



FOUNDATIONS  
ADVANCES

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**Supporting information for article:**

**Hydrogen-bond-reversal symmetry and its violation in ice  
nanotubes**

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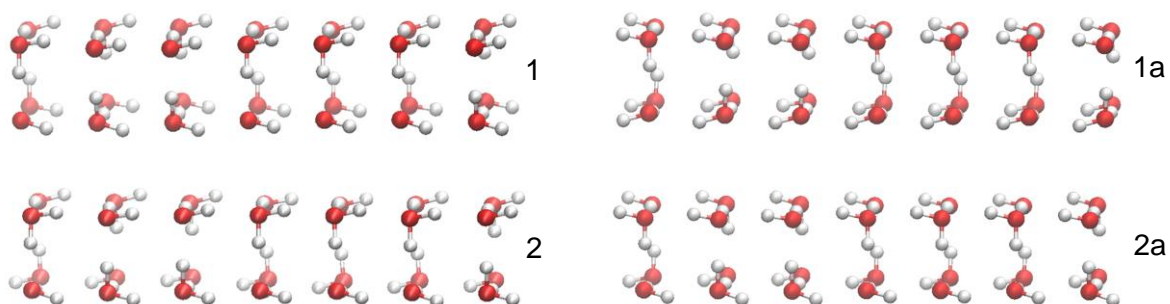
**Table S1** Potential energy of different proton configurations (Fig. 1s and Fig. 2s) and of their antipodes with opposite direction of all hydrogen bonds (U, Ua, kcal/mol), dipole moment magnitude (D, Debyes), potential energy difference ( $\Delta U=U-Ua$ ) for different unit cells of ice nanotubes. The data correspond to geometric optimization with the TIP3f potential. Calculations were performed with the Tinker molecular modeling package, version 6.2.

#	U	Ua	D*	$\Delta U$	$\Delta U, \%$
1 (Sqr_7)	-324,0818113	-324,0807791	51,101	0,00103214	0,000318
		-324,0807792**			
2 (Sqr_7)	-324,9154636	-324,9148134	25,484	0,00065022	0,000200
		-324,9148135**			
3 (Hep_1)	-435,1633162	-435,1394891	9,429	0,02382701	0,005475
4 (Hep_3)	-516,3028391	-516,3018827	10,955	0,00095646	0,000185
5 (Hep_4)	-687,3832866	-687,3875465	14,554	0,00425993	0,000620
6 (Oct_1)	-400,1513589	-400,1527342	14,655	0,00137527	0,000344
7 (Oct_1)	-400,1129961	-400,1205237	14,708	0,00752758	0,001881
8 (Oct_3)	-590.94038454	-590.93872279	19.705	0,00166175	0,000281
9 (Oct_3)	-590,7757918	-590,7855906	19.742	0,00979877	0,001659
10 (Oct_4)	-401,0135529	-401,0262741	14,409	0,01272124	0,003172
11 (Oct_4)	-400,8979889	-400,9059695	14,442	0,00798062	0,001991

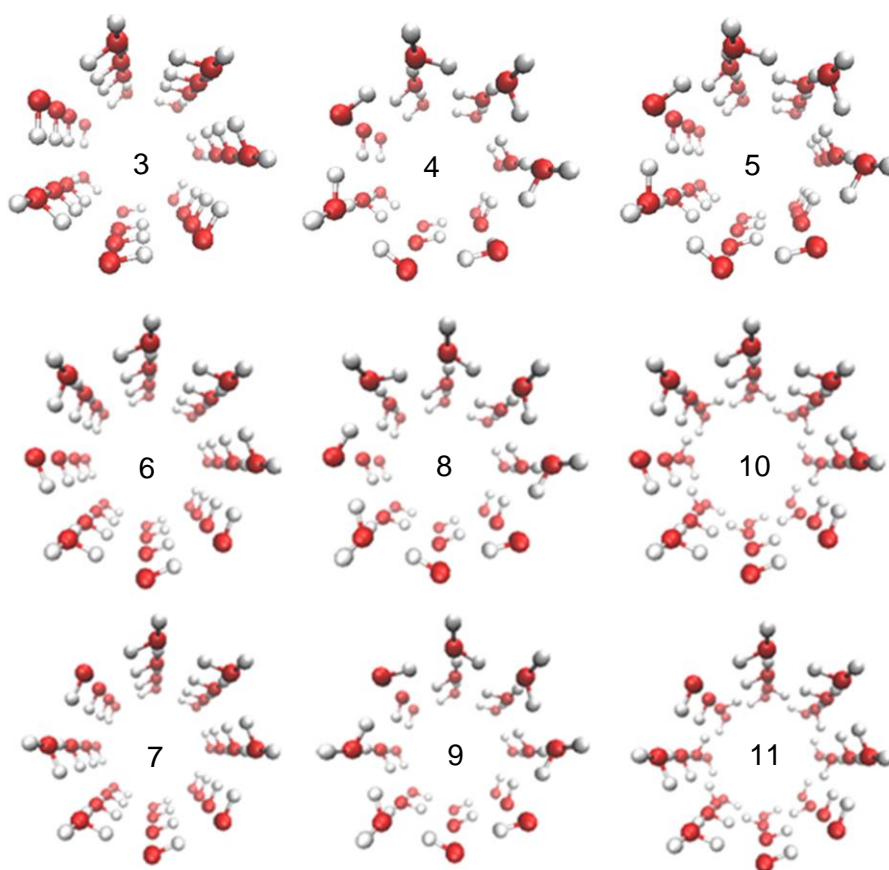
\*practically the same for both antipodes; \*\*potential energy of the indirect antipode with opposite direction of only longitudinal hydrogen bonds (the direct and indirect antipodal configurations are related by the usual spatial symmetry).

**Table S2** Parameters of modeling: period, number of sections (rings) in modeling cell, length of longitudinal hydrogen bonds (distance between rings), length of modeling cell, cut-off of the interaction ( $\text{\AA}$ ).

#	Tube	Period	N_Sections	HB-length	Length	R_cut
1-2	Sqr	7	7	2.75	19.25	9.5
3	Hep	1	5	2.70	13.50	6.5
4	Hep	3	6	2.70	16.20	8.0
5	Hep	4	8	2.70	21.60	9.5
6-7	Oct	1	4	2.75	11.00	5.2
8-9	Oct	3	6	2.70	16.20	8.0
10-11	Oct	4	4	2.75	11.00	5.2



**Figure 1s** Nonequivalent pairs of antipodal configurations of square ice nanotube (1-1a, 2-2a). Configurations 1a and 2a are indirect antipodes (H-bond reversal and reflection in perpendicular plane in the middle of the tube).



**Figure 2s** Nonantisymmetrical configurations of heptagonal and octagonal ice nanotubes with a different size of the unit cell: 1 (left), 3 (middle) and 4 (right).

**Table S3** Initial coordinates of the proton configurations with opposite direction of all hydrogen bonds. Additionally, the coordinates of the indirect antipode are given for configurations 1 and 2 (Fig. 1s).

		Configuration # 1			Antipode			Indirect antipode ( # 1a)		
		x	y	z	x	y	z	x	y	z
1	O	3,876	1,862	-8,299	3,885	1,87	-8,185	3,859	1,897	-8,206
2	H	4,18	1,888	-7,369	4,174	1,843	-9,118	4,183	1,911	-9,106
3	H	3,334	2,677	-8,302	3,291	1,092	-8,182	3,273	2,652	-8,15
4	O	2,011	3,882	-8,303	2,013	3,883	-8,179	1,953	3,86	-8,205
5	H	1,976	4,207	-7,38	2,031	4,195	-9,105	1,941	4,185	-9,106
6	H	1,2	3,335	-8,296	2,797	3,294	-8,194	1,197	3,274	-8,152
7	O	-0,004	2,008	-8,294	-0,001	2,007	-8,184	-0,01	1,952	-8,207
8	H	-0,328	1,963	-7,37	-0,318	2,021	-9,11	-0,336	1,939	-9,107
9	H	0,535	1,19	-8,3	0,57	2,801	-8,2	0,576	1,198	-8,152
10	O	1,867	0	-8,291	1,875	-0,003	-8,185	1,898	-0,009	-8,208
11	H	1,906	-0,309	-7,364	1,856	-0,303	-9,116	1,912	-0,332	-9,109
12	H	2,682	0,542	-8,303	1,086	0,576	-8,19	2,652	0,577	-8,151
13	O	3,889	2,02	-5,551	3,892	2,068	-5,432	3,861	1,961	-5,455
14	H	4,18	2,051	-4,617	4,203	2,081	-6,36	4,194	1,949	-6,352
15	H	3,358	1,199	-5,533	3,282	2,833	-5,454	3,281	1,201	-5,404
16	O	1,857	3,884	-5,554	1,824	3,89	-5,433	1,89	3,859	-5,456
17	H	1,817	4,161	-4,617	1,822	4,177	-6,37	1,902	4,191	-6,353
18	H	2,68	3,356	-5,539	1,052	3,289	-5,449	2,65	3,279	-5,404
19	O	0,002	1,862	-5,553	-0,002	1,833	-5,435	-0,008	1,891	-5,458
20	H	-0,29	1,833	-4,62	-0,297	1,826	-6,368	-0,34	1,904	-6,356
21	H	0,532	2,684	-5,539	0,604	1,064	-5,453	0,573	2,65	-5,406
22	O	2,018	-0,002	-5,545	2,057	-0,01	-5,432	1,959	-0,01	-5,458
23	H	2,041	-0,3	-4,613	2,058	-0,323	-6,359	1,947	-0,343	-6,355
24	H	1,192	0,523	-5,534	2,832	0,587	-5,462	1,2	0,571	-5,406
25	O	3,895	2,046	-2,798	3,877	1,832	-2,694	3,86	1,959	-2,704
26	H	4,216	2,005	-1,874	4,179	1,85	-3,624	4,167	1,982	-3,611
27	H	3,365	1,224	-2,801	3,365	2,667	-2,685	3,281	1,198	-2,666
28	O	1,844	3,882	-2,806	2,045	3,881	-2,694	1,889	3,859	-2,705
29	H	1,87	4,186	-1,877	2,039	4,157	-3,633	1,867	4,165	-3,612
30	H	2,67	3,357	-2,811	1,204	3,379	-2,681	2,65	3,28	-2,665
31	O	0,009	1,855	-2,803	-0,004	2,045	-2,689	-0,01	1,889	-2,708
32	H	-0,307	1,896	-1,877	-0,294	2,047	-3,624	-0,315	1,869	-3,615
33	H	0,543	2,677	-2,812	0,51	1,211	-2,689	0,569	2,65	-2,666
34	O	2,035	0,001	-2,791	1,831	-0,004	-2,692	1,959	-0,011	-2,707
35	H	1,981	-0,328	-1,869	1,83	-0,309	-3,621	1,98	-0,317	-3,614
36	H	1,211	0,531	-2,804	2,672	0,497	-2,699	1,198	0,568	-2,667
37	O	3,872	1,86	-0,049	3,87	1,834	0,059	3,859	1,89	0,049
38	H	4,152	1,828	0,888	3,261	1,067	0,059	3,278	2,648	0,101
39	H	3,33	2,673	-0,034	4,181	1,779	-0,867	4,188	1,9	-0,85
40	O	1,997	3,87	-0,053	2,029	3,868	0,062	1,96	3,859	0,049

41	H	2,03	4,151	0,884	2,792	3,254	0,059	1,201	3,279	0,101
42	H	1,178	3,335	-0,037	2,093	4,194	-0,858	1,95	4,189	-0,849
43	O	-0,013	2,001	-0,053	-0,017	2,031	0,056	-0,01	1,96	0,049
44	H	-0,3	2,031	0,882	0,592	2,797	0,054	0,572	1,201	0,1
45	H	0,517	1,18	-0,039	-0,324	2,081	-0,871	-0,341	1,949	-0,849
46	O	1,858	-0,013	-0,049	1,829	-0,018	0,054	1,89	-0,009	0,048
47	H	1,827	-0,299	0,886	1,06	0,586	0,056	2,649	0,572	0,1
48	H	2,677	0,521	-0,034	1,783	-0,317	-0,877	1,901	-0,339	-0,85
49	O	3,865	1,84	2,696	3,866	2,01	2,803	3,86	1,882	2,801
50	H	4,156	1,811	3,63	4,17	2,007	1,872	4,17	1,858	1,896
51	H	3,344	2,668	2,711	3,345	1,181	2,798	3,287	2,648	2,838
52	O	2,017	3,867	2,697	1,851	3,867	2,795	1,968	3,86	2,801
53	H	2,043	4,163	3,629	1,856	4,177	1,867	1,992	4,17	1,896
54	H	1,193	3,341	2,712	2,682	3,35	2,788	1,202	3,288	2,838
55	O	-0,009	2,017	2,702	-0,009	1,851	2,795	-0,01	1,968	2,8
56	H	-0,3	2,043	3,636	-0,319	1,848	1,868	-0,321	1,991	1,895
57	H	0,511	1,188	2,714	0,506	2,683	2,783	0,562	1,202	2,838
58	O	1,841	-0,008	2,698	2,009	-0,007	2,804	1,883	-0,01	2,8
59	H	1,814	-0,299	3,632	2,013	-0,312	1,874	1,859	-0,32	1,895
60	H	2,669	0,514	2,711	1,181	0,513	2,794	2,649	0,563	2,838
61	O	3,866	1,846	5,453	3,876	2,047	5,554	3,86	1,89	5,552
62	H	4,177	1,88	6,381	4,146	2,073	4,615	4,162	1,865	4,644
63	H	3,336	2,668	5,446	3,375	1,206	5,554	3,28	2,651	5,592
64	O	2,018	3,874	5,455	1,817	3,871	5,547	1,96	3,86	5,552
65	H	1,975	4,194	6,379	1,796	4,149	4,608	1,985	4,163	4,644
66	H	1,201	3,335	5,449	2,659	3,374	5,549	1,199	3,281	5,59
67	O	-0,006	2,014	5,461	-0,005	1,816	5,547	-0,011	1,96	5,551
68	H	-0,326	1,97	6,385	-0,29	1,786	4,612	-0,313	1,984	4,643
69	H	0,527	1,193	5,451	0,491	2,659	5,537	0,569	1,199	5,59
70	O	1,85	-0,004	5,457	2,048	-0,007	5,554	1,89	-0,01	5,551
71	H	1,891	-0,315	6,385	2,081	-0,283	4,617	1,866	-0,311	4,642
72	H	2,67	0,53	5,446	1,208	0,494	5,545	2,651	0,57	5,591
73	O	3,88	2,007	8,203	3,876	2,003	8,309	3,86	1,953	8,302
74	H	4,193	1,973	9,13	4,182	2,058	7,381	4,185	1,94	7,402
75	H	3,336	1,194	8,201	3,288	2,786	8,317	3,273	1,198	8,356
76	O	1,86	3,874	8,207	1,869	3,876	8,305	1,898	3,859	8,301
77	H	1,887	4,172	9,139	1,806	4,174	7,376	1,911	4,182	7,4
78	H	2,679	3,339	8,198	1,098	3,273	8,316	2,652	3,272	8,356
79	O	-0,001	1,865	8,211	-0,005	1,871	8,304	-0,009	1,898	8,3
80	H	-0,31	1,905	9,139	-0,303	1,824	7,374	-0,331	1,912	7,398
81	H	0,541	2,681	8,199	0,585	1,09	8,31	0,578	2,652	8,356
82	O	2,005	-0,005	8,21	1,996	0	8,31	1,952	-0,01	8,3
83	H	1,961	-0,327	9,134	2,046	-0,314	7,385	1,939	-0,334	7,4
84	H	1,189	0,536	8,203	2,782	0,584	8,313	1,198	0,577	8,355

Configuration # 2

Antipode

Indirect antipode

(# 1a)

1	O	3,906	1,965	-8,271	3,869	1,979	-8,208	3,860	1,902	-8,218
2	H	4,189	2,011	-7,334	4,220	1,965	-9,121	4,178	1,908	-9,120
3	H	3,330	2,756	-8,292	3,306	1,180	-8,268	3,269	2,653	-8,166
4	O	1,933	3,868	-8,293	1,882	3,877	-8,204	1,950	3,859	-8,205
5	H	1,870	4,169	-7,363	1,937	4,179	-9,133	1,955	4,181	-9,106
6	H	1,140	3,291	-8,316	2,688	3,322	-8,182	1,197	3,268	-8,166
7	O	0,023	1,933	-8,289	-0,004	1,900	-8,195	-0,006	1,945	-8,212
8	H	-0,332	1,908	-7,376	-0,303	1,933	-9,127	-0,354	1,967	-9,103
9	H	0,596	1,141	-8,240	0,554	2,704	-8,190	0,594	1,199	-8,206
10	O	1,965	-0,011	-8,213	1,964	-0,011	-8,300	1,911	-0,006	-8,284
11	H	1,951	-0,337	-9,135	1,974	-0,351	-7,384	1,870	-0,351	-7,392
12	H	2,758	0,558	-8,265	1,172	0,560	-8,226	2,656	0,595	-8,275
13	O	3,857	2,011	-5,511	3,872	1,887	-5,434	3,858	1,957	-5,462
14	H	4,169	2,054	-4,584	4,177	1,912	-6,363	4,205	1,975	-6,354
15	H	3,323	1,193	-5,450	3,327	2,700	-5,437	3,270	1,202	-5,447
16	O	1,849	3,885	-5,546	2,004	3,891	-5,446	1,891	3,857	-5,455
17	H	1,837	4,168	-4,609	1,947	4,208	-6,370	1,887	4,185	-6,354
18	H	2,668	3,350	-5,535	1,203	3,328	-5,433	2,648	3,273	-5,416
19	O	-0,047	1,885	-5,549	0,013	1,974	-5,462	-0,008	1,892	-5,464
20	H	-0,309	1,861	-4,606	-0,338	1,968	-6,376	-0,337	1,895	-6,363
21	H	0,483	2,708	-5,546	0,570	1,172	-5,530	0,575	2,650	-5,420
22	O	1,951	0,004	-5,462	1,893	-0,009	-5,553	1,947	-0,010	-5,538
23	H	1,968	-0,335	-6,380	1,819	-0,318	-4,627	2,019	-0,331	-4,639
24	H	1,149	0,562	-5,535	2,697	0,541	-5,458	1,197	0,585	-5,520
25	O	3,879	1,943	-2,774	3,886	1,880	-2,685	3,858	1,954	-2,709
26	H	4,215	1,934	-1,855	4,165	1,842	-3,622	4,181	2,006	-3,609
27	H	3,284	1,166	-2,712	3,345	2,695	-2,709	3,263	1,204	-2,711
28	O	1,962	3,877	-2,802	2,009	3,886	-2,692	1,892	3,859	-2,705
29	H	1,990	4,193	-1,876	2,026	4,177	-3,624	1,856	4,162	-3,612
30	H	2,745	3,289	-2,780	1,192	3,346	-2,701	2,651	3,276	-2,677
31	O	-0,007	1,950	-2,806	0,006	1,995	-2,716	-0,012	1,894	-2,717
32	H	-0,324	1,973	-1,882	-0,310	2,046	-3,642	-0,312	1,864	-3,625
33	H	0,556	2,750	-2,795	0,549	1,185	-2,792	0,572	2,652	-2,682
34	O	1,986	0,003	-2,718	1,901	0,005	-2,808	1,957	-0,007	-2,789
35	H	2,047	-0,311	-3,644	1,882	-0,332	-1,890	1,993	-0,350	-1,896
36	H	1,169	0,535	-2,793	2,705	0,559	-2,728	1,200	0,580	-2,789
37	O	3,905	1,884	-0,057	3,860	1,975	0,045	3,859	1,890	0,043
38	H	4,160	1,837	0,888	3,301	1,173	-0,019	3,275	2,648	0,088
39	H	3,369	2,702	-0,039	4,205	1,968	-0,871	4,189	1,894	-0,856
40	O	2,008	3,873	-0,053	1,858	3,864	0,055	1,960	3,858	0,049
41	H	2,033	4,148	0,885	2,669	3,317	0,065	1,203	3,273	0,089
42	H	1,190	3,336	-0,041	1,906	4,178	-0,871	1,963	4,185	-0,850
43	O	0,004	1,991	-0,014	-0,019	1,870	0,069	-0,007	1,956	0,043
44	H	-0,316	2,042	0,908	0,533	2,679	0,070	0,581	1,201	0,057
45	H	0,543	1,177	0,053	-0,326	1,905	-0,858	-0,352	1,975	-0,850
46	O	1,921	-0,007	0,043	1,979	-0,016	-0,053	1,903	-0,010	-0,033

47	H	2,721	0,555	-0,018	2,050	-0,326	0,872	1,827	-0,329	0,866
48	H	1,927	-0,349	-0,874	1,173	0,531	0,038	2,651	0,587	-0,013
49	O	3,883	1,864	2,669	3,865	2,007	2,789	3,860	1,883	2,795
50	H	4,178	1,823	3,601	4,179	2,055	1,864	4,169	1,848	1,889
51	H	3,358	2,688	2,708	3,329	1,191	2,718	3,285	2,648	2,823
52	O	2,003	3,868	2,694	1,847	3,869	2,813	1,967	3,859	2,801
53	H	2,041	4,163	3,627	1,819	4,158	1,880	2,004	4,167	1,895
54	H	1,183	3,336	2,736	2,670	3,341	2,796	1,203	3,284	2,828
55	O	-0,008	2,009	2,761	-0,007	1,852	2,835	-0,009	1,966	2,795
56	H	-0,324	2,053	3,687	-0,299	1,814	1,903	-0,328	2,013	1,894
57	H	0,538	1,200	2,831	0,516	2,678	2,806	0,574	1,207	2,803
58	O	1,862	-0,020	2,785	2,002	-0,007	2,695	1,885	-0,008	2,717
59	H	1,794	-0,337	1,861	2,067	-0,319	3,620	1,818	-0,327	3,617
60	H	2,674	0,517	2,691	1,184	0,524	2,784	2,646	0,571	2,723
61	O	3,873	1,947	5,423	3,871	1,994	5,542	3,862	1,895	5,541
62	H	4,185	1,955	6,349	4,187	2,044	4,617	4,159	1,860	4,632
63	H	3,309	2,747	5,445	3,322	1,188	5,469	3,278	2,653	5,574
64	O	1,908	3,864	5,438	1,865	3,872	5,560	1,957	3,860	5,551
65	H	1,888	4,187	6,360	1,837	4,155	4,625	1,997	4,160	4,643
66	H	1,121	3,280	5,465	2,683	3,334	5,544	1,198	3,277	5,578
67	O	-0,005	1,934	5,489	-0,013	1,871	5,575	-0,008	1,955	5,546
68	H	-0,356	1,925	6,403	-0,290	1,833	4,637	-0,328	2,009	4,646
69	H	0,581	1,152	5,552	0,526	2,686	5,552	0,586	1,205	5,545
70	O	1,898	-0,023	5,531	1,977	-0,010	5,450	1,893	-0,005	5,469
71	H	1,823	-0,325	4,602	1,986	-0,346	6,367	1,856	-0,346	6,363
72	H	2,711	0,514	5,452	1,175	0,548	5,523	2,649	0,581	5,467
73	O	3,862	1,923	8,205	3,882	1,891	8,304	3,856	1,945	8,296
74	H	4,218	1,908	9,115	4,178	1,928	7,373	4,203	1,969	7,404
75	H	3,272	1,142	8,262	3,317	2,690	8,313	3,258	1,198	8,300
76	O	1,947	3,877	8,193	1,991	3,880	8,303	1,901	3,857	8,301
77	H	1,997	4,188	9,119	1,939	4,187	7,375	1,897	4,180	7,400
78	H	2,724	3,281	8,190	1,184	3,325	8,319	2,653	3,265	8,341
79	O	-0,036	1,965	8,218	-0,001	1,968	8,300	-0,010	1,903	8,290
80	H	-0,312	1,981	9,158	-0,345	1,959	7,383	-0,331	1,912	7,388
81	H	0,540	2,756	8,214	0,566	1,173	8,235	0,582	2,653	8,341
82	O	1,916	0,002	8,279	1,907	-0,004	8,208	1,939	-0,007	8,221
83	H	1,902	-0,340	7,361	1,894	-0,338	9,128	1,984	-0,350	9,113
84	H	1,111	0,555	8,238	2,703	0,560	8,281	1,195	0,595	8,233

## Configuration # 3

## Antipode

1	O	6,2941	3,0185	-5,5934	6,2724	3,1862	-5,4891
2	H	6,5652	2,9346	-4,6541	6,5243	3,255	-6,4348
3	H	5,9004	3,9156	-5,5256	5,889	2,283	-5,5232
4	O	5,1619	5,4642	-5,2113	4,9591	5,5554	-5,5122
5	H	5,3431	5,6	-4,2565	5,0493	5,7566	-6,4684
6	H	4,2225	5,7489	-5,218	5,463	4,7134	-5,4944

7	O	2,5479	6,1706	-5,1791	2,3328	6,1433	-5,0631
8	H	2,5588	6,4349	-4,2342	2,1837	6,3939	-6,0002
9	H	1,7608	5,5852	-5,1383	3,2906	5,9446	-5,1482
10	O	0,3865	4,5288	-5,1166	0,2622	4,3792	-5,2197
11	H	0,1847	4,7183	-6,0582	-0,0105	4,4187	-4,2777
12	H	0,3402	3,5503	-5,1793	1,0054	5,0172	-5,1559
13	O	0,2712	1,8133	-5,2841	0,3428	1,6618	-5,0783
14	H	-0,0031	1,7735	-4,3426	0,1356	1,4737	-6,0187
15	H	1,009	1,169	-5,2221	0,3089	2,6408	-5,1389
16	O	2,3262	0,0311	-5,1421	2,5559	0,0862	-5,1293
17	H	2,1736	-0,2247	-6,077	2,5814	-0,1587	-4,1793
18	H	3,2792	0,2474	-5,2344	1,745	0,6387	-5,0978
19	O	4,9507	0,6582	-5,5957	5,1852	0,6992	-5,514
20	H	5,0292	0,4342	-6,5478	5,421	0,5396	-4,575
21	H	5,4557	1,4998	-5,6168	4,2356	0,4608	-5,4417
22	O	6,2941	3,0185	-2,8934	6,2724	3,1862	-2,7891
23	H	6,5652	2,9346	-1,9541	6,5243	3,255	-3,7348
24	H	5,9004	3,9156	-2,8256	5,889	2,283	-2,8232
25	O	5,1619	5,4642	-2,5113	4,9591	5,5554	-2,8122
26	H	5,3431	5,6	-1,5565	5,0493	5,7566	-3,7684
27	H	4,2225	5,7489	-2,518	5,463	4,7134	-2,7944
28	O	2,5479	6,1706	-2,4791	2,3328	6,1433	-2,3631
29	H	2,5588	6,4349	-1,5342	2,1837	6,3939	-3,3002
30	H	1,7608	5,5852	-2,4383	3,2906	5,9446	-2,4482
31	O	0,3865	4,5288	-2,4166	0,2622	4,3792	-2,5197
32	H	0,1847	4,7183	-3,3582	-0,0105	4,4187	-1,5777
33	H	0,3402	3,5503	-2,4793	1,0054	5,0172	-2,4559
34	O	0,2712	1,8133	-2,5841	0,3428	1,6618	-2,3783
35	H	-0,0031	1,7735	-1,6426	0,1356	1,4737	-3,3187
36	H	1,009	1,169	-2,5221	0,3089	2,6408	-2,4389
37	O	2,3262	0,0311	-2,4421	2,5559	0,0862	-2,4293
38	H	2,1736	-0,2247	-3,377	2,5814	-0,1587	-1,4793
39	H	3,2792	0,2474	-2,5344	1,745	0,6387	-2,3978
40	O	4,9507	0,6582	-2,8957	5,1852	0,6992	-2,814
41	H	5,0292	0,4342	-3,8478	5,421	0,5396	-1,875
42	H	5,4557	1,4998	-2,9168	4,2356	0,4608	-2,7417
43	O	6,2941	3,0185	-0,1934	6,2724	3,1862	-0,0891
44	H	6,5652	2,9346	0,7459	5,8891	2,283	-0,1232
45	H	5,9004	3,9156	-0,1256	6,5244	3,2549	-1,0348
46	O	5,1619	5,4642	0,1887	4,9591	5,5554	-0,1122
47	H	5,3431	5,6	1,1435	5,463	4,7134	-0,0944
48	H	4,2225	5,7489	0,182	5,0493	5,7566	-1,0684
49	O	2,5479	6,1706	0,2209	2,3328	6,1433	0,3369
50	H	2,5588	6,4349	1,1658	3,2906	5,9446	0,2518
51	H	1,7608	5,5852	0,2617	2,1837	6,394	-0,6002
52	O	0,3866	4,5288	0,2833	0,2622	4,3792	0,1803



53	H	0,3403	3,5503	0,2207	-0,0105	4,4187	1,1223
54	H	0,1847	4,7183	-0,6582	1,0054	5,0172	0,244
55	O	0,2712	1,8133	0,1159	0,3428	1,6618	0,3217
56	H	-0,0031	1,7735	1,0574	0,3089	2,6408	0,2611
57	H	1,009	1,169	0,1779	0,1356	1,4737	-0,6187
58	O	2,3262	0,0312	0,2579	2,5559	0,0861	0,2707
59	H	3,2792	0,2474	0,1657	2,5814	-0,1587	1,2207
60	H	2,1736	-0,2247	-0,677	1,745	0,6387	0,3022
61	O	4,9507	0,6582	-0,1957	5,1852	0,6992	-0,114
62	H	5,4557	1,4998	-0,2168	5,421	0,5396	0,825
63	H	5,0292	0,4342	-1,1478	4,2356	0,4607	-0,0417
64	O	6,2941	3,0185	2,5066	6,2724	3,1862	2,6109
65	H	6,5652	2,9346	3,4459	6,5244	3,2549	1,6652
66	H	5,9004	3,9156	2,5744	5,8891	2,283	2,5768
67	O	5,1619	5,4642	2,8887	4,9591	5,5554	2,5878
68	H	5,3432	5,6	3,8435	5,0493	5,7566	1,6316
69	H	4,2225	5,7489	2,882	5,463	4,7134	2,6056
70	O	2,5479	6,1706	2,9209	2,3328	6,1433	3,0369
71	H	2,5588	6,4349	3,8658	2,1837	6,3939	2,0998
72	H	1,7608	5,5852	2,9617	3,2906	5,9446	2,9518
73	O	0,3866	4,5288	2,9833	0,2622	4,3792	2,8803
74	H	0,1847	4,7183	2,0418	-0,0105	4,4187	3,8223
75	H	0,3403	3,5503	2,9207	1,0054	5,0171	2,9441
76	O	0,2712	1,8133	2,8159	0,3428	1,6618	3,0217
77	H	-0,0031	1,7735	3,7574	0,1356	1,4737	2,0812
78	H	1,009	1,169	2,8779	0,3089	2,6408	2,9611
79	O	2,3262	0,0311	2,9579	2,5559	0,0861	2,9707
80	H	2,1736	-0,2247	2,023	2,5814	-0,1587	3,9207
81	H	3,2792	0,2474	2,8657	1,7451	0,6386	3,0022
82	O	4,9507	0,6582	2,5043	5,1852	0,6992	2,586
83	H	5,0292	0,4342	1,5522	5,421	0,5396	3,525
84	H	5,4557	1,4998	2,4832	4,2356	0,4607	2,6583
85	O	6,2941	3,0185	5,2066	6,2724	3,1862	5,3109
86	H	6,5651	2,9346	6,1459	6,5244	3,2549	4,3652
87	H	5,9004	3,9156	5,2744	5,8891	2,283	5,2768
88	O	5,1619	5,4642	5,5887	4,9591	5,5554	5,2878
89	H	5,3431	5,6	6,5435	5,0493	5,7566	4,3316
90	H	4,2225	5,7489	5,582	5,463	4,7134	5,3056
91	O	2,5479	6,1706	5,6209	2,3328	6,1433	5,7369
92	H	2,5588	6,4349	6,5658	2,1837	6,3939	4,7998
93	H	1,7608	5,5852	5,6617	3,2906	5,9446	5,6518
94	O	0,3866	4,5288	5,6833	0,2622	4,3792	5,5804
95	H	0,1847	4,7183	4,7418	-0,0105	4,4187	6,5223
96	H	0,3403	3,5503	5,6207	1,0054	5,0172	5,644
97	O	0,2712	1,8133	5,5159	0,3428	1,6618	5,7217
98	H	-0,0031	1,7735	6,4574	0,1356	1,4737	4,7813

99	H	1,009	1,169	5,5779	0,3089	2,6408	5,6611
100	O	2,3262	0,0311	5,6579	2,5559	0,0861	5,6707
101	H	2,1735	-0,2247	4,723	2,5814	-0,1587	6,6207
102	H	3,2792	0,2474	5,5657	1,745	0,6387	5,7022
103	O	4,9506	0,6582	5,2043	5,1852	0,6992	5,286
104	H	5,0292	0,4342	4,2522	5,421	0,5396	6,225
105	H	5,4557	1,4998	5,1832	4,2356	0,4607	5,3583

		Configuration # 8			Antipode		
1	O	6,6270	3,2402	-0,0314	6,6158	3,3018	0,0344
2	H	6,9145	3,1878	0,8618	6,1841	2,4677	0,0684
3	H	6,1931	4,0717	-0,0909	6,9362	3,3656	-0,8468
4	O	5,6608	5,6222	-0,0369	5,6130	5,6652	0,0411
5	H	5,9015	5,7735	0,8589	5,8923	4,7703	0,1077
6	H	4,7681	5,9107	-0,0929	5,7923	5,9023	-0,8505
7	O	3,2963	6,6188	-0,0376	3,2297	6,6268	0,0426
8	H	3,3595	6,8934	0,8590	4,0637	6,1989	0,1109
9	H	2,4633	6,1873	-0,0937	3,1879	6,9206	-0,8491
10	O	0,9170	5,6602	-0,0330	0,8597	5,6264	0,0374
11	H	0,7671	5,9378	0,8522	1,7541	5,9051	0,1131
12	H	0,6469	4,7601	-0,0466	0,6251	5,8259	-0,8505
13	O	-0,0835	3,2998	0,0062	-0,0952	3,2415	-0,0026
14	H	0,3614	2,4730	0,0490	-0,4030	3,1467	0,8802
15	H	-0,4061	3,3484	-0,8752	0,3453	4,0716	-0,0107
16	O	0,8698	0,9093	-0,0002	0,9133	0,8668	0,0053
17	H	0,5899	0,7481	0,8823	0,6450	1,7666	0,0460
18	H	1,7701	0,6398	-0,0148	0,7084	0,5993	-0,8720
19	O	3,2338	-0,0933	0,0308	3,2954	-0,0819	-0,0347
20	H	4,0602	0,3485	0,1020	3,3950	-0,3894	0,8478
21	H	3,1973	-0,3823	-0,8627	2,4653	0,3588	-0,0384
22	O	5,6211	0,8637	0,0327	5,6603	0,9138	-0,0114
23	H	5,9021	1,7604	0,0481	5,8997	0,7506	0,8826
24	H	5,7918	0,5784	-0,8463	4,7620	0,6433	-0,0679
25	O	6,6305	3,2317	2,6631	6,6184	3,2980	2,7311
26	H	6,9436	3,2106	3,5489	6,9243	3,3921	1,8475
27	H	6,1955	4,0612	2,5867	6,1801	2,4667	2,7414
28	O	5,6684	5,6147	2,6581	5,6203	5,6609	2,7366
29	H	5,9058	5,7922	3,5499	5,7706	5,9024	1,8409
30	H	4,7761	5,9018	2,5901	5,9015	4,7657	2,7897
31	O	3,3041	6,6161	2,6567	3,2413	6,6237	2,7381
32	H	3,3478	6,9093	3,5485	3,1754	6,9035	1,8433
33	H	2,4718	6,1847	2,5910	4,0771	6,1973	2,7907
34	O	0,9214	5,6623	2,6638	0,8713	5,6274	2,7290
35	H	0,7410	5,9329	3,5456	0,6299	5,7920	1,8357
36	H	0,6448	4,7647	2,6316	1,7662	5,9084	2,7869
37	O	-0,0860	3,2947	2,7008	-0,0923	3,2352	2,6896

38	H	-0,3954	3,3765	1,8172	-0,4238	3,1772	3,5671
39	H	0,3645	2,4700	2,7173	0,3475	4,0651	2,6582
40	O	0,8688	0,9137	2,6926	0,9089	0,8683	2,6995
41	H	0,5990	0,7134	3,5703	0,7466	0,5958	1,8148
42	H	1,7671	0,6403	2,6541	0,6466	1,7705	2,7200
43	O	3,2414	-0,0898	2,7204	3,3021	-0,0810	2,6640
44	H	3,1813	-0,3712	1,8257	3,3734	-0,4046	3,5434
45	H	4,0710	0,3485	2,7743	2,4690	0,3532	2,6395
46	O	5,6287	0,8692	2,7279	5,6644	0,9195	2,6791
47	H	5,7688	0,5797	1,8448	5,8970	0,7272	3,5691
48	H	5,9053	1,7674	2,7280	4,7673	0,6490	2,6063
49	O	6,6133	3,2836	5,3666	6,6265	3,2509	5,4347
50	H	6,9454	3,3601	6,2425	6,9444	3,2333	4,5506
51	H	6,1670	2,4566	5,3553	6,1796	4,0744	5,5081
52	O	5,6251	5,6515	5,3620	5,6535	5,6271	5,4405
53	H	5,8036	5,8905	6,2533	5,8923	5,8059	4,5493
54	H	5,8927	4,7527	5,3010	4,7579	5,9046	5,5047
55	O	3,2497	6,6227	5,3577	3,2863	6,6153	5,4390
56	H	3,2049	6,9214	6,2476	3,3292	6,9073	4,5468
57	H	4,0792	6,1851	5,2974	2,4599	6,1723	5,5025
58	O	0,8772	5,6381	5,3664	0,9107	5,6443	5,4353
59	H	0,6400	5,8441	6,2522	0,7304	5,9278	4,5577
60	H	1,7761	5,9030	5,2955	0,6513	4,7411	5,4492
61	O	-0,0939	3,2595	5,4118	-0,0794	3,2745	5,3986
62	H	-0,4458	3,1881	4,5433	-0,4205	3,3272	6,2727
63	H	0,3623	4,0811	5,4145	0,3847	2,4577	5,3756
64	O	0,8969	0,8857	5,3950	0,8881	0,8967	5,4040
65	H	0,6835	0,6035	6,2657	0,6009	0,6891	4,5335
66	H	0,6501	1,7923	5,3740	1,7926	0,6424	5,4206
67	O	3,2769	-0,0744	5,4399	3,2580	-0,0902	5,3763
68	H	3,3619	-0,4162	4,5685	3,2266	-0,3852	6,2680
69	H	2,4517	0,3752	5,4371	4,0769	0,3658	5,3076
70	O	5,6463	0,9078	5,4132	5,6379	0,8791	5,3658
71	H	5,8784	0,7053	4,5253	5,8084	0,5713	6,2372
72	H	4,7442	0,6543	5,4846	5,9021	1,7809	5,3785
73	O	6,6270	3,2402	7,9214	6,6158	3,3018	7,9872
74	H	6,9145	3,1878	8,8146	6,1841	2,4677	8,0211
75	H	6,1931	4,0717	7,8619	6,9362	3,3656	7,1060
76	O	5,6608	5,6222	7,9158	5,6130	5,6652	7,9938
77	H	5,9015	5,7735	8,8116	5,8923	4,7703	8,0604
78	H	4,7681	5,9107	7,8598	5,7923	5,9023	7,1023
79	O	3,2963	6,6188	7,9152	3,2297	6,6268	7,9954
80	H	3,3595	6,8934	8,8117	4,0637	6,1989	8,0636
81	H	2,4633	6,1873	7,8590	3,1879	6,9206	7,1037
82	O	0,9170	5,6602	7,9197	0,8597	5,6264	7,9902
83	H	0,7671	5,9378	8,8050	1,7541	5,9051	8,0659

84	H	0,6469	4,7601	7,9061	0,6251	5,8259	7,1023
85	O	-0,0835	3,2998	7,9589	-0,0952	3,2415	7,9501
86	H	0,3614	2,4730	8,0017	-0,4030	3,1467	8,8330
87	H	-0,4061	3,3484	7,0775	0,3453	4,0716	7,9420
88	O	0,8698	0,9093	7,9525	0,9133	0,8668	7,9580
89	H	0,5899	0,7481	8,8351	0,6450	1,7666	7,9987
90	H	1,7701	0,6398	7,9380	0,7084	0,5993	7,0807
91	O	3,2338	-0,0933	7,9835	3,2954	-0,0819	7,9181
92	H	4,0602	0,3485	8,0548	3,3950	-0,3894	8,8005
93	H	3,1973	-0,3823	7,0900	2,4653	0,3588	7,9144
94	O	5,6211	0,8637	7,9854	5,6603	0,9138	7,9413
95	H	5,9021	1,7604	8,0008	5,8997	0,7506	8,8353
96	H	5,7918	0,5784	7,1064	4,7620	0,6433	7,8849
97	O	6,6305	3,2317	10,6158	6,6184	3,2980	10,6838
98	H	6,9436	3,2106	11,5017	6,9243	3,3921	9,8002
99	H	6,1955	4,0612	10,5394	6,1801	2,4667	10,6942
100	O	5,6684	5,6147	10,6108	5,6203	5,6609	10,6893
101	H	5,9058	5,7922	11,5026	5,7706	5,9024	9,7936
102	H	4,7761	5,9018	10,5429	5,9015	4,7657	10,7424
103	O	3,3041	6,6161	10,6094	3,2413	6,6237	10,6908
104	H	3,3478	6,9093	11,5012	3,1754	6,9035	9,7960
105	H	2,4718	6,1847	10,5437	4,0771	6,1973	10,7434
106	O	0,9214	5,6623	10,6165	0,8713	5,6274	10,6817
107	H	0,7410	5,9329	11,4983	0,6299	5,7920	9,7885
108	H	0,6448	4,7647	10,5843	1,7662	5,9084	10,7396
109	O	-0,0860	3,2947	10,6535	-0,0923	3,2352	10,6423
110	H	-0,3954	3,3765	9,7699	-0,4238	3,1772	11,5198
111	H	0,3645	2,4700	10,6700	0,3475	4,0651	10,6109
112	O	0,8688	0,9137	10,6454	0,9089	0,8683	10,6522
113	H	0,5990	0,7134	11,5230	0,7466	0,5958	9,7675
114	H	1,7671	0,6403	10,6068	0,6466	1,7705	10,6728
115	O	3,2414	-0,0898	10,6731	3,3021	-0,0810	10,6167
116	H	3,1813	-0,3712	9,7785	3,3734	-0,4046	11,4962
117	H	4,0710	0,3485	10,7270	2,4690	0,3532	10,5922
118	O	5,6287	0,8692	10,6806	5,6644	0,9195	10,6319
119	H	5,7688	0,5797	9,7976	5,8970	0,7272	11,5219
120	H	5,9053	1,7674	10,6808	4,7673	0,6490	10,5591
121	O	6,6133	3,2836	13,3194	6,6265	3,2509	13,3875
122	H	6,9454	3,3601	14,1952	6,9444	3,2333	12,5033
123	H	6,1670	2,4566	13,3080	6,1796	4,0744	13,4608
124	O	5,6251	5,6515	13,3148	5,6535	5,6271	13,3932
125	H	5,8036	5,8905	14,2060	5,8923	5,8059	12,5020
126	H	5,8927	4,7527	13,2537	4,7579	5,9046	13,4574
127	O	3,2497	6,6227	13,3104	3,2863	6,6153	13,3917
128	H	3,2049	6,9214	14,2003	3,3292	6,9073	12,4995
129	H	4,0792	6,1851	13,2502	2,4599	6,1723	13,4552

130	O	0,8772	5,6381	13,3191	0,9107	5,6443	13,3881
131	H	0,6400	5,8441	14,2049	0,7304	5,9278	12,5104
132	H	1,7761	5,9030	13,2482	0,6513	4,7411	13,4019
133	O	-0,0939	3,2595	13,3646	-0,0794	3,2745	13,3513
134	H	-0,4458	3,1881	12,4961	-0,4205	3,3272	14,2255
135	H	0,3623	4,0811	13,3672	0,3847	2,4577	13,3283
136	O	0,8969	0,8857	13,3478	0,8881	0,8967	13,3567
137	H	0,6835	0,6035	14,2184	0,6009	0,6891	12,4862
138	H	0,6501	1,7923	13,3268	1,7926	0,6424	13,3734
139	O	3,2769	-0,0744	13,3926	3,2580	-0,0902	13,3290
140	H	3,3619	-0,4162	12,5213	3,2266	-0,3852	14,2207
141	H	2,4517	0,3752	13,3899	4,0769	0,3658	13,2604
142	O	5,6463	0,9078	13,3659	5,6379	0,8791	13,3185
143	H	5,8784	0,7053	12,4780	5,8084	0,5713	14,1899
144	H	4,7442	0,6543	13,4373	5,9021	1,7809	13,3312

		Configuration # 11			Antipode		
1	O	6,6847	3,3411	-5,5063	6,5906	3,3498	-5,6458
2	H	6,9437	3,3039	-4,5631	6,8539	3,3686	-6,5873
3	H	6,3627	4,2668	-5,5311	6,2763	2,4230	-5,5901
4	O	5,8317	5,9468	-5,448	5,7390	5,9495	-5,6014
5	H	6,024	6,0804	-4,497	5,9210	6,1162	-6,5475
6	H	4,9354	6,3443	-5,4728	6,0235	5,0113	-5,5597
7	O	3,3024	6,9874	-5,3834	3,2366	7,0227	-5,5492
8	H	3,3103	7,2042	-4,4282	3,2028	7,2257	-6,5073
9	H	2,4181	6,5676	-5,4378	4,1471	6,6567	-5,5121
10	O	0,8431	5,7818	-5,6561	0,7844	5,8053	-5,3122
11	H	0,7169	5,9543	-6,6004	0,6073	5,9300	-4,3574
12	H	0,4365	4,8913	-5,6045	1,6608	6,2423	-5,3578
13	O	-0,2851	3,2494	-5,4203	-0,2268	3,2186	-5,5609
14	H	-0,5154	3,2897	-4,4694	-0,4595	3,2025	-6,5100
15	H	0,0719	2,3372	-5,4432	0,1304	4,1287	-5,5032
16	O	0,7284	0,6873	-5,3588	0,7566	0,6558	-5,5209
17	H	0,5718	0,5642	-4,3999	0,6326	0,4940	-6,4822
18	H	1,6144	0,2709	-5,4217	0,3940	1,5667	-5,4827
19	O	3,2117	-0,43	-5,6461	3,2770	-0,3886	-5,2830
20	H	3,1951	-0,6559	-6,5928	3,3007	-0,6050	-4,3281
21	H	4,093	0,0028	-5,6132	2,3654	-0,0300	-5,3329
22	O	5,6477	0,786	-5,7214	5,7755	0,7191	-5,3923
23	H	5,8355	0,6043	-6,678	5,9858	0,5855	-4,4456
24	H	5,9908	1,7027	-5,6707	4,8821	0,3148	-5,3983
25	O	6,8057	3,1993	-2,7516	6,7615	3,4154	-2,9071
26	H	7,0959	3,1762	-1,8175	6,9113	3,4104	-3,8757
27	H	6,4173	2,3011	-2,8129	6,4094	4,3271	-2,8257
28	O	5,9346	5,7953	-2,6995	5,7848	5,9830	-2,8455
29	H	6,1412	5,939	-1,7528	5,9281	6,1613	-3,7978

30	H	6,2368	4,8652	-2,7739	4,8644	6,3152	-2,7737
31	O	3,4374	6,9097	-2,6415	3,2150	6,9100	-2,7969
32	H	3,4455	7,1033	-1,681	3,1749	7,1969	-3,7319
33	H	4,3311	6,511	-2,7124	2,3362	6,4795	-2,7337
34	O	0,9069	5,8486	-2,8967	0,7522	5,7137	-2,5659
35	H	0,7492	5,9979	-3,8514	0,5980	5,8734	-1,6125
36	H	1,8102	6,2234	-2,8284	0,3942	4,8032	-2,6300
37	O	-0,2949	3,389	-2,6639	-0,2669	3,1682	-2,8102
38	H	-0,5413	3,409	-1,7165	-0,4777	3,1613	-3,7669
39	H	0,1356	4,2677	-2,7271	0,1320	2,2745	-2,7437
40	O	0,7388	0,8499	-2,619	0,8455	0,6664	-2,7656
41	H	0,6028	0,7179	-1,6578	0,6715	0,4662	-3,7076
42	H	0,3756	1,7582	-2,6911	1,7621	0,3238	-2,7018
43	O	3,1972	-0,3541	-2,8769	3,4080	-0,2976	-2,5408
44	H	3,1611	-0,6278	-3,8156	3,4257	-0,4817	-1,5788
45	H	2,3198	0,0776	-2,8059	4,3016	0,0977	-2,6284
46	O	5,7326	0,6732	-2,9692	5,9101	0,8082	-2,6392
47	H	5,8544	0,5396	-3,9319	6,1329	0,6442	-1,7006
48	H	4,8277	0,3037	-2,8856	6,2081	1,7391	-2,7111
49	O	6,9485	3,2549	0,0097	6,9230	3,2855	-0,1615
50	H	7,1321	3,2164	0,9715	6,5962	2,3632	-0,0923
51	H	6,6115	4,1759	-0,0337	7,1070	3,3083	-1,1231
52	O	5,956	5,8053	0,0528	5,9139	5,8429	-0,0995
53	H	6,1307	5,9622	1,0039	6,2890	4,9376	-0,0721
54	H	5,0401	6,1549	0,0139	6,0580	6,0318	-1,0499
55	O	3,4082	6,8095	0,1014	3,3528	6,8404	-0,0381
56	H	3,4188	7,0603	1,0475	4,2625	6,4757	-0,0180
57	H	2,4983	6,4501	0,046	3,3197	7,0942	-0,9829
58	O	0,8398	5,8102	-0,1465	0,8168	5,7702	0,1841
59	H	0,4272	4,9214	-0,1027	0,6393	5,9091	1,1370
60	H	0,6959	5,9926	-1,0974	1,7163	6,1583	0,1377
61	O	-0,3135	3,343	0,0823	-0,3072	3,2913	-0,0714
62	H	-0,5381	3,3633	1,0358	0,0902	4,1867	-0,0196
63	H	0,0984	2,4524	0,0473	-0,5329	3,2787	-1,0245
64	O	0,8491	0,8755	0,1277	0,8078	0,7955	-0,0079
65	H	0,661	0,7075	1,0735	0,4087	1,6911	0,0125
66	H	1,7404	0,4714	0,0719	0,6504	0,5905	-0,9520
67	O	3,3419	-0,294	-0,124	3,3904	-0,1724	0,2067
68	H	4,25	0,0753	-0,1159	3,3988	-0,4329	1,1503
69	H	3,3003	-0,5476	-1,0687	2,4814	0,1906	0,1574
70	O	5,8815	0,7365	-0,2275	5,9652	0,7325	0,1182
71	H	6,2754	1,6331	-0,1788	6,1389	0,5886	1,0718
72	H	6,0166	0,5643	-1,1822	5,0401	0,4040	0,0924
73	O	6,8118	3,2995	2,7601	6,7610	3,3104	2,6103
74	H	6,9715	3,2521	3,7262	7,0564	3,3458	1,6786
75	H	6,4882	4,2249	2,7162	6,4435	2,3827	2,6380

76	O	5,8928	5,8754	2,8038	5,8325	5,8892	2,6492
77	H	6,0784	6,0255	3,754	5,9960	6,0685	1,7001
78	H	4,9856	6,2483	2,7758	6,1620	4,9657	2,6791
79	O	3,3585	6,8996	2,8516	3,3030	6,9128	2,7031
80	H	3,3717	7,1778	3,7896	3,2635	7,1048	1,7430
81	H	2,4607	6,5069	2,8207	4,2160	6,5542	2,7387
82	O	0,8502	5,7864	2,6075	0,8066	5,7770	2,9376
83	H	0,7275	5,9874	1,6572	0,6080	5,8993	3,8887
84	H	0,4379	4,8967	2,6314	1,6965	6,1883	2,9119
85	O	-0,2876	3,2922	2,8335	-0,2765	3,2564	2,6893
86	H	-0,5018	3,3309	3,7889	-0,5270	3,2292	1,7436
87	H	0,0941	2,3889	2,8063	0,1027	4,1600	2,7222
88	O	0,7984	0,7782	2,8786	0,7899	0,7352	2,7321
89	H	0,5761	0,611	3,8167	0,6842	0,5657	1,7725
90	H	1,687	0,364	2,8509	0,3995	1,6347	2,7639
91	O	3,2851	-0,3658	2,6143	3,3352	-0,2847	2,9549
92	H	3,2456	-0,5634	1,655	3,3600	-0,5688	3,8910
93	H	4,1844	0,0264	2,6385	2,4250	0,0797	2,9320
94	O	5,7758	0,7565	2,5326	5,8734	0,7199	2,8703
95	H	5,9532	0,549	1,5927	6,0443	0,6097	3,8293
96	H	6,1431	1,6654	2,5578	4,9649	0,3492	2,8482