791	-1.52805078
H	1.35134605	-3.79194002	-1.57631209
H	2.76973954	-4.15409130	-2.06461194
O	-.90140862	4.02505289	-1.20396405
H	.02598094	3.87734647	-1.43638641
H	-1.38875902	3.23952642	-1.48761127
O	-1.03687470	4.13081860	1.49392831
H	-1.04921910	4.19357371	.52410522
H	-1.43790165	4.93856349	1.82361577
O	-.13472017	-.32075622	1.21413811
H	.78574690	-.40894569	1.50094029
H	-.08540974	-.30845373	.24626960
O	2.18961537	-3.40817084	1.33196210
H	2.37271470	-2.49401725	1.58726097
H	2.39084809	-3.45807172	.38776899
O	-2.30778001	1.55641868	-1.32688136
H	-3.08854705	1.06577013	-1.61770914
H	-2.35046903	1.54943978	-.35800273
O	-2.29506401	-2.20607792	-1.37659752
H	-3.08236194	-1.71868072	-1.65522547

H	-2.34123982	-2.23354746	-.40819510
O	-.32108205	-4.26815521	-1.36914976
H	-1.02615909	-3.65442959	-1.61377591
H	-.44250484	-4.44087499	-.42551311
O	-2.14464376	1.54628807	1.44375339
H	-1.83608076	2.43903300	1.65446207
H	-1.36930145	.97350021	1.54308480
O	-2.06718823	-2.27054889	1.37239032
H	-1.36220595	-1.61222598	1.46355839
H	-1.63417186	-3.11747785	1.54675090
O	-.30886638	-4.46153901	1.48163715
H	.58650429	-4.08586596	1.53517972
H	-.28802534	-5.26983980	1.99980749
O	-4.43132745	-.33393660	-1.50330097
H	-4.49510228	-.35523092	-.53370613
H	-5.33162854	-.33171536	-1.83644958
O	-4.20098195	-.39089460	1.18642530
H	-3.66036076	.37537005	1.42216522
H	-3.66166254	-1.16215000	1.40660351

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O	2.37338062	.69090097	1.42287399
H	2.99257782	-.03157519	1.60549896
H	1.48858186	.32458698	1.57549336
O	4.11887641	-1.50483682	1.57475268
H	3.64360511	-2.35305747	1.56916182
H	4.86305463	-1.62233130	2.17053087
O	2.51376743	3.49626832	1.22160569
H	2.52364924	2.55266307	1.43375019
H	2.63525920	3.55049992	.26470959
O	-.19382342	-.32283284	1.30324277
H	-.99719756	.14797244	1.57114658
H	-.21503466	-.29873086	.33441362
O	4.11323355	-1.38124892	-1.28879085
H	4.26532715	-1.32046152	-.33617324
H	3.57893671	-.60735391	-1.51404435
O	2.72381616	-3.80245550	1.28621139
H	1.78280066	-3.66890730	1.46706628
H	2.78797289	-3.99161777	.34071131
O	2.35367370	3.63443239	-1.64154695
H	1.47356473	4.04509745	-1.59374262
H	2.87673399	4.20069822	-2.21428731
O	.22052459	4.89200882	1.60181765
H	1.04203873	4.37302326	1.57859711
H	.41488727	5.66697142	2.13458831
O	-2.57247517	1.02640954	1.38232388
H	-2.56655045	1.95781126	1.65183820
H	-2.59828354	1.05713543	.41520663
O	.01458861	-3.06147615	1.43756841
H	-.05695372	-2.10226404	1.55928341
H	-.87784921	-3.39959847	1.60046058
O	2.37962764	.84887525	-1.33101719
H	2.41547214	1.77594320	-1.60697652
H	2.39828145	.87524438	-.36209515

O	2.92762797	-3.79724138	-1.57299132
H	3.38889200	-2.94121037	-1.57534938
H	3.42595666	-4.37111448	-2.15994782
O	-.04659596	4.81669458	-1.21081339
H	-.03483302	4.97477881	-.25692392
H	-.89387991	4.38788794	-1.39003673
O	-2.39879653	3.75777360	1.46947867
H	-1.51147460	4.10280563	1.63191024
H	-2.55802441	3.86858614	.52441238
O	-4.06309419	-1.35998875	1.35898574
H	-3.61447446	-.53604147	1.59574563
H	-4.25262053	-1.28670355	.41441220
O	-2.71120807	-3.69658731	1.54280601
H	-3.20796843	-2.86124569	1.58114854
H	-3.19405371	-4.31644739	2.09521328
O	-.07533265	-.38535609	-1.47054243
H	.79993814	.01422369	-1.59720005
H	.05156781	-1.34094510	-1.58058866
O	.22930090	-3.11611092	-1.31209102
H	1.09604625	-3.45619455	-1.57499630
H	.22495615	-3.15876257	-.34361513
O	-2.61695737	3.60181624	-1.40020603
H	-2.63988396	2.63673147	-1.49873825
H	-3.32001636	3.94692595	-1.95578588
O	-4.15630822	-1.41745045	-1.51782396
H	-3.59217053	-2.20937233	-1.54081156
H	-4.91146391	-1.61645026	-2.07693831
O	-2.56500434	-3.59578607	-1.31342481
H	-2.58727198	-3.80316147	-.36930768
H	-1.62903448	-3.49845834	-1.53558142
O	-2.53127574	.85213126	-1.40182898
H	-1.66146491	.44486058	-1.54210588
H	-3.16526172	.13533487	-1.55539209

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O	-.02828076	2.30564646	1.38020547
H	.85947546	2.63820239	1.57968542
H	.00934119	1.35284617	1.55780937
O	2.62890716	3.19021421	1.58535887
H	3.33183683	2.51863772	1.59907001
H	2.95437450	3.91951895	2.11905409
O	.05150401	-.45385832	1.49639999
H	.81748687	-1.03759580	1.60817913
H	-.71979968	-1.03643088	1.58090881
O	-2.63815902	3.35609110	1.22942870
H	-1.74040535	3.05464622	1.42675780
H	-2.65838183	3.51356341	.27637503
O	4.63858362	1.39066859	1.31088301
H	4.64410520	.46712599	1.59397337
H	4.77403572	1.36656498	.35368784
O	2.52645013	3.14598620	-1.28331780
H	2.49531525	3.31126928	-.33148938
H	1.61622570	2.94530934	-1.53969107
O	2.12270472	-2.26126668	1.34173269



H	3.01388799	-2.04641200	1.64963967
H	2.18533974	-2.26893148	.37438289
O	-2.03718482	-2.21258939	1.28218206
H	-2.92129563	-1.91479306	1.54690504
H	-2.07159914	-2.23333921	.31537173
O	-4.72775305	1.66301979	1.57698232
H	-3.95814443	2.25675798	1.56587371
H	-5.38797557	2.10066342	2.11999389
O	-2.86047608	3.33474001	-1.63187270
H	-3.53343834	2.63369387	-1.60035199
H	-3.23321648	4.03237809	-2.17648279
O	4.80707852	-1.45465867	1.53483363
H	4.86513999	-1.50080048	.56565705
H	5.57316906	-1.92091474	1.87765597
O	4.62161083	1.44183570	-1.52871028
H	3.83971136	2.01918126	-1.55010985
H	5.28688332	1.88732814	-2.05920938
O	-.21130410	2.45022775	-1.35961820
H	-1.07521091	2.79466735	-1.62667813
H	-.21989437	2.46871423	-.39033037
O	.00924068	-4.15701049	1.30515021
H	.78504996	-3.62705762	1.53350991
H	-.75894216	-3.61117173	1.52374471
O	-4.56554492	-1.17989776	1.38352483
H	-4.58933666	-.23100769	1.56253982
H	-4.72470494	-1.27672589	.43685547
O	-4.75910481	1.43749122	-1.23969672
H	-4.89870944	1.48286508	-.28393505
H	-4.64173384	.49929245	-1.43911681
O	4.63861574	-1.37562737	-1.15197862
H	4.59786614	-.44097363	-1.39773937
H	3.78552410	-1.75473344	-1.40453767
O	.06309815	-.27280663	-1.25816812
H	-.00062413	.65313242	-1.53599257
H	.06383396	-.23292897	-.28868265
O	.01547864	-4.31262915	-1.39151291
H	.01291073	-4.37836107	-.42077084
H	.01689677	-5.21492117	-1.72052978
O	-4.49022092	-1.39476257	-1.48984039
H	-3.59148694	-1.74196540	-1.60365732
H	-5.05812729	-1.92328794	-2.05578030
O	1.96826411	-2.25345008	-1.44315547
H	1.36289446	-1.50383429	-1.54503425
H	1.42711686	-3.03790495	-1.60877383
O	-1.85446081	-2.20885448	-1.53251187
H	-1.21400219	-1.48172015	-1.57994999
H	-1.32601032	-3.01053215	-1.65844266

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O	.06312175	2.35337551	1.42251558
H	-.80517915	2.74037308	1.61071277
H	-.03704575	1.40060810	1.57229605
O	-2.47218769	3.53145689	1.62966985
H	-3.27715664	2.98620098	1.63841279

H	-2.67342927	4.30105525	2.16813759
O	-.21502529	-.39584956	1.30096073
H	-1.01708034	-.86533523	1.57351166
H	-.24167754	-.40736666	.33151352
O	2.54452411	3.65417519	1.20613036
H	1.70217249	3.22800097	1.41799515
H	2.51522974	3.83530024	.25741821
O	-4.74214455	2.08386101	1.35616674
H	-4.84574883	1.16334394	1.63053826
H	-4.88047956	2.08386248	.39898813
O	-2.36819379	3.48523417	-1.23791400
H	-2.31765208	3.64281304	-.28575179
H	-1.50661645	3.12223008	-1.48433974
O	-2.57390496	-1.82623576	1.41643783
H	-3.42570719	-1.48608301	1.72253317
H	-2.62667506	-1.80534768	.44835757
O	2.23257065	-1.69346944	1.39582644
H	1.41141697	-1.19990873	1.54305038
H	1.99950344	-2.62029135	1.55365380
O	4.82617129	2.22777046	1.47387290
H	3.99583605	2.73301967	1.48580708
H	5.42702453	2.69641658	2.05831418
O	2.69124593	3.72084641	-1.65548358
H	3.48581908	3.16067109	-1.66006258
H	2.89966655	4.47739513	-2.20916625
O	-5.15975067	-.72497712	1.58082313
H	-5.20329015	-.77183735	.61076326
H	-5.96600707	-1.12872579	1.91048579
O	-4.70043926	2.12971242	-1.48420719
H	-3.84416260	2.58923381	-1.50808420
H	-5.28820357	2.64407817	-2.04301847
O	.23501036	2.40995025	-1.33342254
H	1.04804035	2.85935151	-1.60485839
H	.24837109	2.42654099	-.36439172
O	-1.35172938	-4.35798349	1.33437455
H	-1.80085863	-3.53205636	1.56149136
H	-1.50397213	-4.48124767	.38792062
O	1.34276350	-4.34806151	1.53742910
H	.37102394	-4.37294245	1.56595287
H	1.64264246	-5.05309167	2.11665710
O	4.80913271	-.58410934	1.11766549
H	3.95079525	-.95516618	1.36729277
H	4.78160680	.35090049	1.36393814
O	4.89996349	2.18323472	-1.36760012
H	5.03299990	2.18135340	-.40974147
H	4.91047938	1.25353026	-1.62986679
O	-4.94322408	-.67209458	-1.09980617
H	-4.83765926	.25590196	-1.35082117
H	-4.11028392	-1.10696249	-1.33101792
O	-.09445097	-.32791358	-1.47474332
H	.02357641	.62484819	-1.61414382
H	.77879739	-.72501164	-1.61900281
O	-1.33948442	-4.43836233	-1.53222275
H	-.36919988	-4.38110141	-1.56026773

H	-1.58053192	-5.15188360	-2.12821070
O	1.34496940	-4.21418919	-1.32364793
H	1.50591857	-4.34392001	-.37956722
H	1.71434796	-3.34445299	-1.52967795
O	5.00806139	-.65559474	-1.56257524
H	5.05038990	-.70429018	-.59256492
H	5.76421373	-1.14565773	-1.89414735
O	-2.40288702	-1.85334332	-1.33220689
H	-1.62945466	-1.29600895	-1.51070578
H	-2.11128680	-2.75769399	-1.52042256
O	2.36224813	-1.59288771	-1.36513001
H	3.22424527	-1.27921282	-1.67179669
H	2.41888028	-1.58052509	-.39702723

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O	.13894608	-.09307371	-1.45680812
H	-.62758242	.47968154	-1.61675935
H	.91611913	.47158876	-1.58523141
O	-2.09497189	1.54654749	-1.39219542
H	-2.17913645	2.46075393	-1.69615654
H	-2.11218691	1.59914787	-.42400410
O	2.36795191	1.58528715	-1.27657714
H	2.34738387	2.51854865	-1.53580344
H	2.31992966	1.59465651	-.30668139
O	-.04352885	-2.86817838	-1.30323991
H	.04677434	-1.92258484	-1.50020761
H	.81573993	-3.26635248	-1.50942870
O	-2.50036668	4.32805148	-1.60443448
H	-2.58785632	4.34587062	-.63636312
H	-3.29914634	4.72654038	-1.95816773
O	.00272678	5.64265016	-1.36018583
H	-.81300176	5.20042177	-1.62969576
H	-.07905949	5.77350756	-.40532008
O	2.36311130	4.35805189	-1.61286024
H	1.50654181	4.81812826	-1.61739867
H	2.95050026	4.89873716	-2.14650503
O	-4.45607676	.01767258	-1.27043294
H	-3.64603284	.48810678	-1.50947321
H	-4.55823678	.15060206	-.31855557
O	-4.70352720	-2.66488484	-1.51499174
H	-4.59504621	-1.69933031	-1.54008659
H	-5.44109490	-2.86179204	-2.09756984
O	-2.44332929	-4.32526140	-1.11767865
H	-1.63922471	-3.82989407	-1.32871878
H	-3.18315914	-3.75786466	-1.37450517
O	2.43414138	-4.14529600	-1.55686990
H	3.24734657	-3.61337789	-1.52927382
H	2.61675376	-4.87350299	-2.15599575
O	4.68132407	-2.68975691	-1.19696008
H	4.66472651	-1.74364580	-1.39322808
H	4.82837211	-2.75590489	-.24348529
O	4.69123190	.13721269	-1.46795354
H	3.86685842	.64518036	-1.53230791
H	5.34600278	.61910454	-1.97894118

O	.04598636	-.24055740	1.33589027
H	-.02005145	-1.16489189	1.61699055
H	.08321750	-.27687916	.36768071
O	-2.17244724	1.42336964	1.36531072
H	-1.40663211	.85588837	1.54461289
H	-2.95344690	.88243251	1.55687208
O	2.28957647	1.41828719	1.45705291
H	1.53365935	.83629762	1.62910012
H	3.08087069	.87407481	1.60582494
O	-.20147654	-3.00555833	1.44513561
H	-.98768919	-3.49377464	1.72479271
H	-.23308431	-3.00549283	.47623361
O	-2.40406255	4.21359769	1.07792621
H	-2.29321567	3.28529608	1.32835586
H	-1.58940683	4.66380393	1.34099961
O	.01769092	5.61692474	1.48077212
H	.84172940	5.10227468	1.51349222
H	.14342412	6.35362204	2.08384460
O	2.31115088	4.21032656	1.26287406
H	2.51335652	4.26327347	.32008350
H	2.30455932	3.26608005	1.47618673
O	-4.55720850	-.03333340	1.59029707
H	-4.59349025	-1.00480388	1.60268396
H	-5.29383672	.26156210	2.13178731
O	-4.71499695	-2.71952743	1.32990312
H	-4.79408427	-2.83679122	.37326714
H	-3.99778498	-3.30678786	1.60221231
O	-2.55745476	-4.54986211	1.55994951
H	-2.52184902	-4.60835657	.59024994
H	-2.62436339	-5.45039204	1.88616329
O	2.31149098	-4.24829654	1.31224919
H	2.26805587	-4.36840839	.35443690
H	1.47855365	-3.82131649	1.55521356
O	4.63212141	-2.89936064	1.62644427
H	3.79080372	-3.38613802	1.62774247
H	5.22429202	-3.39440204	2.19784843
O	4.58342415	-.07455560	1.40672335
H	4.78762759	-.00131443	.46650765
H	4.57341487	-1.02065238	1.60137923