

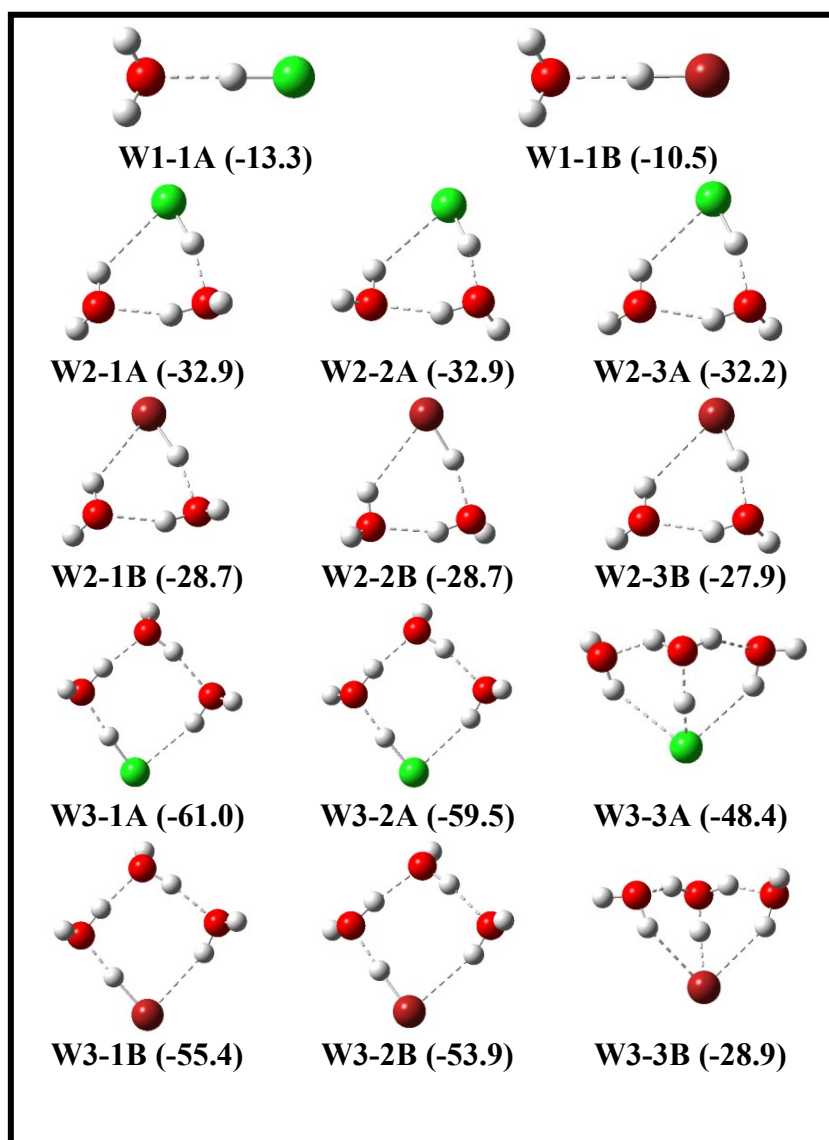
Electronic Supplementary Information for

## Insights into Acid Dissociation with Internal Electric Fields

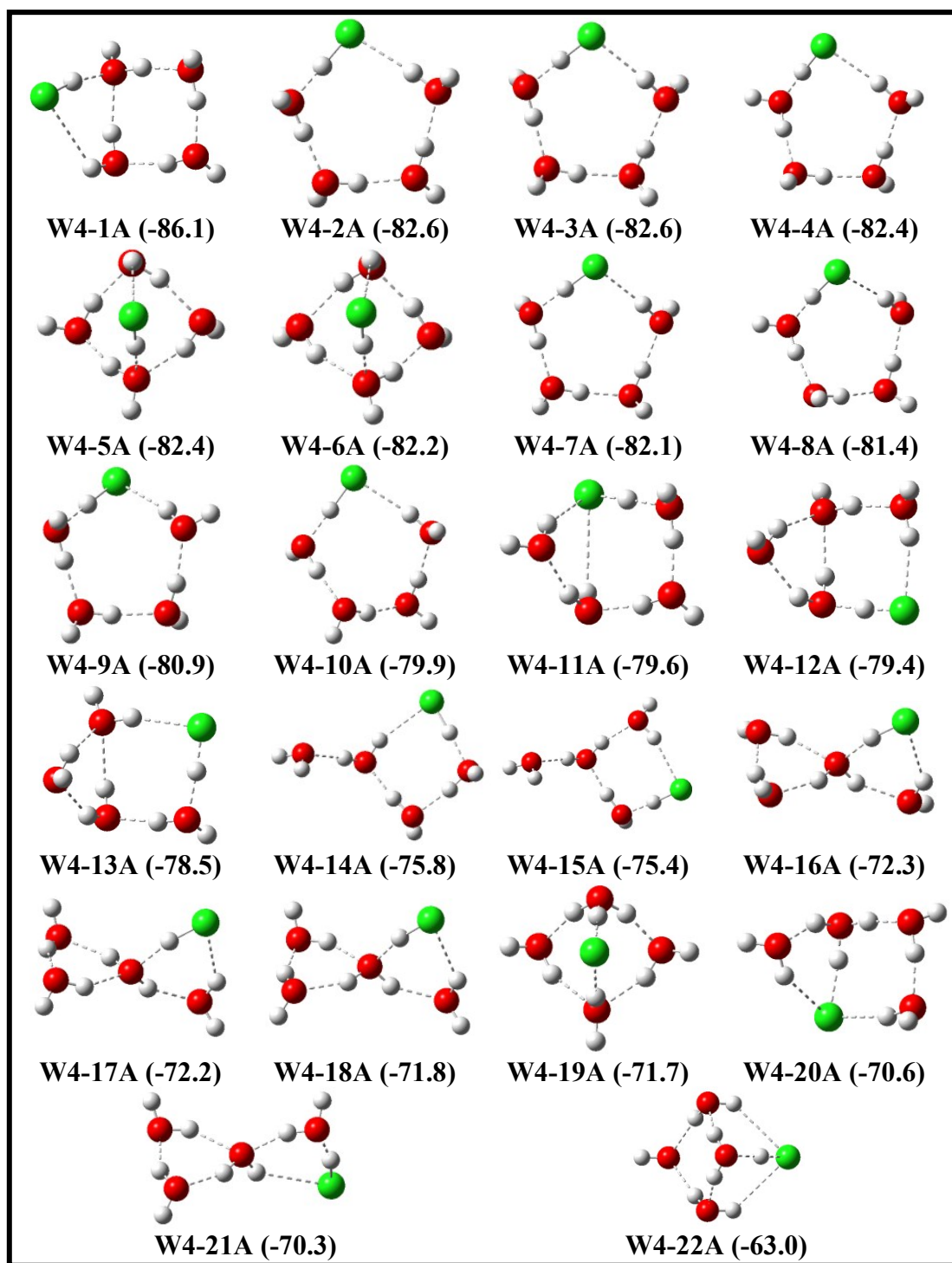
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India

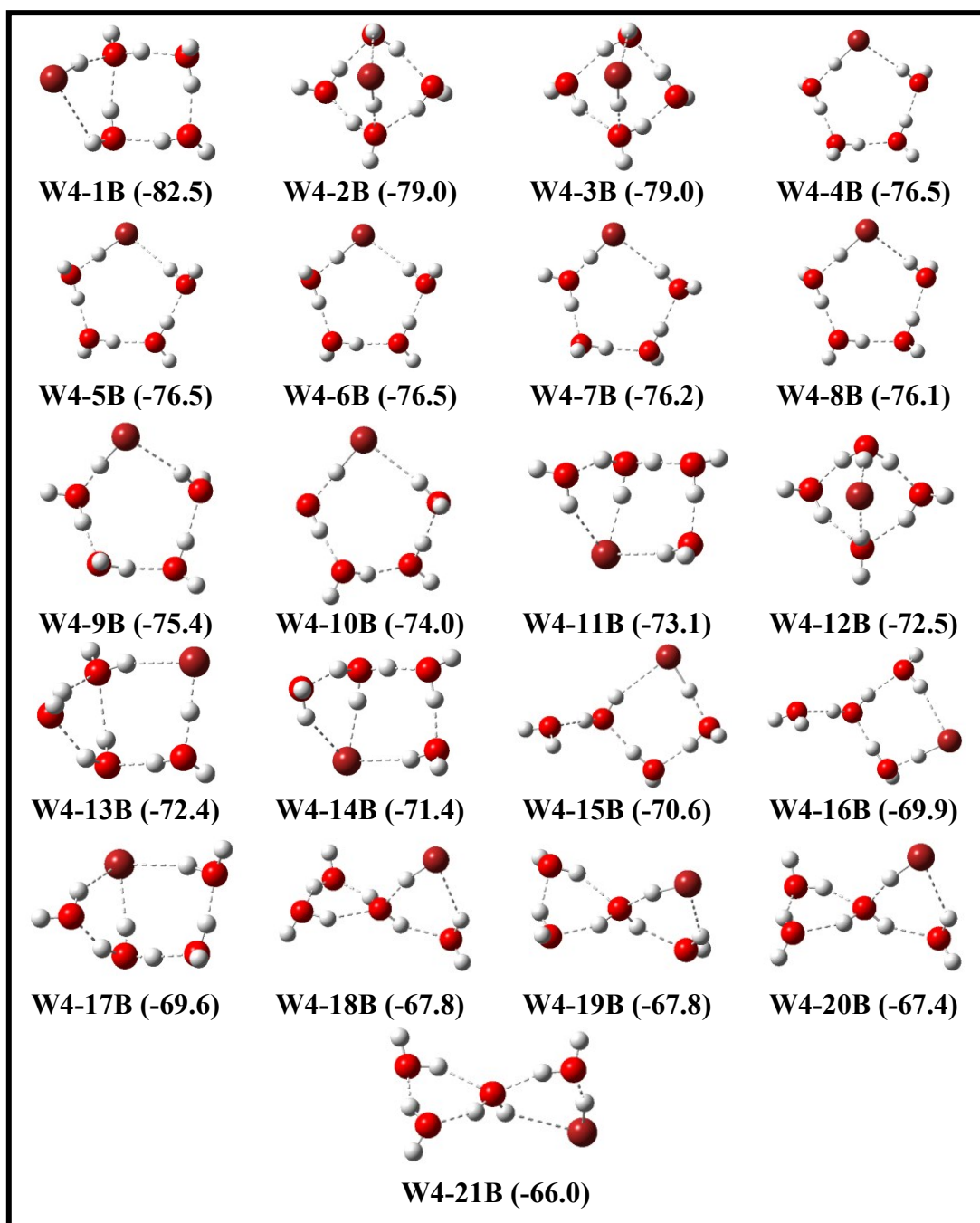
E-mail: naresh@chem.iitb.ac.in



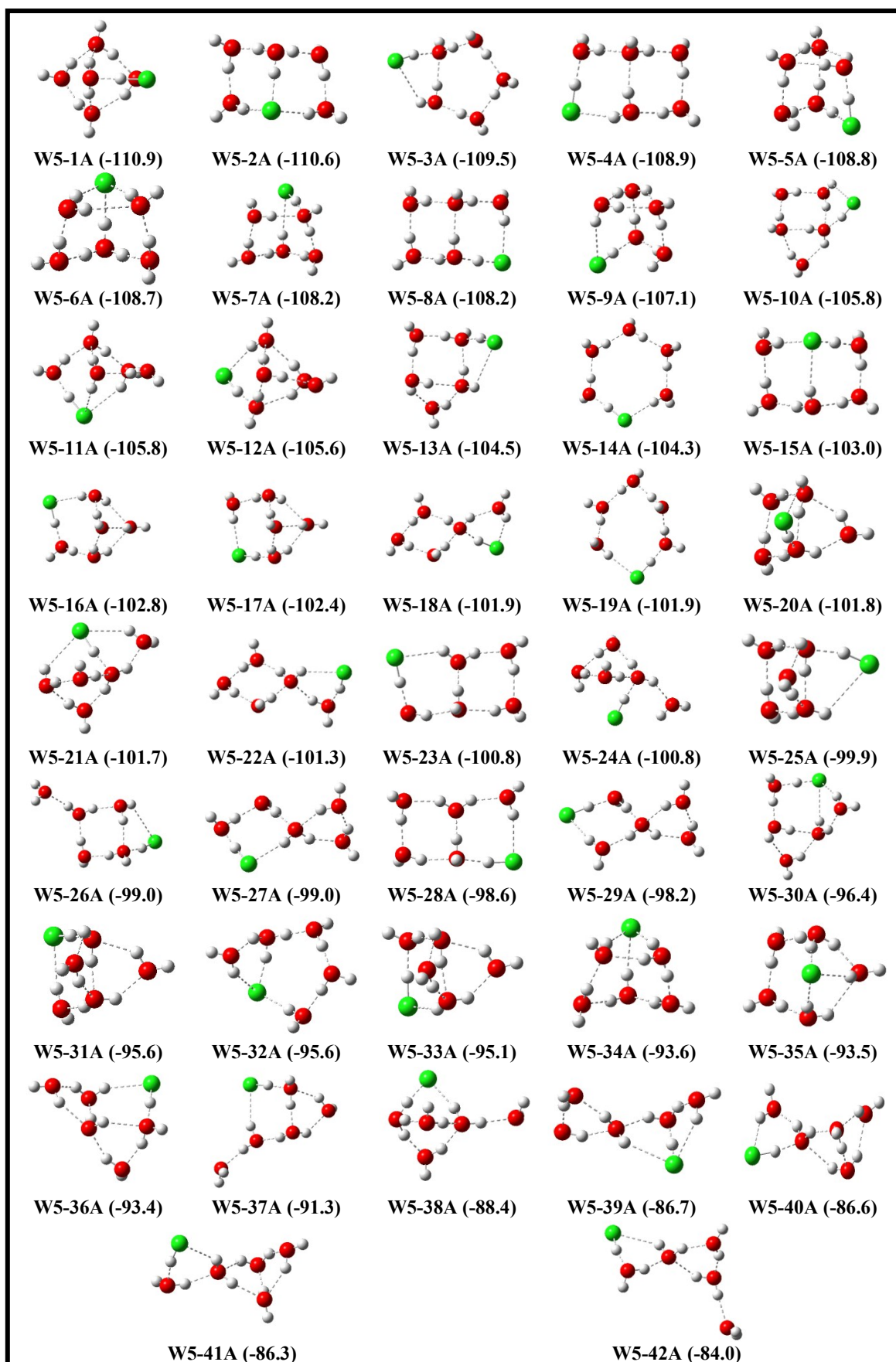
**Fig. S1.** Optimized structures of  $\text{HCl}-(\text{H}_2\text{O})_{1-3}$  and  $\text{HBr}-(\text{H}_2\text{O})_{1-3}$  clusters. The stabilization energies calculated at MP2/aug-cc-pVDZ level are shown in parenthesis. The structures with labels ending with A and B denote water clusters of HCl and HBr, respectively.



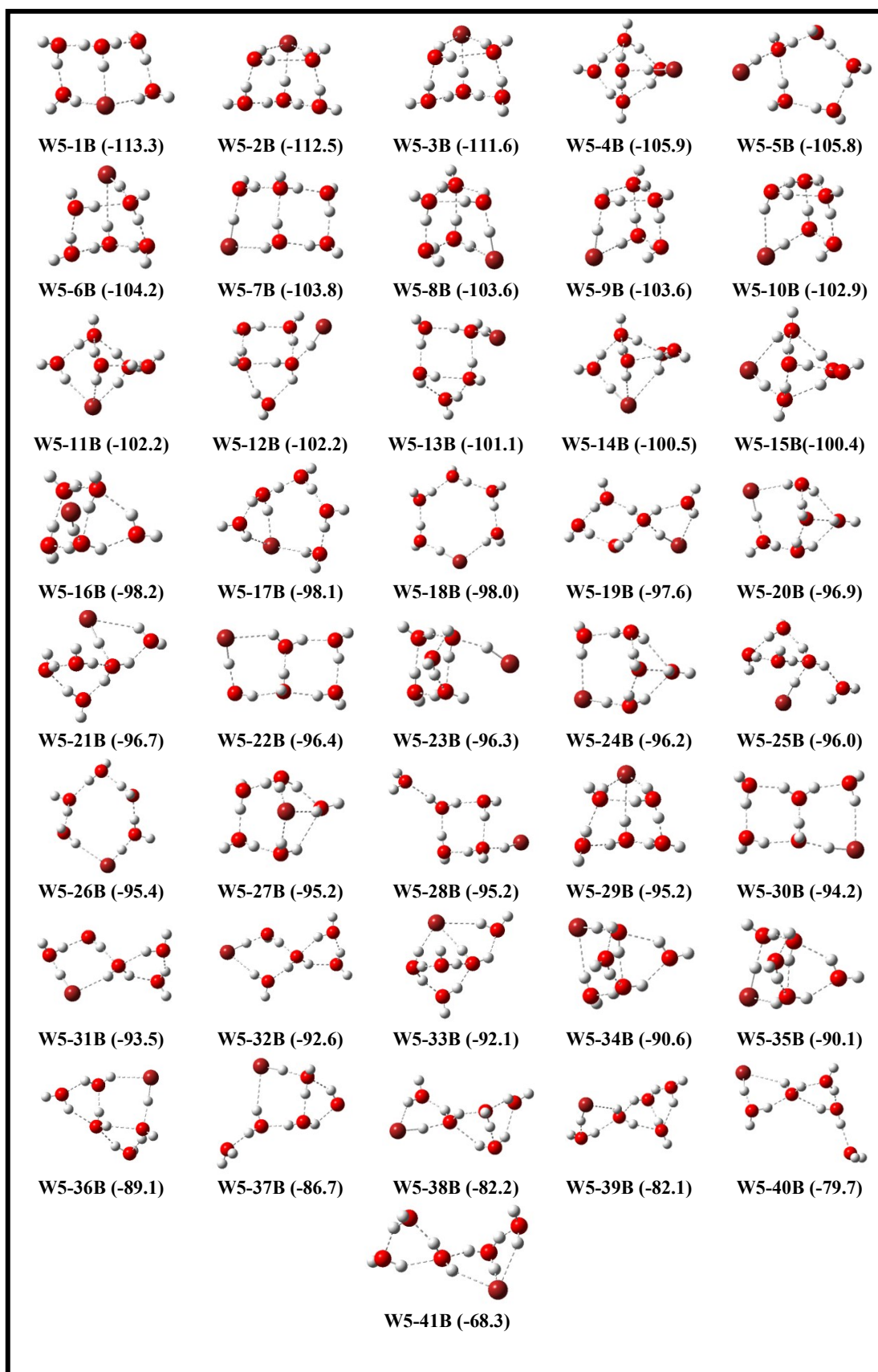
**Fig. S2.** Optimized structures of HCl-(H<sub>2</sub>O)<sub>4</sub> cluster. The stabilization energies calculated at MP2/aug-cc-pVDZ level are shown in parenthesis.



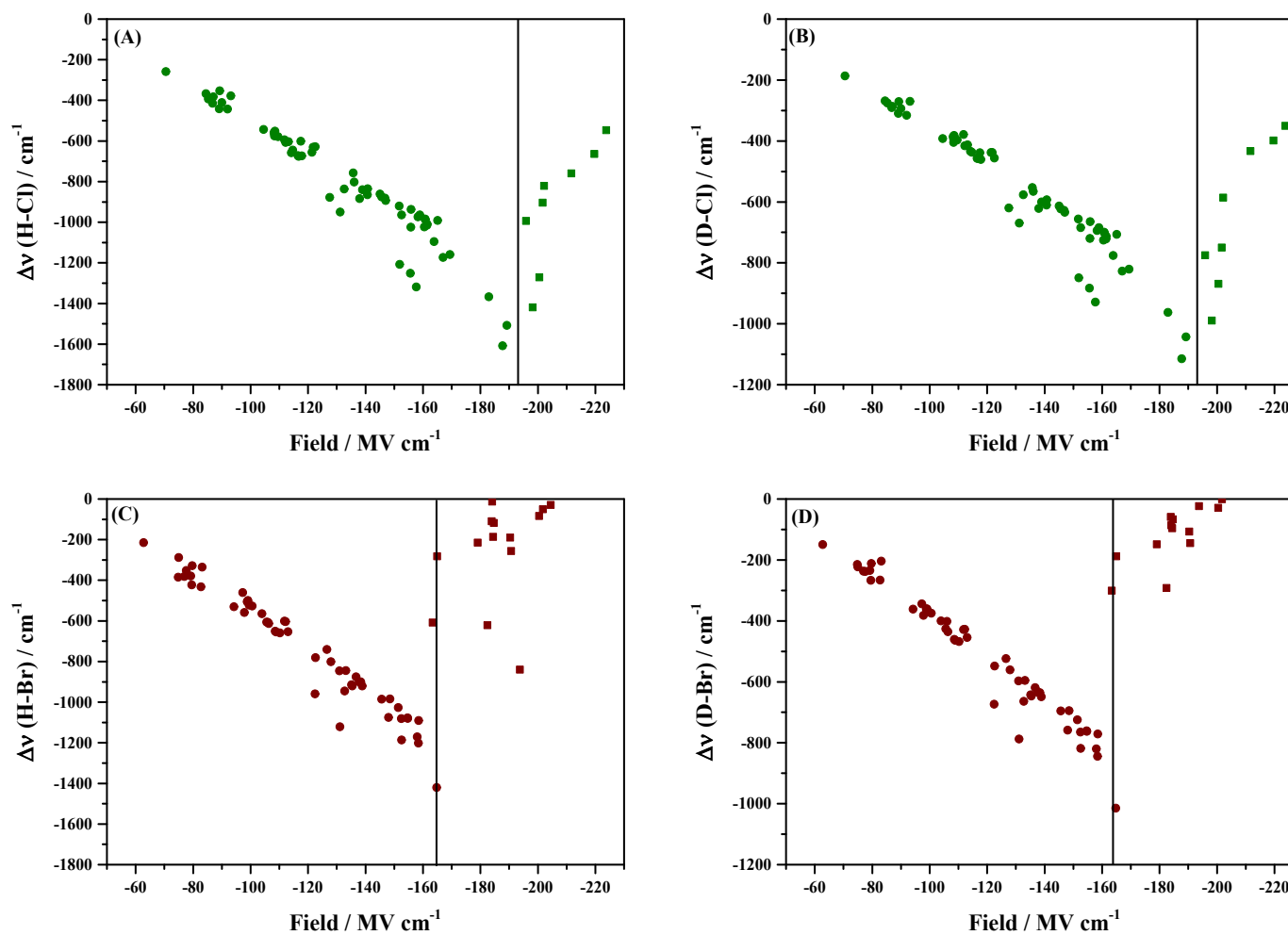
**Fig. S3.** Optimized structures of  $\text{HBr}-(\text{H}_2\text{O})_4$  cluster. The stabilization energies calculated at MP2/aug-cc-pVDZ level are shown in parenthesis.



**Fig. S4.** Optimized structures of  $\text{HCl}-(\text{H}_2\text{O})_5$  cluster. The stabilization energies calculated at MP2/aug-cc-pVDZ level are shown in parenthesis.



**Fig. S5.** Optimized structures of  $\text{HBr}-(\text{H}_2\text{O})_5$  cluster. The stabilization energies calculated at MP2/aug-cc-pVDZ level are shown in parenthesis.



**Fig. S6.** Plot of red-shift in the X–H stretching frequencies against electric field calculated at MP2/aug-cc-pVDZ level for (A) HCl–(D<sub>2</sub>O)<sub>1-5</sub>, (B) DCl–(H<sub>2</sub>O)<sub>1-5</sub>, (C) HBr–(D<sub>2</sub>O)<sub>1-5</sub>, and (D) DBr–(H<sub>2</sub>O)<sub>1-5</sub> clusters. The vertical line at about 193  $\text{MV cm}^{-1}$  for HCl/DCl clusters and at about 163  $\text{MV cm}^{-1}$  for HBr/DBr clusters separates the region of reversal in the frequency shift trend.

**Table S1: ZPE and BSSE corrected stabilization energy (kJ mol<sup>-1</sup>), unscaled vibrational frequencies and their shifts (cm<sup>-1</sup>) for hydrogen bonded H-Cl molecule in HCl-(H<sub>2</sub>O)<sub>1-5</sub> clusters, for D-Cl molecule in DCl-(H<sub>2</sub>O)<sub>1-5</sub> clusters and for H-Cl molecule in HCl-(D<sub>2</sub>O)<sub>1-5</sub> clusters calculated at the MP2/aug-cc-pVDZ level of theory.**

Structure	$\Delta E$	$\nu$	$\Delta\nu$	$\nu$	$\Delta\nu$	$\nu$	$\Delta\nu$
		HCl/H <sub>2</sub> O	HCl/H <sub>2</sub> O	DCl/H <sub>2</sub> O	DCl/H <sub>2</sub> O	HCl/D <sub>2</sub> O	HCl/D <sub>2</sub> O
W1-1A	-13.3	2761	-264	1982	-187	2765	-259
W2-1A	-32.9	2478	-547	1784	-386	2465	-559
W2-2A	-32.9	2478	-547	1784	-386	2466	-559
W2-3A	-32.2	2483	-542	1787	-382	2473	-552
W3-1A	-61.0	2156	-869	1541	-628	2142	-882
W3-2A	-59.5	2177	-848	1555	-614	2164	-861
W3-3A	-48.4	1784	-1241	1787	-883	1773	-1252
W4-1A	-86.1	2610	-414	1879	-291	2610	-415
W4-2A	-82.6	2056	-968	1470	-700	2041	-984
W4-3A	-82.6	2053	-972	1467	-702	2037	-987
W4-4A	-82.4	2067	-958	1475	-694	2051	-974
W4-5A	-82.4	2606	-418	1875	-294	2613	-411
W4-6A	-82.2	2633	-392	1894	-276	2631	-394
W4-7A	-82.1	2074	-951	1484	-685	2060	-965
W4-8A	-81.4	2077	-948	1484	-685	2061	-964
W4-9A	-80.9	2104	-921	1444	-726	2000	-1024
W4-10A	-79.9	2101	-924	1504	-665	2088	-937
W4-11A	-79.6	1884	-1141	1348	-821	1865	-1160
W4-12A	-79.4	1857	-1167	1342	-827	1850	-1174
W4-13A	-78.5	1947	-1077	1394	-776	1929	-1096
W4-14A	-75.8	2207	-818	1576	-593	2190	-835
W4-15A	-75.4	2019	-1005	1449	-720	2000	-1025
W4-16A	-72.3	2365	-659	1711	-458	2349	-676
W4-17A	-72.2	2367	-657	1712	-457	2351	-673
W4-18A	-71.8	2396	-628	1732	-437	2380	-645
W4-19A	-71.7	1769	-1255	1301	-869	1752	-1272
W4-20A	-70.6	2181	-844	1583	-586	2204	-821
W4-21A	-70.3	2461	-564	1772	-397	2445	-579
W4-22A	-63.0	1823	-1201	1320	-849	1817	-1208
W5-1A	-110.9	2148	-877	1547	-622	2140	-884
W5-2A	-110.6	2423	-601	1819	-351	2478	-547
W5-3A	-109.5	2583	-442	1859	-310	2582	-442
W5-4A	-108.9	2392	-632	1731	-438	2369	-656
W5-5A	-108.8	2168	-856	1559	-611	2160	-865
W5-6A	-108.7	2352	-672	1771	-399	2361	-664
W5-7A	-108.2	2462	-562	1777	-392	2480	-544
W5-8A	-108.2	1411	-1614	1054	-1115	1417	-1608
W5-9A	-107.1	2441	-584	1764	-405	2459	-566
W5-10A	-105.8	2639	-385	1899	-271	2672	-353
W5-11A	-105.8	2199	-826	1569	-600	2184	-840
W5-12A	-105.6	2242	-783	1593	-577	2188	-837
W5-13A	-104.5	2640	-384	1900	-269	2656	-368
W5-14A	-104.3	2049	-975	1462	-707	2033	-992

W5-15A	-103.0	1725	-1300	1207	-963	1658	-1367
W5-16A	-102.8	2119	-906	1513	-656	2103	-921
W5-17A	-102.4	2023	-1001	1456	-713	2016	-1009
W5-18A	-101.9	2402	-623	1736	-434	2366	-658
W5-19A	-101.9	2026	-999	1447	-722	2010	-1015
W5-20A	-101.8	2634	-391	1900	-270	2647	-378
W5-21A	-101.7	2091	-934	1499	-670	2075	-950
W5-22A	-101.3	2436	-589	1756	-413	2421	-604
W5-23A	-100.8	2396	-628	1732	-438	2394	-631
W5-24A	-100.8	2162	-863	1549	-620	2146	-878
W5-25A	-99.9	2618	-406	1882	-287	2642	-383
W5-26A	-99.0	2574	-451	1854	-316	2582	-443
W5-27A	-99.0	2163	-862	1546	-623	2149	-876
W5-28A	-98.6	2396	-629	1730	-439	2423	-601
W5-29A	-98.2	2145	-879	1536	-634	2131	-894
W5-30A	-96.4	1487	-1537	1126	-1043	1517	-1508
W5-31A	-95.6	2239	-785	1603	-566	2222	-802
W5-32A	-95.6	2279	-746	1737	-433	2265	-760
W5-33A	-95.1	2279	-745	1616	-553	2266	-758
W5-34A	-93.6	1940	-1085	1395	-775	2030	-994
W5-35A	-93.5	2071	-954	1419	-750	2121	-904
W5-36A	-93.4	2482	-542	1791	-379	2429	-595
W5-37A	-91.3	2357	-667	1713	-456	2396	-629
W5-38A	-88.4	1583	-1442	1179	-990	1606	-1419
W5-39A	-86.7	1723	-1301	1241	-929	1706	-1319
W5-40A	-86.6	2362	-662	1709	-461	2351	-674
W5-41A	-86.3	2466	-558	1776	-393	2449	-575
W5-42A	-84.0	2434	-591	1754	-416	2416	-608

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**Table S2: ZPE and BSSE corrected stabilization energy (kJ mol<sup>-1</sup>), unscaled vibrational frequencies and their shifts (cm<sup>-1</sup>) for hydrogen bonded H-Br molecule in HBr-(H<sub>2</sub>O)<sub>1-5</sub> clusters, for D-Br molecule in DBr-(H<sub>2</sub>O)<sub>1-5</sub> clusters and for H-Br molecule in HBr-(D<sub>2</sub>O)<sub>1-5</sub> clusters calculated at the MP2/aug-cc-pVDZ level of theory.**

Structure	$\Delta E$	$\nu$ HBr/H <sub>2</sub> O	$\Delta\nu$ HBr/H <sub>2</sub> O	$\nu$ DBr/H <sub>2</sub> O	$\Delta\nu$ DBr/H <sub>2</sub> O	$\nu$ HBr/D <sub>2</sub> O	$\Delta\nu$ HBr/D <sub>2</sub> O
W1-1B	-10.5	2513	-214	1790	-150	2512	-215
W2-1B	-28.7	2225	-501	1579	-362	2221	-506
W2-2B	-28.7	2225	-502	1578	-362	2220	-506
W2-3B	-27.9	2230	-496	1580	-361	2226	-500
W3-1B	-55.4	1839	-887	1305	-636	1825	-901
W3-2B	-53.9	1863	-863	1321	-619	1850	-876
W3-3B	-28.9	2237	-489	1640	-301	2117	-609
W4-1B	-82.5	2376	-351	1704	-237	2344	-382
W4-2B	-79.0	2381	-345	1706	-235	2347	-379
W4-3B	-79.0	2402	-324	1717	-223	2438	-288
W4-4B	-76.5	1595	-1132	1180	-761	1648	-1078
W4-5B	-76.5	1594	-1133	1178	-763	1646	-1080
W4-6B	-76.5	1593	-1133	1178	-763	1646	-1080
W4-7B	-76.2	1592	-1134	1176	-765	1645	-1082
W4-8B	-76.1	1617	-1109	1216	-725	1699	-1027
W4-9B	-75.4	1596	-1130	1181	-759	1650	-1076
W4-10B	-74.0	1763	-963	1246	-695	1742	-984
W4-11B	-73.1	2494	-232	1874	-67	2609	-118
W4-12B	-72.5	2255	-472	1649	-292	2105	-622
W4-13B	-72.4	1268	-1458	925	-1015	1305	-1421
W4-14B	-71.4	2487	-240	1854	-87	2594	-13
W4-15B	-70.6	1893	-834	1345	-596	1881	-845
W4-16B	-69.9	1521	-1205	1122	-819	1539	-1187
W4-17B	-69.6	2516	-210	1881	-59	2616	-110
W4-18B	-67.8	2083	-643	1480	-461	2076	-651
W4-19B	-67.8	2079	-647	1477	-464	2072	-655
W4-20B	-67.4	2121	-605	1505	-436	2114	-613
W4-21B	-66.0	2204	-522	1565	-375	2200	-527
W5-1B	-113.3	2610	-116	1957	17	2697	-30
W5-2B	-112.5	2580	-146	1940	-1	2676	-51
W5-3B	-111.6	2569	-157	1912	-29	2642	-84
W5-4B	-105.9	1788	-939	1277	-664	1781	-945
W5-5B	-105.8	2342	-384	1674	-267	2304	-423
W5-6B	-104.2	2222	-504	1578	-362	2196	-531
W5-7B	-103.8	2131	-595	1512	-429	2125	-601
W5-8B	-103.6	1820	-907	1297	-643	1811	-915
W5-9B	-103.6	1814	-912	1293	-647	1806	-921
W5-10B	-102.9	2202	-525	1559	-382	2167	-559
W5-11B	-102.2	2418	-308	1796	-145	2469	-257
W5-12B	-102.2	2406	-320	1728	-212	2399	-328
W5-13B	-101.1	2407	-319	1725	-215	2341	-385
W5-14B	-100.5	1891	-835	1343	-597	1880	-846

W5-15B	-100.4	1963	-763	1393	-548	1945	-781
W5-16B	-98.2	2405	-322	1736	-204	2390	-336
W5-17B	-98.1	2513	-213	1917	-24	1887	-840
W5-18B	-98.0	1583	-1143	1170	-771	1636	-1091
W5-19B	-97.6	2130	-596	1515	-426	2120	-606
W5-20B	-96.9	1769	-957	1244	-696	1740	-986
W5-21B	-96.7	1566	-1160	1152	-788	1604	-1122
W5-22B	-96.4	2129	-597	1513	-428	2123	-604
W5-23B	-96.3	2387	-339	1702	-238	2374	-352
W5-24B	-96.2	1552	-1175	1120	-820	1555	-1171
W5-25B	-96.0	1784	-942	1266	-674	1767	-960
W5-26B	-95.4	1499	-1227	1095	-845	1525	-1202
W5-27B	-95.2	2426	-300	1845	-96	2540	-187
W5-28B	-95.2	2331	-396	1675	-266	2295	-432
W5-29B	-95.2	2510	-216	1792	-149	2511	-215
W5-30B	-94.2	2163	-564	1539	-402	2118	-608
W5-31B	-93.5	1840	-886	1306	-635	1826	-900
W5-32B	-92.6	1821	-906	1291	-649	1805	-921
W5-33B	-92.1	2483	-243	1834	-107	2537	-190
W5-34B	-90.6	1934	-792	1379	-561	1925	-801
W5-35B	-90.1	1994	-733	1417	-524	1986	-741
W5-36B	-89.1	2273	-453	1596	-344	2265	-461
W5-37B	-86.7	2095	-631	1486	-455	2072	-654
W5-38B	-82.2	2072	-654	1473	-468	2066	-660
W5-39B	-82.1	2209	-517	1569	-371	2204	-522
W5-40B	-79.7	2167	-560	1541	-400	2161	-565
W5-41B	-68.3	2370	-357	1752	-188	2444	-282

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**Table S3: Bond distances (Å) and electric fields along the H-X bond (MV cm<sup>-1</sup>) at the MP2/aug-cc-pVDZ level of theory for the HCl-(H<sub>2</sub>O)<sub>n</sub> and HBr-(H<sub>2</sub>O)<sub>n</sub> clusters respectively.**

Structure	d(H-Cl)	H-Cl Field	Structure	d(H-Br)	H-Br Field
<b>HCl-H<sub>2</sub>O</b>			<b>HBr-H<sub>2</sub>O</b>		
W1-1A	1.307	-70.6	W1-1B	1.438	-62.8
<b>HCl-(H<sub>2</sub>O)<sub>2</sub></b>			<b>HBr-(H<sub>2</sub>O)<sub>2</sub></b>		
W2-1A	1.328	-108.2	W2-1B	1.462	-98.8
W2-2A	1.328	-108.2	W2-2B	1.462	-98.9
W2-3A	1.328	-108.5	W2-3B	1.4624	-99.1
<b>HCl-(H<sub>2</sub>O)<sub>3</sub></b>			<b>HBr-(H<sub>2</sub>O)<sub>3</sub></b>		
W3-1A	1.353	-146.8	W3-1B	1.498	-138.4
W3-2A	1.352	-145.1	W3-2B	1.496	-136.7
W3-3A	1.386	-155.6	W3-3B	1.956	-163.4
<b>HCl-(H<sub>2</sub>O)<sub>4</sub></b>			<b>HBr-(H<sub>2</sub>O)<sub>4</sub></b>		
W4-1A	1.317	-86.9	W4-1B	1.448	-77.0
W4-2A	1.362	-160.7	W4-2B	1.448	-79.3
W4-3A	1.362	-160.9	W4-3B	1.446	-75.0
W4-4A	1.361	-158.3	W4-4B	1.515	-154.7
W4-5A	1.318	-90.0	W4-5B	1.515	-154.8
W4-6A	1.315	-85.31	W4-6B	1.515	-154.8
W4-7A	1.360	-159.0	W4-7B	1.515	-152.5
W4-8A	1.360	-152.6	W4-8B	1.510	-151.4
W4-9A	1.365	-160.5	W4-9B	1.514	-148.0
W4-10A	1.358	-155.9	W4-10B	1.506	-148.5
W4-11A	1.377	-169.6	W4-11B	2.010	-184.7
W4-12A	1.379	-167.0	W4-12B	1.943	-182.4
W4-13A	1.371	-163.9	W4-13B	1.553	-164.8
W4-14A	1.349	-140.8	W4-14B	2.003	-184.1
W4-15A	1.364	-155.8	W4-15B	1.492	-133.2
W4-16A	1.336	-116.7	W4-16B	1.525	-152.6
W4-17A	1.336	-116.5	W4-17B	2.017	-183.9
W4-18A	1.334	-114.7	W4-18B	1.474	-108.6
W4-19A	1.715	-200.5	W4-19B	1.474	-108.9
W4-20A	1.790	-202.2	W4-20B	1.471	-106.4
W4-21A	1.329	-109.6	W4-21B	1.464	-100.6
W4-22A	1.381	-151.9			
<b>HCl-(H<sub>2</sub>O)<sub>5</sub></b>			<b>HBr-(H<sub>2</sub>O)<sub>5</sub></b>		
W5-1A	1.354	-138.0	W5-1B	2.022	-204.5
W5-2A	1.830	-223.9	W5-2B	2.018	-201.8
W5-3A	1.319	-89.1	W5-3B	2.010	-200.4
W5-4A	1.334	-121.4	W5-4B	1.502	-132.8
W5-5A	1.352	-140.7	W5-5B	1.451	-79.6
W5-6A	1.817	-219.7	W5-6B	1.461	-94.2
W5-7A	1.328	-104.6	W5-7B	1.470	-111.8
W5-8A	1.420	-187.8	W5-8B	1.499	-135.2
W5-9A	1.330	-108.3	W5-9B	1.500	-135.4
W5-10A	1.315	-89.3	W5-10B	1.463	-97.9
W5-11A	1.350	-139.0	W5-11B	1.980	-190.7
W5-12A	1.346	-132.6	W5-12B	1.446	-79.7
W5-13A	1.315	-84.5	W5-13B	1.446	-74.8
W5-14A	1.362	-165.1	W5-14B	1.493	-131.0

W5-15A	1.395	-182.9	W5-15B	1.485	-122.7
W5-16A	1.356	-151.7	W5-16B	1.447	-83.2
W5-17A	1.364	-161.5	W5-17B	2.014	-193.8
W5-18A	1.333	-114.2	W5-18B	1.516	-158.7
W5-19A	1.364	-161.4	W5-19B	1.470	-105.6
W5-20A	1.316	-93.1	W5-20B	1.505	-145.6
W5-21A	1.357	-131.2	W5-21B	1.518	-131.1
W5-22A	1.331	-113.3	W5-22B	1.470	-112.2
W5-23A	1.334	-121.8	W5-23B	1.448	-77.7
W5-24A	1.352	-127.6	W5-24B	1.524	-158.0
W5-25A	1.317	-87.1	W5-25B	1.518	-122.5
W5-26A	1.320	-92.0	W5-26B	1.527	-158.5
W5-27A	1.352	-145.6	W5-27B	1.999	-184.5
W5-28A	1.333	-117.5	W5-28B	1.452	-82.8
W5-29A	1.354	-147.1	W5-29B	1.985	-179.1
W5-30A	1.410	-189.2	W5-30B	1.466	-106.8
W5-31A	1.346	-136.1	W5-31B	1.498	-137.8
W5-32A	1.801	-211.7	W5-32B	1.499	-138.9
W5-33A	1.343	-135.8	W5-33B	1.991	-190.4
W5-34A	1.749	-196.0	W5-34B	1.487	-128.0
W5-35A	1.766	-201.7	W5-35B	1.483	-126.6
W5-36A	1.327	-111.8	W5-36B	1.458	-97.3
W5-37A	1.336	-122.6	W5-37B	1.473	-113.1
W5-38A	1.691	-198.2	W5-38B	1.475	-110.2
W5-39A	1.392	-157.7	W5-39B	1.463	-99.6
W5-40A	1.336	-117.7	W5-40B	1.467	-104.0
W5-41A	1.329	-108.4	W5-41B	1.990	-165.0
W5-42A	1.331	-112.2			

**Cartesian coordinates of various hydrogen bonded HCl-water clusters considered in the present investigation at MP2/aug-cc-pVDZ level of theory.**

**HCl-H<sub>2</sub>O**

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**W1-1A**

O -1.95574500 0.00002800 -0.09287200  
H -2.35970500 -0.76462500 0.33983700  
H -2.36033000 0.76422600 0.34005600  
Cl 1.20394400 0.00000000 0.00711600  
H -0.10106400 0.00017900 -0.05787900

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**HCl-(H<sub>2</sub>O)<sub>2</sub>**

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**W2-1A**

Cl -1.53607400 -0.22192900 0.00190200  
H -0.57606800 0.69455400 -0.03901400  
O 0.91871900 1.53688100 -0.10887900  
H 1.46805600 0.72995600 -0.02576700  
O 1.72239300 -1.12078900 0.09417800  
H 0.79060100 -1.39273000 0.06436500  
H 1.14398000 2.07877500 0.65913200  
H 2.15778300 -1.66650000 -0.57344200

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**W2-2A**

Cl 1.53617200 -0.22180100 0.00188100  
H 0.57612700 0.69461700 -0.03915200  
O -0.91893300 1.53655000 -0.10888500  
H -1.46761600 0.72925000 -0.02463700  
O -1.72257700 -1.12107100 0.09450100  
H -0.79074300 -1.39295700 0.06525400  
H -1.14418500 2.07910600 0.65866100  
H -2.15643500 -1.66322600 -0.57702500

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**W2-3A**

Cl 1.53126600 -0.22443100 0.00838100  
H 0.56977400 0.69010300 -0.03173900  
O -0.91792800 1.54923200 -0.09217300  
H -1.48739500 0.75906300 -0.00087600  
O -1.70672800 -1.11605400 -0.05728700  
H -0.78211100 -1.40475200 0.00308700  
H -1.12091800 2.09930300 0.67606800  
H -2.21361800 -1.79382100 0.40666800

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**HCl-(H<sub>2</sub>O)<sub>3</sub>**

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**W3-1A**

O 2.32986400 -0.36241300 0.01709300  
H 2.91790200 -0.36333700 0.78266800  
H 1.91993200 0.53121100 0.00948500  
Cl -1.89902600 0.18081800 0.05309200  
H -1.00431900 -0.83346900 0.00636600  
O 0.85600400 1.97042200 -0.01381700  
H -0.05489500 1.62657700 0.03031700  
H 0.85390500 2.56043500 -0.77854900  
O 0.12905400 -1.94224400 -0.01780300  
H 0.13933900 -2.46364700 -0.83178400

H 0.99220300 -1.45780000 -0.00485000

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**W3-2A**

O -0.85972900 1.96854300 0.02885000  
H -0.86852100 2.49354300 0.83984200  
H 0.05194300 1.62890900 -0.02766400  
H 1.00578200 -0.81758800 0.06375600  
O -2.33244500 -0.36491000 -0.06206200  
H -1.91620500 0.52584400 -0.04699700  
H -2.94796800 -0.34353500 -0.80491800  
O -0.12672700 -1.92288300 0.23636200  
H -0.06849600 -2.63149500 -0.41820300  
H -0.99363500 -1.47711500 0.07146500  
Cl 1.89931200 0.18679000 -0.07661700

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**W3-3A**

H 0.01043100 -0.40914100 0.72081600  
O 2.07593500 1.00635300 -0.61764000  
H 3.03892400 1.06395100 -0.57296600  
H 1.88885300 0.06141900 -0.74245900  
O -2.22445400 0.83942600 -0.50231200  
H -1.91734500 -0.04537700 -0.75746200  
H -2.53785500 1.23991000 -1.32314100  
O -0.03493500 1.00311100 1.21806900  
H 0.73676400 1.33894900 0.71839600  
H -0.81401900 1.30032300 0.70482200  
Cl 0.06246400 -1.60830300 0.02747400

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**HCl-(H<sub>2</sub>O)<sub>4</sub>**

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**W4-1A**

O -1.84431200 1.67523600 -0.34995200  
H -1.69158500 2.05262800 -1.22550600  
H -2.21036800 0.77432300 -0.52103600  
O -2.53117800 -0.93964500 -0.66339600  
H -1.79300300 -1.35956800 -0.16469500  
H -3.33547800 -1.34954500 -0.32266300  
H 1.62162100 0.54157000 0.18274700  
O 0.25602700 1.03388200 1.17800400  
H -0.49767800 1.38788800 0.63495400  
H 0.36761000 1.64350000 1.91821300  
O -0.33712300 -1.73278100 0.79332300  
H -0.08610000 -0.85799400 1.14521500  
H 0.44179800 -1.99996200 0.28467400  
Cl 2.51975700 -0.06625800 -0.56445500

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**W4-2A**

O 1.94790400 -1.69046200 -0.18579000  
H 2.22669800 -0.74496700 -0.16373400  
H 2.23645100 -2.02055300 -1.04549100  
O 2.54757200 0.96284200 0.03276300  
H 1.72094400 1.49401100 0.07484400  
H 3.13514100 1.45971200 -0.54909700  
O 0.17277800 2.34588800 0.17938300  
H -0.59394100 1.77034900 0.00027600  
H -0.04341100 2.76955500 1.02006300  
O -0.65081700 -2.08251600 0.36595400  
H 0.31238000 -1.94116500 0.17131700  
H -0.68863100 -2.36555700 1.28927500

H -1.51922000 -0.83984700 0.06074200  
Cl -2.28975900 0.24308500 -0.23509800

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**W4-3A**

O -1.94848200 -1.69057400 -0.18325300  
H -2.24099400 -2.02297200 -1.04071300  
H -2.22740800 -0.74515200 -0.16236400  
Cl 2.29074800 0.24320100 -0.23450300  
H 1.51927800 -0.83990000 0.05975800  
O -2.54879100 0.96398500 0.03131600  
H -3.13419800 1.46011200 -0.55336000  
H -1.72139500 1.49398800 0.07356200  
O 0.65096200 -2.08170100 0.36351400  
H 0.68973200 -2.36559100 1.28654600  
H -0.31253100 -1.94027600 0.17004500  
H 0.59489100 1.76990500 0.00079500  
O -0.17261000 2.34449300 0.17969100  
H 0.04127000 2.76584200 1.02213400

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**W4-4A**

O 2.52958700 0.92188600 -0.10753800  
H 1.70784100 1.45930400 -0.15940600  
H 2.99055200 1.09049400 -0.93859000  
O 0.16245700 2.33431100 -0.19393600  
H -0.61427900 1.75042200 -0.11640900  
H 0.01499600 3.01438000 0.47583300  
H -1.47347500 -0.82223500 -0.18659900  
O 1.88146300 -1.64989500 0.50323400  
H 2.17040200 -0.72990700 0.29028000  
H 1.98327100 -1.72500700 1.46004300  
O -0.50192800 -1.91062200 -0.70225700  
H 0.36315000 -1.89090900 -0.21556800  
H -0.82794200 -2.81735600 -0.63265600  
Cl -2.28747900 0.18266900 0.23688500

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**W4-5A**

H 0.70397200 -0.96939600 1.18707800  
O 0.22622700 -0.25127400 1.68073100  
H 0.14362900 -0.55567900 2.59348600  
H 1.25638900 -2.70626000 -0.33934100  
O 1.50930400 -1.82191900 -0.04729100  
H 1.29222900 -1.22152600 -0.80426700  
H 1.07828500 1.32715300 0.98794100  
O 1.36049000 1.94849200 0.29048900  
H 2.23426900 2.25525500 0.56264700  
H -1.25040200 -0.07172800 0.70705000  
H -0.12681700 0.20584700 -1.83921000  
O 0.83947400 0.14599600 -1.79813300  
H 1.08606000 0.89408000 -1.21437200  
Cl -2.22950400 0.03952300 -0.16749300

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**W4-6A**

H -0.85222100 -0.92554400 1.18639900  
O -0.27728900 -0.29321200 1.69165000  
H -0.15097800 -0.68234000 2.56639600  
H -2.57136600 -1.93261500 -0.16772100  
O -1.62863400 -1.74043100 -0.09670900  
H -1.43337000 -1.09550900 -0.82188500  
H 1.20368700 -0.22083100 0.67066200  
H -1.72200300 2.62365700 0.66010500

O	-0.99972100	2.07038000	0.33930000
H	-0.83522400	1.41844200	1.04605300
H	-0.94662400	1.00518400	-1.18227800
O	-0.86119800	0.24122200	-1.78933500
H	0.09684100	0.14972700	-1.90130500
Cl	2.19682300	-0.15081400	-0.18915700

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**W4-7A**

O	-0.67362600	2.11247000	0.32897400
H	-0.74943300	2.34217100	1.26476400
H	0.29602300	1.98001000	0.16966400
H	-1.51502400	0.84700800	-0.00099400
O	1.92849100	1.66121700	-0.19483600
H	2.66342100	2.13883100	0.20759900
H	2.19351500	0.71071100	-0.18124200
O	2.53222000	-0.99325900	-0.14051900
H	1.71581200	-1.50432100	0.05694900
H	2.87151000	-1.38443100	-0.95526000
O	0.17403300	-2.32490000	0.35292200
H	-0.02930800	-2.71652200	1.21167300
H	-0.59884700	-1.76562800	0.15086100
Cl	-2.26686000	-0.25247400	-0.27625500

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**W4-8A**

O	0.19670800	-2.24109100	0.36854100
H	-0.57485900	-1.72827400	0.06627200
H	-0.00478900	-2.43999800	1.29236500
H	-1.46971800	0.72341800	0.22236900
O	-0.50020000	1.66206000	0.98868000
H	0.32856400	1.76935700	0.45115600
H	-0.82595100	2.55556700	1.15907700
O	2.54027500	-0.84641100	-0.04336800
H	1.73418100	-1.39295100	0.09173000
H	3.13469500	-1.39291200	-0.57092300
O	1.74806100	1.72289900	-0.47948200
H	2.11743900	0.81312500	-0.38395400
H	1.61799100	1.83409500	-1.42977300
Cl	-2.23154800	-0.18359300	-0.44548700

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**W4-9A**

O	2.34484900	1.14357800	-0.43249100
H	1.56356100	1.55384200	-0.00179400
H	2.34011200	1.49201400	-1.33286300
O	0.06786500	2.01403000	0.86271000
H	-0.71534600	1.58955400	0.46570600
H	-0.21593000	2.91074400	1.07931100
H	-1.42091000	-0.86012600	0.01497500
O	1.97986400	-1.55137300	-0.23899100
H	2.18218600	-0.58896500	-0.31704000
H	2.77257100	-1.95391200	0.13506700
O	-0.53121600	-1.95421100	0.63294000
H	0.41425400	-1.84559800	0.35194100
H	-0.52022100	-1.86580800	1.59583000
Cl	-2.19359900	0.13835600	-0.50496900

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**W4-10A**

O	0.52841800	2.08455600	-0.23775500
H	-0.38807500	1.89028900	0.08299800
H	0.42201500	2.33235500	-1.16621600
O	-1.92372500	1.41303800	0.67867700



H	-2.25083300	0.62280400	0.19081900
H	-2.67306200	2.01695100	0.74006400
O	-2.34766600	-0.87845700	-0.71463000
H	-1.63192600	-1.44926900	-0.35328900
H	-3.09792200	-1.46695100	-0.85848500
H	1.48141500	0.85028700	-0.11458600
O	-0.21353500	-2.25174700	0.34657500
H	0.59089100	-1.73275700	0.16027800
H	-0.21226500	-2.33258500	1.30952200
Cl	2.31834300	-0.21589700	-0.03376700

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**W4-11A**

O	-2.53830200	-0.21790000	0.04843000
H	-3.29302300	-0.39439900	-0.52585000
H	-2.03379000	0.51347100	-0.38479700
Cl	1.72348100	-0.76160900	-0.54783300
H	0.62450300	-1.34198800	0.04570400
O	-0.86603700	1.65752800	-0.99096700
H	-0.22992900	1.17125200	-1.53582600
H	-0.32598100	1.91895400	-0.21708600
O	-0.60466100	-1.94965600	0.67022900
H	-0.54979800	-1.94452800	1.63606900
H	-1.38547200	-1.37354900	0.45040500
H	1.43236300	1.13020800	0.86218800
O	0.87891900	1.85136600	1.21004700
H	1.50259900	2.53723000	1.48043400

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**W4-12A**

O	0.70352100	2.22034500	0.29083200
H	0.80709100	2.59690500	1.17408200
H	1.29961500	1.44621100	0.28507100
H	0.95926300	-1.05367800	-0.35578700
O	-2.48330000	-1.02402400	0.90555400
H	-2.56713700	-0.94910100	1.86396600
H	-2.39898500	-0.10923100	0.57845900
O	-1.62664100	1.18097400	-0.67576700
H	-0.84836000	1.67240000	-0.32201500
H	-2.08050200	1.79985500	-1.26089800
O	-0.39371400	-1.38474300	-0.92530200
H	-0.76924400	-0.52702700	-1.20498200
H	-1.00156900	-1.62273300	-0.19531500
Cl	2.17652300	-0.65847100	0.15734600

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**W4-13A**

H	1.61501000	0.58749700	-0.23518500
O	0.92844100	1.94651900	-0.24325300
H	0.03646200	1.81266200	0.18186700
H	1.37705700	2.62020600	0.28545400
O	-2.58343800	-0.43401900	-1.06299200
H	-2.37344500	-0.53370900	-2.00002900
H	-1.98898700	-1.05482700	-0.60238800
O	-0.78474500	-1.54566100	0.85739900
H	0.14907900	-1.46391400	0.58379700
H	-0.81922900	-2.35382800	1.38491300
O	-1.44605600	1.33606900	0.82046100
H	-1.27396500	0.50523000	1.29423900
H	-1.98620100	1.01507800	0.07066100
Cl	2.13827100	-0.67986300	-0.23154400

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**W4-14A**

H	0.45949100	1.58967700	-0.47189300
O	-0.10392200	2.35236600	-0.19003500
H	-0.15588800	2.92468200	-0.96565600
H	3.82564900	0.03875400	1.34983400
O	3.60991200	-0.52078200	0.59220300
H	4.43251600	-0.57589100	0.08833400
H	-1.56249200	1.59394400	0.32107600
O	-2.33036300	1.02011500	0.57284400
H	-2.46138600	1.17026500	1.51859700
H	-1.89210700	-0.48420700	0.23017400
H	0.60185000	-0.61003500	-0.73338100
O	1.24483400	0.10396400	-0.87879700
H	2.03012900	-0.15215900	-0.36092600
Cl	-1.44949700	-1.71413700	-0.10269900

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**W4-15A**

H	-0.35445600	1.14522500	0.73621600
O	0.37013600	1.80454400	0.53912000
H	0.59062600	2.20747400	1.38988600
H	-3.42321800	0.57262600	-1.65697300
O	-3.64951600	0.11070600	-0.83862600
H	-4.45498800	0.54621000	-0.53020300
H	1.54102500	0.96894100	-0.03069700
H	0.68643200	-2.78766100	0.88490200
O	0.31152000	-2.16177100	0.25225900
H	1.07350700	-1.63206800	-0.04478400
H	-0.94504800	-0.91595700	0.75745200
O	-1.43513000	-0.09449400	0.96716900
H	-2.20156000	-0.08546100	0.36543500
Cl	2.51244700	0.15934100	-0.54297700

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**W4-16A**

O	2.51179700	0.24507200	1.45602800
H	2.95455200	-0.07725600	0.64599000
H	2.65424700	-0.44586000	2.11508300
H	-0.94704400	-0.67715100	-0.01517700
O	0.33069900	0.38054800	-0.21025900
H	-0.21445200	1.19241100	-0.20371900
H	0.93119200	0.43314400	0.56668500
O	-1.88467800	2.06704900	-0.11822000
H	-2.32597100	2.63938400	-0.75856700
H	-2.44787000	1.27783500	-0.06136800
O	2.84208900	-0.47594000	-1.22270500
H	1.92676400	-0.14487600	-1.28144100
H	3.30085800	-0.09518600	-1.98129100
Cl	-2.13126700	-1.28448700	0.10206100

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**W4-17A**

O	-2.51279500	0.24635800	1.45546100
H	-2.65638600	-0.44402300	2.11481200
H	-2.95324500	-0.07715800	0.64459800
O	-2.83912100	-0.47718200	-1.22359700
H	-3.29874900	-0.09113100	-1.97900400
H	-1.92419900	-0.14448800	-1.28043600
O	-0.33096500	0.38353700	-0.21084800
H	0.21574300	1.19435800	-0.20456000
H	-0.93055700	0.43698200	0.56661400
O	1.88728500	2.06575100	-0.11839300
H	2.44930800	1.27569800	-0.06171600
H	2.33068900	2.63873600	-0.75668700

H	0.94548600	-0.67693500	-0.01478000
Cl	2.12862800	-1.28586800	0.10295100

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**W4-18A**

H	-2.24201900	2.77372900	0.27442300
O	-1.83570700	2.07752200	-0.25713300
H	-2.42058800	1.30974300	-0.14893200
H	-0.98336400	-0.68525100	0.05640400
H	2.89726800	-1.07809900	-1.86224400
O	2.82476500	-0.28462700	-1.31742900
H	1.86891800	-0.09378500	-1.27231100
H	2.98439400	-0.17022200	0.57568200
O	2.57436200	-0.00439300	1.44854600
H	3.17689200	0.59608000	1.90404400
H	-0.18455700	1.17470900	-0.08727800
O	0.33333400	0.34557200	-0.10649500
H	0.95780300	0.37727800	0.65038000
Cl	-2.18992800	-1.25157500	0.10411300

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**W4-19A**

H	0.42684100	0.00199700	1.35586600
O	-0.50117100	0.00121900	1.71897900
H	-0.40490600	0.00258100	2.68030100
H	0.68252300	0.00030700	-1.09890200
H	-1.16596300	1.41543500	0.67940800
O	-1.41098700	1.85805100	-0.16128900
H	-0.98081400	2.72309200	-0.12363600
H	-0.96913000	-2.72510900	-0.11963100
O	-1.40433600	-1.86263300	-0.15861500
H	-1.16183700	-1.41747900	0.68142800
H	-0.73897000	-0.79421800	-1.22622000
O	-0.27064600	-0.00141500	-1.63324900
H	-0.74133700	0.79048700	-1.22739100
Cl	1.98533600	0.00241900	0.01601000

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**W4-20A**

H	-0.52803400	0.25315200	-0.95802900
H	-1.89384800	0.16325400	0.89859000
O	-1.94920800	1.12241600	1.10479600
H	-2.89456100	1.31967100	1.13743700
H	1.06324900	-1.45164800	0.36407300
O	1.95954400	-1.20770000	0.69293500
H	1.96021200	-1.47885800	1.61993400
H	2.78081400	1.47258100	-0.68747000
O	2.04366900	1.34266500	-0.07697800
H	2.13573300	0.41298300	0.26714100
H	0.61623200	1.40114500	-0.64356100
O	-0.35486900	1.30130700	-0.95849600
H	-0.95425200	1.55177900	-0.19579000
Cl	-0.93403700	-1.41844500	-0.46472900

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**W4-21A**

H	2.40701200	0.37154300	-0.01783000
H	1.72720700	2.39534500	-0.90905700
O	1.61870700	1.88591800	-0.09513100
H	0.71874500	1.49726000	-0.14726100
H	-3.40927900	0.00679400	-2.02784200
O	-3.06379800	-0.47883700	-1.26898000
H	-2.10909200	-0.27941700	-1.24602400
H	-3.23212000	-0.14423600	0.61230300

O	-2.78057200	0.09003600	1.44695400
H	-3.12157600	-0.52609700	2.10682900
H	0.12859600	-0.60027600	0.02770000
O	-0.51549500	0.11160800	-0.11611600
H	-1.13298400	0.06704800	0.64685300
Cl	2.70310300	-0.92104500	0.07179400

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**W4-22A**

H	3.52096000	0.00181900	-0.14890900
O	2.70540000	0.00146900	-0.66945900
H	3.00763800	0.00292400	-1.58822400
H	1.37308200	-1.40795000	-0.11467800
O	0.67862000	-1.94726500	0.30045800
H	-0.04012500	-1.93165300	-0.35072700
H	-1.51893100	-0.00105600	0.45195400
H	-0.17939400	-0.76815600	1.53955900
O	-0.75299700	-0.00231700	1.75830700
H	-0.18045700	0.76487100	1.54159600
H	1.37108100	1.40859000	-0.11249500
O	0.67640500	1.94694800	0.30350400
H	-0.04299300	1.93053700	-0.34696500
Cl	-1.98648800	0.00055300	-0.84785800

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**HCl-(H<sub>2</sub>O)<sub>5</sub>**

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**W5-1A**

O	0.37811200	-0.42622000	1.56236300
H	-0.11537100	-1.05759700	1.00173700
H	-0.09388000	0.41492000	1.40789000
O	0.13521900	0.52489100	-1.74295100
H	-0.23773200	-0.35878500	-1.56171700
H	1.07728900	0.42312500	-1.52359600
O	-1.17776500	-1.69671100	-0.47384200
H	-2.04674500	-1.27770900	-0.26939600
H	-1.37269800	-2.60477900	-0.73611300
O	-1.08869100	1.72581400	0.32506100
H	-1.04556800	2.68999300	0.34039000
H	-0.61204900	1.44430600	-0.50094000
O	-3.23197300	-0.03674600	0.16970500
H	-2.63681600	0.73236700	0.29824200
H	-3.74975300	-0.09498100	0.98241300
H	1.77290000	-0.23855400	0.81666200
Cl	2.87889400	-0.04709000	0.06010200

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**W5-2A**

O	-2.42846000	1.33381700	-0.09970900
O	-1.94592500	-0.99414900	-1.31557200
O	-0.21378500	1.16318000	1.21172300
O	1.68877500	1.99731200	-0.30285100
O	2.56483400	-0.45972200	-0.88904200
H	-3.26174600	1.36360000	0.38748700
H	-2.42931700	0.46917900	-0.58790200
H	-1.25503600	-1.35898900	-0.71441700
H	-2.50938300	-1.74669700	-1.53422000
H	-0.04074600	0.13498100	1.17074900
H	0.50762200	1.57357400	0.61529700
H	-1.10994200	1.28987000	0.74672800
H	1.46421400	2.44747400	-1.12774400
H	2.11567200	1.14158600	-0.57680900

H	1.87766600	-0.98376500	-0.41555000
H	3.40260200	-0.80097400	-0.55033400
Cl	0.23028700	-1.63843100	0.80884200

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**W5-3A**

O	0.92555500	-2.29638400	-0.00731200
H	0.61357500	-2.61682100	-0.86297900
H	1.74006600	-1.77385800	-0.21026200
H	-2.16221000	-0.41426200	0.19690800
O	-0.86076400	-0.81887500	1.29303000
H	-1.05461900	-1.23589200	2.14213000
H	-0.19607400	-1.40866000	0.84143500
O	3.10842700	-0.74273500	-0.42303700
H	2.88282000	0.21783100	-0.39317000
H	3.70161100	-0.83857900	-1.17771300
O	2.34714700	1.87088200	-0.30126800
H	1.41653700	1.92127500	0.01972100
H	2.83540900	2.47419200	0.27236000
O	-0.21216300	1.86786000	0.66831900
H	-0.40511800	0.97804400	1.02228900
H	-0.95039000	2.03395400	0.06515200
Cl	-2.99336600	0.09510600	-0.69139600

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**W5-4A**

O	0.83374300	1.56804400	0.85125200
H	1.63917700	1.41084300	0.29288500
H	1.12582000	2.13769200	1.57401400
O	0.26833800	-1.25672100	1.08783400
H	0.35534800	-0.28983900	1.17941800
H	-0.63166800	-1.37919100	0.74487200
H	-2.31586500	0.41436400	-0.31222200
O	-1.65252400	1.94013400	-0.27428100
H	-0.73069500	1.90272100	0.06576200
H	-1.59196200	2.36766700	-1.13858000
O	2.97115100	0.87139900	-0.61290500
H	2.89710500	-0.11506700	-0.61704700
H	3.08920600	1.11967000	-1.53792200
O	2.44164900	-1.77782600	-0.46835400
H	1.62537500	-1.72922300	0.08497500
H	3.00821700	-2.42209000	-0.02672400
Cl	-2.78640600	-0.83398800	-0.29281100

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**W5-5A**

O	-1.84409700	0.23338400	1.39938000
H	-1.23094000	-0.54997300	1.48105300
H	-2.42172600	0.20417400	2.17169400
O	-0.04536000	2.00991900	0.15640600
H	-0.54058400	1.90070800	-0.67334100
H	-0.63634900	1.57345700	0.80334800
H	1.28437000	1.13443100	0.06377300
O	-2.02449500	0.46558100	-1.35311700
H	-2.26470000	0.32617900	-0.41303500
H	-2.85777400	0.47048700	-1.84051600
O	-0.09469300	-1.76475700	1.29210400
H	-0.06954000	-1.86226000	0.31088300
H	0.79546500	-1.44164100	1.49641600
O	-0.04770400	-1.61647100	-1.47318900
H	0.79740300	-1.14901100	-1.56086500
H	-0.71819400	-0.92195300	-1.61927400
Cl	2.37137400	0.33495000	-0.02310600

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**W5-6A**

H	-0.14421700	-0.03679000	1.41147900
O	-0.72597800	-1.37502500	-1.59893200
H	-0.12037900	-0.83319400	-2.12716100
H	-0.17211700	-1.61797300	-0.82407800
O	-2.57094300	0.03660800	-0.28564600
H	-1.98933600	-0.52746800	-0.86538100
H	-3.34879000	-0.49870100	-0.08357300
O	1.76242700	0.51249700	-1.29506100
H	1.70426100	-0.14059500	-0.55321800
H	2.70040500	0.53636900	-1.52669100
O	-0.82683500	0.75781900	1.45822100
H	-0.36781000	1.51286600	0.96005300
H	-1.59746600	0.46669000	0.85734300
O	0.47474300	2.49945000	0.03917800
H	-0.00289100	3.08633600	-0.56120600
H	1.01493200	1.90503300	-0.53781400
Cl	1.02447600	-1.37078700	1.01812800

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**W5-7A**

O	-0.00178600	2.03844600	1.18293000
H	0.75931500	2.23269200	0.61750900
H	0.21558900	1.16057200	1.55051700
O	-1.26631300	-2.13889600	0.67106700
H	-2.16997900	-2.04809400	0.99928800
H	-1.28327900	-1.72982400	-0.23245700
O	-1.14036600	-0.78988400	-1.67428700
H	-1.51194000	0.07282500	-1.38672300
H	-0.21066300	-0.59652800	-1.86573400
O	-2.17194900	1.44277900	-0.42802100
H	-2.62269600	2.22817900	-0.75993800
H	-1.45228200	1.77581400	0.15363800
H	1.59319000	-0.36860000	0.26831800
O	0.69512500	-0.68677500	1.68275600
H	-0.06474800	-1.27738000	1.41075800
H	1.15551200	-1.15233900	2.39316200
Cl	2.15731100	0.04572500	-0.86023000

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**W5-8A**

O	-0.73814800	1.63463300	0.89460800
H	0.05688100	1.90882200	0.37019000
H	-0.78713700	2.25512000	1.63297500
O	-0.00672900	-1.10055100	1.09270300
H	-0.29475400	-0.17053800	1.20071900
H	-0.71547600	-1.50884100	0.53466000
O	-2.07491600	-1.90679600	-0.47949200
H	-2.52873400	-1.04092400	-0.57513400
H	-2.74795700	-2.51133700	-0.14288500
O	-2.97906000	0.70441600	-0.50861600
H	-2.24061800	1.17114200	-0.06652800
H	-3.16098300	1.21458500	-1.30727900
O	1.51292200	2.11147900	-0.50318900
H	1.96169500	1.24015500	-0.48162800
H	1.51504100	2.35888900	-1.43678600
H	1.22137600	-1.05157700	0.41675200
Cl	2.47106600	-0.90652600	-0.24195100

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**W5-9A**

O	0.56389100	0.90876900	-1.62617000
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H	-0.25625700	0.34122300	-1.74257300
H	0.86328900	1.14703600	-2.51303900
O	-0.12146900	2.12908800	0.84604200
H	0.64118100	1.85208400	1.37354400
H	0.15778000	1.93795600	-0.07000700
O	-2.22145600	0.36969300	1.05550900
H	-1.53252900	1.07371200	1.09022300
H	-2.92732700	0.67002200	1.64093900
H	1.61305300	0.08482300	-0.58460600
O	-1.58948500	-0.60881800	-1.61997000
H	-1.27667000	-1.34246800	-1.04629300
H	-2.17885400	-0.13990900	-1.00363500
O	-0.77341600	-2.08956600	0.60342400
H	-1.23156700	-1.36172600	1.06330000
H	0.16571700	-1.92055000	0.77329800
Cl	2.29986300	-0.47150200	0.40871600

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**W5-10A**

O	0.50196500	1.69273000	-1.18732800
H	1.40760600	1.92087700	-0.93649000
H	0.45565800	0.72594200	-1.04028800
O	0.17698000	-0.94568000	-0.26801100
H	-0.45542600	-0.69388500	0.43708900
H	-0.32026600	-1.63380700	-0.74465600
O	-2.06684300	-0.13530000	1.18670200
H	-2.23092900	-0.11975100	2.13774200
H	-2.05631700	0.81317100	0.90266100
H	1.88791800	-0.81478500	0.13818300
O	-2.25977500	-2.30614200	-0.66646300
H	-2.54545900	-1.59285400	-0.06780800
H	-3.01737000	-2.48476000	-1.23610300
O	-1.70493000	2.37557400	0.26805900
H	-0.88590000	2.26804000	-0.27169500
H	-2.31945700	2.85689100	-0.29923000
Cl	3.11181000	-0.39379600	0.37158400

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**W5-11A**

O	0.93985600	-0.04137500	1.83853500
H	0.25147500	-0.66978600	1.56844300
H	0.66325400	0.78825800	1.40633400
O	1.02854600	0.24372800	-1.75558900
H	0.37659000	-0.47320700	-1.72334400
H	1.80444600	-0.12239800	-1.27510400
H	-1.97557200	-0.40903400	-0.03531300
O	0.08931500	2.03290300	-0.01367700
H	0.41910000	2.92443300	-0.18180000
H	0.46883400	1.46036700	-0.73811700
O	-2.46891100	1.10961700	0.06023800
H	-1.62428100	1.61911200	0.07062500
H	-2.91700900	1.32658500	0.88912800
O	2.99143100	-0.47156100	0.03122500
H	2.38767100	-0.43371600	0.80621400
H	3.56782200	-1.23022400	0.18028600
Cl	-1.41554200	-1.63334600	-0.13254200

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**W5-12A**

O	-1.20636300	-0.55295400	-1.67600600
H	-0.70827500	-1.15087400	-1.09071900
H	-0.70208000	0.27559800	-1.61194800
O	-1.12115000	0.47419500	1.63681300

H	-0.73414300	-0.41565700	1.56593500
H	-2.01220600	0.36874000	1.23904100
O	0.28922000	-1.85038400	0.51544100
H	1.19842100	-1.51670300	0.40369800
H	0.39442100	-2.78531100	0.73482000
O	0.29487400	1.61633900	-0.28890900
H	0.32795900	2.58055700	-0.23084600
H	-0.25680000	1.30688800	0.48940800
H	1.72256900	0.86991100	-0.18440300
O	-3.29500700	0.22200600	-0.04909300
H	-2.70381200	-0.13314100	-0.75083100
H	-4.12187200	-0.26829300	-0.12403500
Cl	2.81783600	0.09380400	-0.09094600

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**W5-13A**

O	2.15683800	0.54231000	-1.24365800
H	2.84686700	0.10716900	-0.71197500
H	1.45477600	-0.13277000	-1.22330900
O	0.32961900	-1.42559400	-0.14675200
H	-0.06764400	-0.76195700	0.45456200
H	-0.43115100	-1.90614500	-0.50064700
O	-0.79060300	0.75114000	1.22933300
H	-0.81329700	0.91066500	2.18149800
H	-0.25180300	1.49271400	0.83925200
O	3.06049800	-1.45167300	0.61264900
H	2.15731900	-1.77570800	0.44237300
H	3.60512800	-2.24400400	0.69059500
H	-2.23082300	0.17583800	0.36738400
O	0.84130100	2.50369100	0.07731800
H	1.40669600	1.88232100	-0.44782300
H	0.55926800	3.18489100	-0.54539100
Cl	-3.11862200	-0.48776500	-0.33986100

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**W5-14A**

O	-1.13786600	2.56086400	-0.12335200
H	-1.33251300	3.03427800	-0.94134100
H	-1.81598900	1.84469300	-0.07614600
O	1.45406700	2.12416000	0.36820800
H	1.57433400	2.38494000	1.29068600
H	0.48602500	2.24513500	0.18277500
H	2.06785600	0.75585000	0.01978700
O	0.32155600	-2.57652600	0.37925200
H	0.58107700	-2.90653300	1.24853600
H	1.00830200	-1.92240700	0.15367700
O	-3.03715100	0.63333300	-0.01011400
H	-3.66497000	0.66147800	0.72188400
H	-2.77116000	-0.31350400	-0.07837900
O	-2.30873500	-1.98636700	-0.15972900
H	-2.50627700	-2.47841500	-0.96591600
H	-1.36810200	-2.19288900	0.03547000
Cl	2.67096800	-0.42096100	-0.30736200

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**W5-15A**

H	-1.38292600	-1.22485800	-0.07514300
O	0.16555800	1.55640000	1.15299400
H	0.09160300	0.61860000	1.38900600
H	1.03507900	1.61546400	0.69758100
O	2.55673800	1.51936100	-0.24827800
H	2.60157100	0.58248100	-0.53285200
H	3.39037300	1.67846500	0.21161600



O	2.37016600	-1.19152900	-0.83986200
H	1.53494400	-1.49095300	-0.43771700
H	2.40111900	-1.62707500	-1.70062600
O	-2.39907300	-0.57048300	-0.88896700
H	-2.31034800	0.41751200	-0.75180900
H	-2.26620500	-0.71540300	-1.83610300
O	-1.94843500	1.98686000	-0.43543800
H	-1.15845800	1.93657800	0.16510800
H	-2.58277100	2.55550100	0.01792500
Cl	-0.43021300	-1.80889300	0.76055300

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**W5-16A**

O	-0.45046100	-1.87283100	-0.19516200
H	-0.81785100	-1.44714000	-0.98665100
H	0.49546200	-1.64178900	-0.20223900
O	-2.54941000	-0.08752400	-1.31942400
H	-2.84779600	-0.30001000	-0.41538400
H	-3.33501800	-0.16183000	-1.87536400
O	-2.11032600	-0.50839700	1.41133500
H	-2.37429100	-0.89420700	2.25495900
H	-1.43355700	-1.11831100	1.02479400
H	2.18163200	0.49929000	-0.07056200
O	1.59201100	1.94644200	-0.17192800
H	0.61880400	1.95431300	0.02375500
H	1.98669100	2.58509300	0.43626900
O	-1.06185100	1.88039600	0.25823100
H	-1.35286800	1.20607400	0.90043500
H	-1.51748700	1.59326900	-0.55083300
Cl	2.64921000	-0.77290800	-0.02374100

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**W5-17A**

O	1.31296400	1.84812800	-0.14070000
H	1.48523000	1.35279800	-0.95625200
H	0.35208900	2.04890000	-0.16162400
O	2.34527300	-0.72431300	-1.31510000
H	2.69184600	-0.68266400	-0.40410900
H	3.06569400	-1.08049200	-1.84992300
O	2.07305100	-0.17985600	1.41044500
H	2.43824000	0.01665200	2.28120200
H	1.78194200	0.68747100	1.02349400
O	-1.41910000	2.26807800	-0.02406300
H	-1.87539000	1.40640300	-0.02277000
H	-1.93043800	2.81424000	-0.63414500
H	-1.29403200	-1.26718800	0.07176500
O	0.13766100	-1.81706400	0.20362400
H	0.66727800	-1.33307000	0.87010300
H	0.66393700	-1.68401200	-0.60550200
Cl	-2.56736400	-0.79051900	-0.04034700

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**W5-18A**

O	-1.78539500	-1.44480600	1.30520800
H	-1.78948100	-1.50423500	2.26818200
H	-1.00360300	-0.89499100	1.08280000
O	0.15324200	0.26883400	0.27389100
H	0.72521100	0.85445800	0.80844900
H	-0.45173100	0.85179500	-0.24825400
O	-1.75853200	1.53014700	-1.17006100
H	-2.05736500	2.44382100	-1.08800400
H	-2.53582300	0.97905200	-0.91462800
O	2.40977200	1.28491800	1.54609700

H	2.94184400	0.75032300	0.93349900
H	2.87008500	2.13242100	1.59453100
O	-3.67265400	-0.19246100	-0.25092300
H	-3.10753800	-0.71629400	0.36139500
H	-4.05449700	-0.84372800	-0.85250800
H	1.41865200	-0.45534200	-0.57521700
Cl	2.60428100	-0.89237300	-1.00023200

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**W5-19A**

H	1.94509300	0.78860400	-0.38026400
O	-3.19962200	0.45244400	0.12569200
H	-3.75226800	0.75506100	-0.60559600
H	-2.82737100	-0.40740900	-0.17959300
O	-1.99880800	-1.85993600	-0.68973800
H	-1.12301300	-2.02519800	-0.27644400
H	-2.41498400	-2.72819700	-0.74599500
O	0.44331300	-2.31428200	0.52130500
H	0.45806500	-2.30827000	1.48700700
H	1.18735100	-1.73406100	0.27690500
O	0.90093300	1.78625200	-0.89902900
H	1.25958300	2.66218700	-1.09380000
H	0.15400200	1.93748700	-0.26226200
O	-1.17673600	2.15004400	0.74996600
H	-1.92991900	1.54408100	0.54252100
H	-1.07827800	2.11214900	1.70894000
Cl	2.84524100	-0.13603600	0.06253000

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**W5-20A**

O	2.64437400	-0.78848400	-1.24930100
H	2.75898700	-1.49931600	-1.89216000
H	1.83895300	-0.31168100	-1.53810000
H	-1.85694000	-0.45574600	0.57667400
O	0.23034400	0.62937600	-1.49087800
H	-0.51323600	0.45641800	-2.08448500
H	-0.07237200	0.28534200	-0.61827400
O	-0.27963600	0.04886600	1.15980500
H	-0.06805600	0.98597000	1.33047700
H	0.52642800	-0.46604800	1.40268700
O	2.03283700	-1.36882700	1.38873700
H	2.37355900	-1.21951200	0.47856300
H	2.76043300	-1.12582400	1.97443200
O	0.52661800	2.66565500	0.54665100
H	0.20477900	3.57538700	0.54809900
H	0.45316400	2.36704100	-0.37674200
Cl	-2.92011700	-0.71086600	-0.15537000

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**W5-21A**

O	-2.36630100	0.60403600	-0.78990700
H	-1.72146100	1.23653100	-1.13882700
H	-2.25191300	0.66927200	0.18177600
O	3.13473400	-0.94642000	0.33400800
H	3.78362700	-1.44505400	-0.17889800
H	3.06559600	-0.09126900	-0.11935600
H	0.64694200	0.43937500	-0.00253700
O	-1.76769900	0.35004800	1.94149700
H	-1.57771400	1.06771000	2.55863900
H	-0.91554500	-0.10662100	1.81346600
O	0.38115100	-0.95767000	0.68042000
H	-0.15972000	-1.48113200	0.03428000
H	1.29758500	-1.29620500	0.64311100

O	-1.33241000	-1.89897500	-1.14936300
H	-1.99822700	-2.58480200	-1.01621400
H	-1.82843400	-1.04457400	-1.12829800
Cl	1.01549800	1.61344800	-0.57531700

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**W5-22A**

O	1.74942300	-1.93950200	-0.08794700
H	1.54055800	-2.56170400	-0.79567100
H	1.02137100	-1.28072600	-0.10074700
O	-0.00029100	0.22014700	0.05395000
H	-0.66405400	0.36619100	-0.63817100
H	0.66865400	0.94191100	-0.04545400
O	2.10545600	1.91131100	-0.04619800
H	2.29425200	2.58746100	-0.70808100
H	2.84291500	1.26110100	-0.11693800
H	-2.87402300	-0.01741800	0.39857200
O	3.86819800	-0.17787600	-0.20295100
H	3.21556300	-0.91329700	-0.17233900
H	4.48091000	-0.35786900	0.52080100
O	-2.06567200	0.05329000	1.89102500
H	-1.17143500	0.11342800	1.49137900
H	-2.05425000	-0.75338000	2.42324600
Cl	-3.20925600	0.00443200	-0.88939000

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**W5-23A**

O	-2.86066200	-1.73049400	0.05436200
O	-3.32993800	1.02631600	0.07753500
O	-0.56610200	1.43292800	0.55063200
O	-0.31459700	-0.94556200	-0.56681100
O	2.01604100	1.84935100	-0.45683000
H	-3.50570500	-2.26414200	-0.42451400
H	-3.19608500	-0.80968100	0.00706200
H	-2.41403800	1.35162000	0.19690800
H	-3.69439400	1.56367400	-0.63642800
H	-0.44668900	0.49455700	0.22883100
H	-0.45661600	1.38727100	1.51090700
H	0.45860000	-1.46281700	-0.29716100
H	-1.11667300	-1.47854400	-0.37942500
H	2.55113100	0.30005100	-0.09363000
H	1.07668200	1.87415500	-0.17181300
H	1.99549800	2.02318100	-1.40751100
Cl	2.89355000	-0.94350800	0.24680400

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**W5-24A**

O	2.35429400	0.86826400	-0.54148700
H	2.29397500	0.61095200	0.40315400
H	1.68739800	1.56478200	-0.62961800
O	-3.11303900	-1.03766600	0.24008100
H	-3.09281600	-0.10176500	-0.01374700
H	-3.92261700	-1.38761900	-0.15198400
O	1.76031100	-0.13868500	2.00796700
H	0.98348400	-0.64675300	1.70732800
H	2.29716000	-0.76727300	2.50607800
H	-0.67994900	0.43837600	0.05861000
O	-0.34691000	-1.08600600	0.41402200
H	0.15867000	-1.40975700	-0.37320700
H	-1.25274600	-1.44522700	0.35603800
O	1.45002000	-1.51092800	-1.52631500
H	1.36310500	-1.55473100	-2.48608800
H	1.85346100	-0.62926100	-1.33506900

Cl -1.08979600 1.68049700 -0.28209600

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**W5-25A**

O -2.02292200 -1.32165700 -1.43960000  
H -2.67668900 -1.03184300 -2.08779600  
H -1.24092100 -0.75092800 -1.59276300  
O -0.20260800 2.98576300 -0.30641200  
H -0.17570400 3.91520900 -0.05012300  
H -0.30672800 2.49367900 0.52594000  
O 0.25153200 0.30106200 -1.23514800  
H 0.31997200 1.20736400 -1.57855400  
H 0.00632000 0.46494300 -0.29248000  
O -0.31992800 0.69254600 1.42198400  
H 0.43627300 0.28515500 1.86784100  
H -1.07409500 0.06579000 1.54561900  
O -2.43427000 -0.99568100 1.26686900  
H -2.38913100 -1.19505900 0.30374700  
H -2.52266300 -1.85441100 1.69833700  
H 1.76599100 -0.44944300 -0.63040900  
Cl 2.68723200 -0.96745400 0.15465300

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**W5-26A**

O -0.59048200 -2.11877600 -0.33662100  
O 1.25220300 -0.97567400 1.21122700  
O 0.07329600 1.59597400 0.71691500  
O -1.86233200 0.20243800 -0.74315700  
O -4.59696900 0.55732900 0.08660700  
H -1.14024000 -1.31482200 -0.53611200  
H -0.30267400 -2.44228000 -1.19969200  
H 0.60883700 -1.50331800 0.66285100  
H 1.48477200 -1.52987100 1.96660500  
H 0.49364800 0.80625000 1.10448600  
H 0.78584700 1.99196200 0.19549700  
H -1.28249500 0.82688800 -0.25842900  
H -2.76480000 0.36389300 -0.41682800  
H -5.19765300 0.82454800 -0.62155800  
H -5.03159500 -0.20086700 0.49874100  
H 2.48956500 -0.24700100 0.22809500  
Cl 3.27359100 0.49025300 -0.53549500

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**W5-27A**

O -0.63833300 2.33419600 -0.12804600  
H -0.41134500 2.84378700 -0.91598000  
H -0.02679900 1.56228500 -0.13540800  
O 0.79346200 -0.00948700 0.02192600  
H 1.43729800 -0.24120500 -0.68101900  
H 0.09638800 -0.68815200 -0.01250300  
H -2.52373700 -0.45863200 0.02710300  
O 3.14681800 -0.28946500 -1.38086700  
H 3.52891700 -0.24491400 -0.48139000  
H 3.56823800 -1.05068400 -1.79853700  
O -3.02068200 1.05037700 -0.00427000  
H -2.20663000 1.61212700 -0.05121500  
H -3.46640100 1.31403400 0.81208200  
O 3.26740700 -0.10399400 1.40115500  
H 2.30127200 -0.02145400 1.28970200  
H 3.51426300 0.59968500 2.01358500  
Cl -2.01181400 -1.71058200 0.03849400

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**W5-28A**

O	1.89306600	2.28999600	0.20520900
O	-0.11873700	-1.26258200	0.56681300
O	-0.58129700	1.12287500	-0.34199900
O	-3.30221200	1.17316300	0.01246800
O	-2.86088600	-1.59263100	-0.19643000
H	2.36959500	2.91039700	-0.36112800
H	2.34119800	1.43905800	0.05939200
H	1.51468100	-1.20935500	0.12461700
H	-0.30841000	-0.30804400	0.30315700
H	-0.14044300	-1.27100300	1.53469400
H	-1.47094100	1.47116300	-0.13742500
H	0.09491700	1.79379000	-0.13434500
H	-3.91828700	1.35809300	0.73127900
H	-3.27787200	0.19494000	-0.05838900
H	-1.90166400	-1.68305400	-0.03276000
H	-3.00729900	-2.01768800	-1.05090200
Cl	2.79206100	-0.97205100	-0.17333400

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**W5-29A**

O	-0.81891800	1.80606600	-0.23619100
H	-0.74281600	2.25058000	-1.09140200
H	-0.10003900	1.12371400	-0.22819600
O	0.94503700	-0.22898500	-0.02427800
H	1.64312800	-0.36753200	-0.69607600
H	0.37203000	-1.02566700	-0.02916000
O	-1.01594600	-2.16449900	0.16393200
H	-1.22739300	-2.88360900	-0.44478800
H	-1.81476200	-1.60623500	0.16828700
O	3.38029500	-0.06854900	-1.32819300
H	3.67660700	0.11507400	-0.41353400
H	4.01255100	-0.71006000	-1.67438000
H	-2.17352600	0.99923300	-0.08659600
O	3.30226500	0.28456300	1.43699600
H	2.34925100	0.14100800	1.27783800
H	3.35023300	1.06462800	2.00309800
Cl	-3.27571300	0.22765300	0.06569300

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**W5-30A**

O	-1.61007500	0.89524100	1.14612400
H	-2.45729100	0.97469100	0.67716300
H	-1.29902300	0.01996900	0.83361900
O	-0.75618400	-1.38570400	-0.27463400
H	-0.16362900	-0.90983500	-0.88004800
H	-0.12683700	-1.93470000	0.23419100
H	1.28137300	1.39498500	-0.20671900
O	-3.34649800	-0.32473300	-0.79469800
H	-2.64669100	-0.99880800	-0.74496000
H	-4.13054500	-0.79300500	-1.10459700
O	1.55378700	-2.17909500	1.07794400
H	2.01023100	-1.45643900	0.61248700
H	2.17880600	-2.91495100	1.06847100
O	0.47188600	2.35052900	0.47380200
H	-0.37307400	1.88330600	0.74915300
H	0.88898400	2.64830300	1.29467800
Cl	2.01966900	0.42568100	-0.91539600

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**W5-31A**

H	1.21378600	-0.88099000	-0.73490200
O	-2.27059500	-1.84809600	1.02582500
H	-2.64420900	-2.29641800	1.79372300

H	-2.13028500	-0.92771300	1.30977500
O	-0.39026100	-0.92514600	-0.93970300
H	-0.81438400	-1.76406400	-0.69154900
H	-0.68718400	-0.32934600	-0.20651800
O	-1.31301100	0.84510600	0.92713100
H	-1.63643700	1.41782400	0.20850400
H	-0.48147400	1.25661700	1.24732500
O	1.26494400	1.57644400	1.63571800
H	1.80106200	0.97423300	1.08938700
H	1.67612700	2.44183200	1.51429500
O	-1.71380300	1.52479000	-1.78687500
H	-2.33533600	1.72606100	-2.49682200
H	-1.38755900	0.62886700	-1.97727700
Cl	2.51810000	-0.68421700	-0.46780600

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**W5-32A**

O	2.82878500	-0.14014200	0.54665700
H	3.71242600	-0.43616900	0.29698400
H	2.25407800	-0.94361900	0.46946300
H	-1.05829000	0.61051200	-0.84933500
O	1.18867100	-2.25840800	0.27059200
H	0.33138100	-1.96458500	-0.11397500
H	0.93043800	-2.75697000	1.05636800
O	-0.88116700	1.62157900	-0.60493300
H	0.13437500	1.76694600	-0.53793200
H	-1.28378400	1.63738000	0.31185200
O	1.62937000	2.00424500	-0.45570000
H	2.04856700	2.25100600	-1.28987200
H	2.13883000	1.21728200	-0.11700900
O	-2.03351000	0.86031900	1.61241300
H	-2.08267300	0.00576500	1.12867100
H	-2.94331900	1.05332600	1.87462900
Cl	-1.53171900	-1.12597700	-0.77541600

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**W5-33A**

O	-1.57347400	-0.34315900	1.93980900
H	-1.81746600	-1.18608400	2.34498100
H	-0.58863200	-0.34846700	1.89771200
O	2.57400000	-1.85418000	-0.44968700
H	3.08920400	-2.45634700	-0.99936900
H	2.04939700	-1.32432800	-1.07489700
O	1.09816700	-0.12947800	1.36306700
H	1.77536700	-0.81740500	1.45893200
H	0.92611600	-0.15477500	0.39432700
O	0.74151200	0.13451100	-1.38170900
H	0.98170900	1.07306100	-1.25990900
H	-0.22041900	0.12825800	-1.52517400
H	-2.12618200	-0.20083100	0.41089300
O	1.52571300	2.40163400	0.04415900
H	2.16776400	3.10915200	0.17621000
H	1.62278500	1.81121900	0.81139100
Cl	-2.51688200	-0.07694600	-0.86824800

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**W5-34A**

O	1.10840300	0.86179000	-1.40888300
H	0.34148100	1.51768400	-1.15033700
H	0.68276600	0.04479000	-1.76068200
O	-2.35090400	-1.43776900	0.14054700
H	-3.14238300	-1.41527200	-0.41133500
H	-1.61632200	-1.63930100	-0.46926900

O	0.14973900	-1.70316900	-1.23818200
H	0.68826200	-1.58229400	-0.41539100
H	0.47438500	-2.52472600	-1.63134400
H	1.47841800	0.48925900	-0.46704300
O	-0.81646400	2.29061500	-0.63853400
H	-0.68773400	3.21993100	-0.40927600
H	-1.03701600	1.80883700	0.22009300
O	-1.21953200	0.78572600	1.45580200
H	-1.73289600	0.01935400	1.12615800
H	-0.33040200	0.41171600	1.61698700
Cl	1.75950100	-0.39573700	1.01561400

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**W5-35A**

O	-0.39157000	1.80144600	0.07001900
H	0.62938400	1.71000100	-0.02316100
H	-0.67200400	1.42753600	0.94572500
O	0.28600600	-2.01707200	0.45093100
H	-0.35789900	-1.62109600	-0.17589700
H	-0.08121100	-1.79108100	1.31752300
O	-1.56092400	0.16160500	1.82567000
H	-1.95870500	-0.14445500	0.97710200
H	-2.30879500	0.32425100	2.41580300
O	2.11699400	1.56073700	-0.24385800
H	2.73218900	2.06679700	0.30124300
H	2.42183100	0.61111000	-0.20172600
H	-0.86645800	1.09716700	-0.58183900
O	2.73326100	-1.00033900	-0.04525100
H	1.86436800	-1.44171000	0.13331800
H	3.11581100	-1.48426300	-0.78768700
Cl	-1.76403800	-0.28266300	-1.22238200

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**W5-36A**

O	-3.37426000	0.62466600	0.64140000
H	-2.93341400	-0.24145900	0.70812600
H	-4.31925500	0.43031000	0.63732300
O	-1.19854400	-1.26056300	0.29731500
H	-1.10520800	-0.46813100	-0.28832100
H	-0.57183500	-1.08037900	1.01689100
H	1.79565200	0.65406500	0.42348900
O	0.88143100	-2.77541400	-0.78021600
H	0.98803900	-2.71393400	-1.73800200
H	-0.01408200	-2.41772500	-0.59610900
O	-1.24566900	1.01863200	-1.19602400
H	-2.03375900	1.31838900	-0.70735200
H	-0.52798100	1.61577200	-0.93261500
O	1.71152100	-0.93590400	1.03074600
H	1.63296300	-1.63422800	0.33650800
H	2.45595300	-1.19782800	1.58802700
Cl	1.79041700	1.90375400	-0.02316100

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**W5-37A**

O	0.38046500	-1.80752300	0.62086500
O	1.95404800	0.24911800	1.10233600
O	-1.53505800	-0.38246500	-0.74535900
O	-4.22035200	-0.59537500	0.20624300
O	2.88107400	-1.72901600	-0.84121400
H	-0.35516600	-1.39476200	0.11213400
H	0.98947900	-2.14862300	-0.05730500
H	1.32146900	-0.52994400	1.08339100
H	2.19838100	0.37903600	2.02813200

H	1.09104500	1.48566200	0.41236900
H	-1.23128000	0.53732900	-0.69065600
H	-2.45358100	-0.37223000	-0.41884900
H	-4.82772100	-1.00922800	-0.42134100
H	-4.29893300	-1.13162500	1.00654200
H	2.92573800	-0.89580400	-0.34213300
H	3.15653200	-1.49605200	-1.73658200
Cl	0.34133000	2.39401900	-0.21874500

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**W5-38A**

O	-2.28402300	-0.20544900	-0.16328900
H	-1.95798000	-0.57118600	0.71467300
H	-1.83604600	-0.80371800	-0.83449100
O	3.80743800	-0.09166300	0.03067300
H	4.02789700	0.34173800	-0.80539700
H	4.15170200	0.50824300	0.70627800
O	-0.98243300	-1.14776600	1.93323100
H	-0.11071700	-0.96796100	1.51197900
H	-0.98895300	-0.60506200	2.73315600
O	-0.68780200	-1.66954300	-1.66255200
H	-0.69861500	-2.63500300	-1.67606500
H	0.10076900	-1.41587600	-1.12912600
O	1.01880500	-0.52277300	0.15341200
H	0.66727000	0.39325900	0.01269200
H	1.99115200	-0.42184500	0.14743900
H	-1.72019500	0.74396600	-0.23013300
Cl	-0.62365700	2.03123500	-0.20487100

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**W5-39A**

O	3.71625200	-0.92132600	0.53135500
H	2.74366400	-0.98646100	0.57049200
H	4.01978300	-1.10207600	1.42939400
O	1.01422100	-0.18877400	0.00288200
H	1.53948800	0.47619000	-0.49295900
H	0.43695700	-0.61634100	-0.64918000
O	-2.78034100	1.87642300	0.00628700
H	-2.95923900	1.09933500	-0.54834600
H	-3.62868100	2.33253800	0.07507500
O	-1.22385800	0.17139800	1.58318600
H	-1.69089300	0.99091500	1.32209500
H	-0.31366000	0.27399400	1.22851200
O	3.07885900	1.41316000	-0.85362400
H	3.62748800	0.72581600	-0.42551700
H	3.48543500	1.56544900	-1.71547900
H	-1.73241500	-0.70342800	0.50069600
Cl	-2.11582300	-1.34488100	-0.67385200

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**W5-40A**

H	-1.79427000	-0.62178700	-0.05948000
O	-0.26309300	0.02293000	-0.18767100
H	-0.53489800	0.95523100	-0.06948300
H	0.32889400	-0.19184000	0.55940400
O	3.44834800	1.13344000	0.10568900
H	3.16574000	0.58212500	0.85591400
H	4.27574600	1.54268900	0.38637200
O	2.25043900	-1.00631200	-1.39676100
H	2.81061900	-0.21602600	-1.29337700
H	1.35878200	-0.63440000	-1.50731200
O	-1.89024800	2.27185000	-0.08670500
H	-2.66254200	1.68967500	0.00003200



H	-2.07745300	3.02131300	0.49240900
O	1.93161200	-0.97043200	1.29309500
H	2.11495500	-1.26613200	0.36763100
H	1.98000600	-1.76104100	1.84445100
Cl	-3.10482700	-0.86538900	0.03542700

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**W5-41A**

O	-2.54111000	-1.78227800	0.08944100
H	-1.58305200	-1.58117600	0.01044200
H	-2.75685800	-2.30990500	-0.69102700
O	-0.09007000	-0.51559900	-0.09045300
H	-0.53310500	0.34670100	-0.04196200
H	0.56534200	-0.51038000	0.63414800
O	2.99960500	1.70298900	-0.04783700
H	2.93618500	1.17286900	0.76497800
H	3.52746500	2.47533000	0.18777800
O	2.60422900	-0.81562400	-1.34937100
H	2.89470800	0.11379200	-1.32217000
H	1.63755600	-0.73890800	-1.42122000
H	-2.99928700	-0.13269400	0.02710500
O	2.33670100	-0.69080100	1.34926000
H	2.60711300	-0.97758800	0.44365300
H	2.66371500	-1.36457000	1.95775900
Cl	-3.02556600	1.19512000	-0.00928300

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**W5-42A**

O	2.51232500	0.41274500	-0.85322100
H	1.63163800	0.00523900	-0.79793900
H	3.14180900	-0.29478600	-0.62635600
O	-1.98741200	-1.23361500	1.52291200
H	-1.20542100	-0.75758000	1.16286200
H	-1.75597800	-2.17101600	1.48261700
O	4.45721300	-1.59406800	-0.19024100
H	4.95394100	-1.45911700	0.62761900
H	5.13400500	-1.76324500	-0.85894700
O	-0.28501800	0.33238200	0.03295700
H	0.11770600	1.16075200	0.37624800
H	-1.03135400	0.61355500	-0.51895100
O	1.47047200	2.29713400	0.84245200
H	1.53673400	3.21389600	0.54843300
H	2.07660600	1.79029500	0.25774100
H	-3.02346500	-0.68453700	0.29356100
Cl	-3.58334400	-0.08059200	-0.75210300

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**Cartesian coordinates of various hydrogen bonded HBr-water clusters considered in the present investigation at MP2/aug-cc-pVDZ level of theory.**

**HBr-H<sub>2</sub>O**

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**W1-1B**

O	-2.57087400	0.00003900	-0.09323000
H	-2.96879300	-0.76426600	0.34576500
H	-2.96960700	0.76380300	0.34601600
H	-0.65980800	0.00005000	-0.06588700
Br	0.77614900	0.00000300	0.00342700

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**HBr-(H<sub>2</sub>O)<sub>2</sub>**

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**W2-1B**

H	0.05122800	0.81799900	-0.04333000
O	1.64717700	1.50817400	-0.10897600
H	2.10343800	0.64465500	-0.03060500
O	2.20595100	-1.21954600	0.09387700
H	1.25683000	-1.42474000	0.07502500
H	1.91639700	2.00852600	0.67330000
H	2.59191300	-1.79231800	-0.58166300
Br	-1.10699500	-0.07323300	0.00080200

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**W2-2B**

H	-0.05131100	0.81809400	-0.04360300
O	-1.64737100	1.50723700	-0.10904800
H	-2.10339700	0.64393700	-0.02634700
O	-2.20556100	-1.21948000	0.09406900
H	-1.25695000	-1.42688100	0.07486900
H	-1.91595400	2.01138500	0.67100900
H	-2.59254600	-1.78864000	-0.58394200
Br	1.10696100	-0.07314100	0.00079600

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**W2-3B**

H	-0.05735400	0.81257600	-0.03967900
O	-1.64894300	1.51869200	-0.09250000
H	-2.12603200	0.66915000	-0.00319600
O	-2.18831600	-1.21701900	-0.05831100
H	-1.24484000	-1.43793300	-0.00210100
H	-1.89406200	2.02979800	0.69060200
H	-2.64063300	-1.92464600	0.41765000
Br	1.10460000	-0.07321000	0.00409200

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**HBr-(H<sub>2</sub>O)<sub>3</sub>**

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**W3-1B**

O	2.89837600	-0.27005300	0.03116400
H	3.48485100	-0.24292600	0.79749700
H	2.45372600	0.60701400	0.01700100
H	-0.37207800	-0.97966800	-0.01028600
O	1.36121800	2.02080000	-0.02025800
H	0.45913800	1.65401800	0.02537300
H	1.34683800	2.59417700	-0.79767600

O	0.82208600	-2.00036100	-0.02464700
H	0.86622600	-2.49024000	-0.85761900
H	1.64256000	-1.44451300	-0.00261900
Br	-1.44384900	0.06568700	0.02680700

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**W3-2B**

O	-1.36257800	2.02205400	0.01837400
H	-1.35944700	2.54427300	0.83144100
H	-0.46010200	1.65760300	-0.03425600
H	0.37240300	-0.96644200	0.09508900
O	-2.89879200	-0.26933600	-0.05658600
H	-2.44875400	0.60512900	-0.04767000
H	-3.53426600	-0.21998400	-0.78104000
O	-0.82237600	-1.99058300	0.22720800
H	-0.79306200	-2.65065900	-0.47901300
H	-1.64745200	-1.46723300	0.06846400
Br	1.44401900	0.06857800	-0.03328500

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**W3-3B**

H	0.48402100	-0.00503200	1.00299500
O	1.34616100	-1.94489300	-0.60517100
H	1.28835200	-2.89631100	-0.44429100
H	0.41511600	-1.64073300	-0.70139000
O	1.40529200	1.98724500	-0.47966600
H	0.47197500	1.71468400	-0.62251300
H	1.78592600	2.05626700	-1.36567800
O	1.53651800	-0.03237100	1.12992200
H	1.72007900	-0.84972000	0.56566500
H	1.76719000	0.75868800	0.54208900
Br	-1.20675500	0.02235200	0.01892700

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**HBr-(H<sub>2</sub>O)<sub>4</sub>**

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**W4-1B**

O	-2.44991200	1.64635800	-0.48006100
H	-2.17793700	2.00199200	-1.33559500
H	-2.77300500	0.73407400	-0.67511300
O	-3.03931500	-0.99040600	-0.81577600
H	-2.36618200	-1.38031300	-0.21148400
H	-3.87285000	-1.41363300	-0.57684200
H	0.93996800	0.61782300	0.45814100
O	-0.56622500	1.07933800	1.33860600
H	-1.24789500	1.40884800	0.69496500
H	-0.56556700	1.70263200	2.07603500
O	-1.04069700	-1.70025900	0.93443700
H	-0.85649400	-0.81103500	1.29306100
H	-0.20221500	-1.95165700	0.52102000
Br	1.99689600	-0.03397100	-0.28748100

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**W4-2B**

H	1.37092100	-0.97612500	1.18093700
O	0.95430500	-0.25653700	1.72456300
H	0.96513200	-0.56520200	2.63960500
H	1.71358400	-2.70713000	-0.40581300
O	2.03961700	-1.84231500	-0.12782900

H	1.80476800	-1.22404400	-0.86457200
H	1.71617800	1.31287700	0.96040000
O	1.93809900	1.94308000	0.24831000
H	2.81762200	2.27467000	0.46766400
H	-0.63843200	-0.08198900	0.84463400
H	0.38158900	0.22869200	-1.85327800
O	1.34806100	0.16253300	-1.83338300
H	1.61128600	0.90234800	-1.24552800
Br	-1.77095200	0.02233800	-0.05192400

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**W4-3B**

H	-1.49286000	-0.91367500	1.19687100
O	-0.99797000	-0.24225300	1.73419200
H	-0.93910000	-0.60080200	2.62887900
H	-3.03624500	-2.04368400	-0.27228800
O	-2.11555800	-1.78984000	-0.13571700
H	-1.90732000	-1.14851400	-0.86031500
H	0.60177400	-0.14651500	0.80920400
H	-2.39658900	2.60214000	0.50615800
O	-1.64651700	2.05139800	0.25155500
H	-1.52630200	1.41754500	0.98401300
H	-1.48777600	0.96289600	-1.23860400
O	-1.35281700	0.19371400	-1.83057900
H	-0.38870200	0.13575000	-1.90686200
Br	1.75645700	-0.05626500	-0.05721900

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**W4-4B**

O	2.55591800	1.62138900	-0.29061500
H	2.76076500	1.87079900	-1.20023300
H	2.79150900	0.66581000	-0.22400100
H	-0.86217900	1.04865400	0.18672900
O	3.06338300	-1.03130600	0.05801400
H	3.67649600	-1.55914200	-0.46741800
H	2.23503900	-1.56057900	0.09534100
O	0.06126900	2.20910500	0.46686200
H	0.10085200	2.42237200	1.40950600
H	0.99549800	1.99107600	0.20096700
H	-0.06647400	-1.79373200	0.03634000
O	0.68195100	-2.40049400	0.19068200
H	0.46465500	-2.82807300	1.02935100
Br	-1.79989500	-0.09847800	-0.12760400

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**W4-5B**

O	2.55556700	1.62086200	0.29281900
H	2.79135600	0.66539800	0.22485800
H	2.75943000	1.86891200	1.20302500
O	3.06369900	-1.03093700	-0.06021700
H	2.23510700	-1.55991200	-0.09632400
H	3.67714600	-1.55883600	0.46478300
O	0.68153900	-2.39965500	-0.18915200
H	-0.06683700	-1.79274600	-0.03514300
H	0.46357500	-2.82870800	-1.02688300
O	0.06198200	2.20786400	-0.46808000
H	0.99598200	1.99040400	-0.20082900
H	0.10247100	2.41955400	-1.41104800
H	-0.86161100	1.04851000	-0.18741400

Br -1.79996900 -0.09821900 0.12748600

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**W4-6B**

O -2.55546700 1.62094200 -0.29261200  
H -2.79122500 0.66546100 -0.22486700  
H -2.75901500 1.86909700 -1.20286200  
O -3.06345500 -1.03102400 0.05993700  
H -2.23492900 -1.56010400 0.09622400  
H -3.67678700 -1.55871600 -0.46540400  
O -0.68150600 -2.39970500 0.18946000  
H 0.06685700 -1.79279900 0.03535500  
H -0.46348800 -2.82871200 1.02719900  
O -0.06187300 2.20792000 0.46808400  
H -0.99591200 1.99042500 0.20094000  
H -0.10233200 2.42009100 1.41094500  
H 0.86157100 1.04858500 0.18748300  
Br 1.79981900 -0.09824000 -0.12754200

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**W4-7B**

O 3.07505200 0.94967700 -0.04945200  
H 2.26008100 1.49019600 -0.15391400  
H 3.58529100 1.10883900 -0.85310500  
O 0.72485400 2.36924600 -0.28431900  
H -0.04825600 1.77845200 -0.21835100  
H 0.54719100 3.06282300 0.36414800  
H -0.82598800 -0.98147900 -0.33323500  
O 2.41880800 -1.61167400 0.57475800  
H 2.70529800 -0.69125100 0.35760200  
H 2.42278300 -1.64964800 1.53927600  
O 0.17441700 -2.00035300 -0.81657300  
H 0.99777900 -1.93072300 -0.26075300  
H -0.14225100 -2.90862800 -0.71668600  
Br -1.78991400 0.08760700 0.13942000

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**W4-8B**

O 0.04732600 2.24824000 0.41097300  
H 0.02668900 2.43571600 1.35971300  
H 0.99430400 2.02710000 0.20679700  
H -0.86791200 1.06206100 0.11593300  
O 2.56293600 1.57885300 -0.22914200  
H 3.35002300 2.01306300 0.12033500  
H 2.77066400 0.61365900 -0.22663400  
O 3.03343400 -1.09879700 -0.20047500  
H 2.21550300 -1.58423600 0.04907900  
H 3.30952600 -1.50241700 -1.03285600  
O 0.67302400 -2.36323400 0.43404300  
H 0.49743300 -2.72406000 1.31238500  
H -0.08541500 -1.77579700 0.25700200  
Br -1.79270200 -0.09958800 -0.15671200

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**W4-9B**

O 0.80337500 -2.27397800 0.44670300  
H 0.01587600 -1.75637600 0.19674200  
H 0.65299400 -2.48852500 1.37687200  
H -0.83441500 0.87275400 0.46608600  
O 0.17807200 1.77448700 1.13332700

H	0.94154500	1.83112900	0.49493500
H	-0.13693400	2.68046300	1.25762300
O	3.08645100	-0.82933600	-0.10387800
H	2.30639000	-1.39720400	0.08571000
H	3.67265400	-1.37116800	-0.64535100
O	2.20271600	1.69320600	-0.60570500
H	2.59588400	0.79543600	-0.48796600
H	1.92173800	1.71491700	-1.52955500
Br	-1.75144700	-0.10847000	-0.23367600

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**W4-10B**

O	-0.17410100	2.20404800	-0.24348700
H	-1.07083800	1.93644600	0.08607400
H	-0.29925800	2.40272900	-1.18207000
O	-2.54717100	1.34800300	0.69541000
H	-2.83669900	0.54606500	0.20236600
H	-3.33152400	1.90098200	0.79030900
O	-2.87472000	-0.94326900	-0.71753900
H	-2.15496400	-1.51186300	-0.36037000
H	-3.60828100	-1.54148300	-0.90160000
H	0.82789400	1.04179400	-0.11118300
O	-0.73240100	-2.31370900	0.32608300
H	0.05506300	-1.76382600	0.15476400
H	-0.73162600	-2.41449100	1.28729800
Br	1.82221100	-0.08448400	-0.01283800

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**W4-11B**

O	2.84451800	0.15095800	-0.24574200
H	3.46790800	-0.18124900	-0.90476200
H	2.44925000	-0.65505900	0.18796900
H	0.07183300	0.69110100	-0.95795800
O	1.49807900	-1.89408000	0.78835200
H	0.57742100	-1.65076300	0.53626300
H	1.44964800	-2.06586100	1.73783900
O	0.79114700	1.43869800	-1.00197300
H	0.48625500	1.99432700	-0.21746700
H	1.66973800	0.96478500	-0.73690300
H	-0.93567400	1.46769200	1.05187000
O	-0.40159000	2.28987300	1.13886700
H	-1.04928200	3.00640000	1.17907600
Br	-1.31555200	-0.55585600	-0.20891300

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**W4-12B**

H	-0.11216900	-0.00249200	1.39868100
O	-1.04825000	-0.00142500	1.73966400
H	-0.97175600	-0.00258600	2.70319600
H	0.07558300	0.00011600	-1.21910800
H	-1.66342000	1.42200000	0.69599800
O	-1.88787100	1.87674700	-0.14481400
H	-1.37580100	2.69744600	-0.12614500
H	-1.39886100	-2.69579000	-0.13081100
O	-1.90034200	-1.86860700	-0.14838200
H	-1.67072700	-1.41761800	0.69311500
H	-1.31995000	-0.79693600	-1.20336400
O	-0.88712500	0.00211400	-1.65357100
H	-1.31680700	0.80205900	-1.20179200

Br 1.58693200 -0.00219500 0.00134500

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**W4-13B**

H 0.90642600 1.02817500 -0.15036600  
O 0.09425400 2.19418000 -0.17538500  
H -0.79114300 1.90035400 0.19832400  
H 0.43655400 2.86673900 0.43125100  
O -2.91530500 -0.73191600 -1.16330100  
H -2.58483200 -0.82843000 -2.06545900  
H -2.31241700 -1.26785400 -0.61546000  
O -1.19625900 -1.52496300 0.98015600  
H -0.26597000 -1.34385900 0.73874600  
H -1.15712300 -2.29488200 1.56198900  
O -2.18070800 1.21442800 0.73016100  
H -1.92542900 0.42120800 1.23262200  
H -2.61499800 0.80814600 -0.04760500  
Br 1.71123100 -0.30009800 -0.12163100

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**W4-14B**

O 1.63122500 -1.88182900 0.66998700  
H 1.60443400 -2.21273800 1.57695500  
H 0.69306700 -1.66924900 0.45558700  
H 0.04042900 0.67824800 -0.94130400  
O -0.72210000 2.40541600 0.95506300  
H -1.17608800 1.53367500 0.92489800  
H -0.45686100 2.51921100 1.87747600  
O 2.82773100 0.34974800 -0.13736700  
H 2.49303900 -0.51856400 0.21915300  
H 3.53463700 0.12589000 -0.75666800  
O 0.70893600 1.47325000 -0.99841200  
H 1.60602900 1.07055800 -0.69461600  
H 0.34914300 2.03366200 -0.24098600  
Br -1.26440500 -0.63809600 -0.18099000

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**W4-15B**

H 1.40199100 1.66271200 -0.49507600  
O 1.09540800 2.56228900 -0.21965200  
H 1.22225700 3.11866500 -0.99825900  
H 4.11498200 -0.80786400 1.39194100  
O 3.77723000 -1.26675200 0.61158600  
H 4.56809900 -1.54205900 0.12959900  
H -0.51645300 2.33089000 0.31209300  
O -1.43074000 2.05809900 0.58512700  
H -1.47659800 2.23544600 1.53473000  
H -1.50823000 0.49820200 0.28000300  
H 0.89915500 -0.47972300 -0.75445700  
O 1.72385400 0.01448200 -0.89683600  
H 2.39371600 -0.45592400 -0.36675100  
Br -1.49785500 -0.95729400 -0.04787500

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**W4-16B**

H -1.02087800 1.11052300 0.86474300  
O -0.28062200 1.77747700 0.74222700  
H -0.07869500 2.10936300 1.62865000  
H -3.83085200 0.58915200 -1.82504600  
O -4.15681200 0.19661400 -1.00408800

H	-4.94912300	0.70651300	-0.79006100
H	0.86368500	0.97624800	0.22602400
H	-0.12546200	-2.87544100	1.01209200
O	-0.43849000	-2.23582700	0.35958800
H	0.36194900	-1.74139200	0.10346700
H	-1.64536300	-0.93382600	0.79715100
O	-2.11935400	-0.09544400	0.97882300
H	-2.83448300	-0.05045200	0.31779400
Br	1.97775600	0.08476400	-0.31277700

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**W4-17B**

O	-1.58888300	-1.96373100	0.55329500
H	-1.58117200	-2.43816900	1.39419800
H	-0.65101400	-1.70458900	0.40368100
O	0.50944500	2.35449700	1.02277400
H	0.99529700	1.49800000	0.99002500
H	1.19851000	3.03253800	1.00752300
H	-0.06460200	0.64456100	-0.97342400
O	-2.84739300	0.26259300	-0.19347600
H	-2.50265500	-0.59278000	0.18023100
H	-3.37411000	0.66685200	0.50788500
O	-0.74664500	1.42347200	-1.04795100
H	-1.63403300	1.02385200	-0.70702100
H	-0.38227300	2.01063300	-0.31259300
Br	1.29668200	-0.59301500	-0.14764700

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**W4-18B**

O	3.05945600	0.05486800	1.48121200
H	3.03246700	0.78714900	2.10980400
H	3.45119300	0.42948800	0.66724200
O	3.32337900	0.72809400	-1.21739500
H	3.87882400	0.41320500	-1.94078300
H	2.49660400	0.21546500	-1.28490000
O	1.00822600	-0.57835000	-0.23154300
H	0.60746300	-1.47007500	-0.19113400
H	1.58070000	-0.48504000	0.56314800
O	-0.85235700	-2.64683300	-0.06424600
H	-1.56610600	-1.98898900	-0.02610900
H	-1.16236800	-3.30873200	-0.69548400
H	-0.43518000	0.25486500	-0.08028600
Br	-1.83409200	0.70544100	0.03240800

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**W4-19B**

O	-3.05783400	0.05838000	1.48196500
H	-3.45035800	0.42927800	0.66661200
H	-3.02869400	0.79417200	2.10636500
H	0.43451300	0.25481300	-0.08052700
O	-1.00761200	-0.57741600	-0.23044600
H	-0.60801300	-1.46956800	-0.18843700
H	-1.58125500	-0.48238700	0.56333700
O	0.85259700	-2.64661100	-0.06146000
H	1.16266000	-3.30789700	-0.69331100
H	1.56564200	-1.98796800	-0.02377700
O	-3.32534300	0.72320800	-1.21726700
H	-2.49776000	0.21225400	-1.28719100
H	-3.87993400	0.41192900	-1.94284700



Br 1.83396400 0.70528200 0.03135500

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**W4-20B**

H -1.06440700 3.36527300 0.36311800  
O -0.80429000 2.63447500 -0.21218100  
H -1.53173100 1.99451400 -0.14179100  
H -0.46284400 -0.27837600 -0.00302100  
H 3.30205900 -1.30531700 -1.87327700  
O 3.36973500 -0.52822500 -1.30472900  
H 2.46814400 -0.15625300 -1.27456800  
H 3.49363100 -0.50451500 0.59374100  
O 3.09920600 -0.29007000 1.46326800  
H 3.79321200 0.16815800 1.95264400  
H 0.63885400 1.43084300 -0.07939100  
O 1.01378000 0.52869400 -0.12874100  
H 1.60953500 0.42010000 0.64446600  
Br -1.87639700 -0.68266900 0.03649000

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**W4-21B**

H 1.66569100 0.85609900 -0.00249500  
H 0.70154200 2.81414700 -0.78944300  
O 0.66440800 2.26535000 0.00543900  
H -0.17166300 1.75594000 -0.06869200  
H -4.12814300 -0.07050900 -2.00702600  
O -3.71735500 -0.56267800 -1.28585200  
H -2.79102700 -0.25775600 -1.25820700  
H -3.88896400 -0.37269400 0.61553000  
O -3.45119700 -0.14374500 1.45894200  
H -3.70819100 -0.83645200 2.07979700  
H -0.51332900 -0.41099700 -0.03393800  
O -1.23231800 0.23543300 -0.12244600  
H -1.82747200 0.07203600 0.64237700  
Br 2.18723600 -0.51156300 0.01066900

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**HBr-(H<sub>2</sub>O)<sub>5</sub>**

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**W5-1B**

O -2.97139000 0.63024500 0.11785400  
O -1.77850600 -0.99696100 -1.62694300  
O -0.76837500 1.13652100 1.33683300  
O 0.51945600 2.86670600 -0.03927800  
O 2.29352100 1.17222400 -1.09378900  
H -3.68731500 0.21564400 0.61632600  
H -2.68951100 -0.03787700 -0.56135500  
H -0.95581500 -1.21860200 -1.13251500  
H -2.05532200 -1.82887400 -2.03128200  
H -0.22245100 0.28660900 1.13627600  
H -0.30419600 1.87903300 0.80049000  
H -1.67904500 0.96156300 0.90797300  
H 0.06160900 3.30881900 -0.76636800  
H 1.23853200 2.32810100 -0.46827600  
H 1.93443900 0.32181600 -0.75113200  
H 3.21902000 1.16789800 -0.81624800  
Br 0.76521200 -1.31011500 0.38596200

**W5-2B**

H	-0.23968700	-1.19448100	1.32735500
O	1.11230400	-0.10372500	-1.63610600
H	0.13359000	-0.16479200	-1.31675800
H	1.43531800	0.78927400	-1.27005200
O	1.82947200	2.10644000	-0.50785600
H	1.24354200	2.13833100	0.28736600
H	1.68676800	2.94074400	-0.97339000
O	0.13344400	1.69354400	1.57656000
H	-0.57046700	1.22977000	1.05814800
H	-0.34051400	2.33967700	2.11686200
O	0.57541400	-1.34050600	1.85408400
H	1.70250500	-1.73936400	0.67178300
H	0.72775700	-0.46371600	2.24122800
O	2.26912500	-1.81188900	-0.14572000
H	1.60860600	-0.83902600	-1.11454500
H	2.30464000	-2.75086700	-0.36873400
Br	-1.63000400	-0.18961300	-0.33677000

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**W5-3B**

H	0.08725300	-0.23831000	-1.33543400
O	0.51338700	-1.20782200	1.94217700
H	0.67776300	-0.32196900	2.30157800
H	-0.29516700	-1.06610100	1.40262800
O	2.18009300	-1.86287100	-0.02865400
H	1.62017900	-1.70768000	0.78227500
H	2.20904700	-2.81971600	-0.15649700
O	0.19143500	1.82731700	1.43225400
H	-0.51320800	1.33519400	0.94101100
H	-0.26647800	2.58884400	1.81314200
O	1.06527500	-0.25338100	-1.66986700
H	1.45458900	0.63124400	-1.35100000
H	1.51995100	-0.97198400	-1.09729800
O	1.90968100	1.97564900	-0.66862400
H	2.82806700	2.05974200	-0.38120800
H	1.36011900	2.06239400	0.14904400
Br	-1.64460200	-0.15379400	-0.31790100

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**W5-4B**

O	-0.27454300	-0.47090900	1.55579700
H	-0.75545600	-1.08629400	0.96529300
H	-0.73983300	0.37702200	1.40969400
O	-0.54671200	0.59135900	-1.75491300
H	-0.90138600	-0.30331100	-1.59177400
H	0.40368100	0.49569600	-1.56981800
O	-1.80807000	-1.68008000	-0.51909700
H	-2.67983200	-1.27460800	-0.29968300
H	-1.99513600	-2.58366400	-0.80198900
O	-1.72208200	1.70869700	0.38401200
H	-1.66798200	2.67068500	0.44297900
H	-1.26246200	1.46030200	-0.46236500
O	-3.86809200	-0.05068000	0.17950400
H	-3.27752100	0.71691800	0.33333800
H	-4.39013700	-0.13481700	0.98720000
H	1.10088800	-0.26293600	0.84144700
Br	2.34060500	-0.02463100	0.02809300

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**W5-5B**

O	-1.57990200	2.29071900	0.02061400
H	-1.15875400	2.58302400	-0.79762600
H	-2.36480500	1.76422700	-0.26945200
H	1.46030600	0.47362500	0.54091200
O	0.03359600	0.83423000	1.55482900
H	0.12987600	1.26024400	2.41619200
H	-0.57557200	1.41781500	1.02439400
O	-3.69891500	0.72654000	-0.62875100
H	-3.47289600	-0.23216300	-0.56299900
H	-4.19837600	0.81156900	-1.44967300
O	-2.93986300	-1.87963600	-0.39312100
H	-2.05161100	-1.91874000	0.03289100
H	-3.48587800	-2.48217400	0.12672700
O	-0.50503700	-1.85152400	0.85415400
H	-0.36115200	-0.96083400	1.22994100
H	0.28759700	-1.99972000	0.31894100
Br	2.43749200	-0.04798600	-0.39634400

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**W5-6B**

O	-0.73895600	1.97052900	1.35010200
H	0.13542500	2.14682000	0.97399300
H	-0.64065000	1.07312500	1.72232700
O	-1.92258200	-2.15480300	0.36112200
H	-2.87884200	-2.10349200	0.48482000
H	-1.75293400	-1.69180400	-0.49960100
O	-1.32220300	-0.68707500	-1.83426000
H	-1.71640800	0.17831600	-1.58641600
H	-0.36800400	-0.52038200	-1.84109800
O	-2.50535600	1.54322600	-0.73422000
H	-2.83845800	2.36351600	-1.11667600
H	-1.92490500	1.81439800	0.01211800
H	0.98240200	-0.45584300	0.72588500
O	-0.25583900	-0.78838100	1.89414600
H	-0.93015300	-1.34971700	1.41510700
H	0.01177900	-1.29600700	2.67156700
Br	1.88229200	0.02208900	-0.32163300

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**W5-7B**

O	1.68702000	1.58143100	0.82359900
H	2.43141200	1.31298800	0.22423000
H	2.09253200	2.12080200	1.51428300
O	0.82161600	-1.14777500	1.20378800
H	1.01872300	-0.19324500	1.24304700
H	-0.09945100	-1.18329900	0.89867300
H	-1.63521600	0.87592400	-0.19818600
O	-0.77359200	2.31683300	-0.18099000
H	0.14769500	2.13755700	0.11298600
H	-0.69083500	2.72041000	-1.05532200
O	3.63368500	0.59519500	-0.73678000
H	3.45288700	-0.37634500	-0.69292200
H	3.71700800	0.79438000	-1.67732500
O	2.83009500	-1.97155200	-0.44198800
H	2.05919200	-1.80923900	0.15313200
H	3.34900200	-2.65623300	-0.00259500

Br -2.32667300 -0.42105000 -0.16745800

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**W5-8B**

O -2.34838900 0.38284100 1.38645400  
H -1.80025800 -0.44517500 1.49378900  
H -2.92556100 0.42487500 2.15858600  
O -0.46023600 2.01808300 0.10191000  
H -0.95259500 1.89326000 -0.72840900  
H -1.07079700 1.62395000 0.75961100  
H 0.79577200 1.07721500 0.04411000  
O -2.50308400 0.53959100 -1.37313600  
H -2.76029500 0.44614200 -0.43192300  
H -3.32986400 0.60353300 -1.86754300  
O -0.77412900 -1.75485500 1.35048500  
H -0.76781300 -1.89976100 0.37501100  
H 0.14077900 -1.48913800 1.52919400  
O -0.72615200 -1.72463100 -1.42213800  
H 0.15903200 -1.34092600 -1.52365000  
H -1.32785300 -0.97566800 -1.59531800  
Br 1.95243900 0.12552800 -0.01605900

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**W5-9B**

O 0.72471700 1.72306300 1.42395500  
H -0.16039400 1.33814300 1.52181500  
H 1.32655600 0.97433300 1.59745600  
O 2.50055300 -0.54290700 1.37435700  
H 3.32690500 -0.61047200 1.86901200  
H 2.75866300 -0.44778100 0.43363500  
O 2.34726800 -0.38107700 -1.38608700  
H 2.92277100 -0.42503100 -2.15934800  
H 1.80070100 0.44805300 -1.49280500  
H -0.79486900 -1.07825000 -0.04679200  
O 0.77592900 1.75867900 -1.34820800  
H 0.77021800 1.90279500 -0.37259500  
H -0.13909500 1.49305200 -1.52646400  
O 0.45929000 -2.01833400 -0.10697700  
H 0.94980200 -1.89777600 0.72506000  
H 1.07081300 -1.61966500 -0.76124400  
Br -1.95126100 -0.12550800 0.01588400

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**W5-10B**

O -0.26483800 1.29532400 -1.56780500  
H -1.01016700 0.63551300 -1.69635400  
H -0.10197200 1.69919800 -2.43018800  
O -0.81375400 2.00286000 1.12496700  
H 0.02852300 1.73818700 1.52197800  
H -0.62016500 1.99989400 0.16754100  
O -2.67076500 -0.01647200 1.23457600  
H -2.06232400 0.75475700 1.31822800  
H -3.34271300 0.10949800 1.91560300  
H 1.00993200 0.46086300 -0.76946300  
O -2.19659100 -0.50012200 -1.60320600  
H -1.75065000 -1.26762300 -1.18268000  
H -2.77039900 -0.20669100 -0.87398300  
O -1.03903400 -2.20083900 0.28975800  
H -1.52194400 -1.60273900 0.89030800

H	-0.10847300	-1.96362600	0.42062600
Br	1.94657700	-0.20009200	0.13977300

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**W5-11B**

O	-0.69074700	2.33393900	0.23262000
H	0.29440600	2.35316200	0.06914000
H	-0.92306700	3.21982200	0.53991800
O	-1.11363700	0.12537100	1.57160600
H	-0.99842100	1.04461900	1.16840900
H	-1.92215200	-0.27914200	1.09232500
O	-2.93062800	-0.87391500	0.08071600
H	-2.51027900	-0.56570300	-0.76527400
H	-3.87041500	-0.66169800	0.02759100
O	-1.32736300	0.08471500	-1.83713000
H	-1.17125400	1.00332900	-1.56628200
H	-0.51136800	-0.37106800	-1.53598600
O	1.92044400	2.04551500	-0.12683900
H	1.91126800	1.06015100	-0.07409100
H	2.38140800	2.23695000	-0.95430600
H	-0.29371600	-0.38968300	1.17896000
Br	1.16425800	-1.09645000	0.04148000

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**W5-12B**

O	0.30314200	1.71836800	1.28416000
H	-0.61220200	1.94474800	1.06793400
H	0.33842900	0.74854700	1.15177000
O	0.53661500	-0.93271600	0.38334900
H	1.12387300	-0.69568600	-0.36462900
H	1.05444800	-1.62613600	0.82923800
O	2.68225100	-0.16262800	-1.24059300
H	2.77218800	-0.15832400	-2.20159000
H	2.70094400	0.78882900	-0.96711800
H	-1.22996400	-0.73648400	0.03186300
O	2.98568900	-2.32657800	0.60473100
H	3.22991700	-1.61820100	-0.01767000
H	3.78665300	-2.51603100	1.10761200
O	2.40883400	2.36135900	-0.32804600
H	1.62925000	2.26639500	0.26990600
H	3.06597000	2.84337200	0.18862100
Br	-2.54833600	-0.18581300	-0.19213500

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**W5-13B**

O	2.79512600	0.39177100	-1.32075800
H	3.49364200	-0.07693700	-0.83069600
H	2.04670300	-0.22189100	-1.20776700
O	0.90993800	-1.36938400	-0.00454500
H	0.60868800	-0.65197200	0.59167200
H	0.08986600	-1.78976800	-0.29795200
O	0.05870600	0.93707800	1.33892400
H	0.10820800	1.13554900	2.28284000
H	0.62851500	1.61659500	0.88639000
O	3.68086100	-1.61078400	0.54045800
H	2.74137500	-1.85566600	0.45600200
H	4.15629000	-2.44676600	0.61493600
H	-1.50791200	0.45039600	0.54112700
O	1.74707400	2.50649700	0.00594900

H	2.21994500	1.82028300	-0.52951900
H	1.47829100	3.18523600	-0.62524900
Br	-2.55992200	-0.22875700	-0.18177200

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**W5-14B**

O	1.36222300	-0.06733000	1.85232800
H	0.49075900	-0.43271600	1.63032400
H	1.36980500	0.78666300	1.38066600
O	1.44997300	0.03675000	-1.76745700
H	0.59129000	-0.40991300	-1.70561600
H	2.06009600	-0.55877400	-1.27725200
H	-1.60994900	0.62724900	0.01090700
O	1.21825200	2.09487600	-0.08839100
H	1.84064100	2.80426400	-0.29208300
H	1.35819900	1.39997900	-0.79213100
O	-1.49434100	2.21214700	0.05387200
H	-0.51694800	2.35146300	0.02852000
H	-1.78894500	2.57686000	0.90024000
O	3.07957600	-1.25022000	0.03269300
H	2.54882300	-0.97659800	0.81376800
H	3.36226500	-2.15552400	0.20737800
Br	-1.56090000	-0.86350700	-0.04483100

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**W5-15B**

O	-1.83417100	-0.49529500	-1.69392000
H	-1.34940500	-1.11776500	-1.12336100
H	-1.32102500	0.32499700	-1.60034500
O	-1.75889400	0.42793100	1.64620900
H	-1.38362000	-0.46473400	1.55053400
H	-2.65019000	0.34526700	1.24357100
O	-0.40142000	-1.90258600	0.47603300
H	0.52312400	-1.60466700	0.39201000
H	-0.33869400	-2.84697400	0.67053500
O	-0.34140700	1.62994900	-0.23938100
H	-0.29977700	2.59103700	-0.14147900
H	-0.89090400	1.29223600	0.52966100
H	1.08955000	0.88855100	-0.13668600
O	-3.92536200	0.25218800	-0.05709000
H	-3.33316800	-0.08668400	-0.76601600
H	-4.75919300	-0.22150000	-0.15730600
Br	2.30866700	0.04579200	-0.04331200

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**W5-16B**

O	3.11630700	-1.11454000	-1.28137100
H	3.09398200	-1.88439500	-1.86317100
H	2.35417200	-0.56447800	-1.55786100
H	-1.21417400	-0.11661300	0.72263400
O	0.87861900	0.56718700	-1.48805000
H	0.07432500	0.43271300	-2.00842600
H	0.60992100	0.33207600	-0.56846700
O	0.48190000	0.25309600	1.22080500
H	0.79897600	1.17142700	1.30982600
H	1.24378100	-0.32589700	1.46167000
O	2.64021800	-1.39825800	1.43256100
H	2.92555700	-1.36549100	0.49215300
H	3.43246200	-1.19310300	1.94418100

O	1.50915900	2.71782600	0.34078200
H	1.29926900	3.65711400	0.27173200
H	1.34667700	2.35063200	-0.54585800
Br	-2.42784500	-0.30561400	-0.04160600

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**W5-17B**

O	3.06626000	-0.80756000	0.47652300
H	3.84242900	-1.35328600	0.30215800
H	2.30205800	-1.43764300	0.50253200
H	-0.47659700	1.12493200	-0.74181700
O	0.92154300	-2.43986700	0.47535400
H	0.14575400	-1.92903100	0.15153500
H	0.61488400	-2.81033300	1.31323800
O	0.05988200	1.99312500	-0.57250800
H	1.06452200	1.75985200	-0.65900500
H	-0.17249800	2.14451800	0.39619200
O	2.51700800	1.43983400	-0.80404000
H	2.82276200	1.37131200	-1.71772200
H	2.77533300	0.58152300	-0.36502500
O	-0.86515600	1.75328700	1.84041800
H	-1.28495200	0.93573500	1.48753600
H	-1.59693600	2.27434400	2.19767900
Br	-1.58951600	-0.51921300	-0.40552200

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**W5-18B**

O	-1.89465200	2.52311300	-0.12955200
H	-2.08683400	2.97018500	-0.96285500
H	-2.50580800	1.74725800	-0.10904200
O	0.68344000	2.35610100	0.50669500
H	0.72209700	2.55070800	1.45311300
H	-0.28318500	2.37507000	0.26803300
H	1.38989200	1.07603100	0.16460300
O	-0.12055900	-2.57282900	0.51447800
H	0.11750900	-2.86740900	1.40254100
H	0.52839100	-1.87450700	0.30852400
O	-3.62256700	0.44454600	-0.08910100
H	-4.29553300	0.43357700	0.60208000
H	-3.29530400	-0.48436900	-0.13802800
O	-2.74071400	-2.12752000	-0.18265900
H	-2.86045000	-2.62813200	-0.99885000
H	-1.80471600	-2.28464600	0.07221200
Br	2.16955300	-0.17145900	-0.20060600

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**W5-19B**

O	-2.39572900	-0.24682200	1.93783000
H	-2.52683600	0.34237100	2.69050300
H	-1.65586400	0.14617100	1.42663600
O	-0.53846000	0.65797100	0.07777700
H	-0.07181300	1.51738700	0.08954100
H	-1.12624000	0.65627100	-0.71831700
O	-2.36512900	0.34597700	-1.89444800
H	-2.77571800	1.03103100	-2.43575200
H	-3.09992500	-0.03481000	-1.35749700
O	1.46314100	2.57582800	0.35933200
H	2.12030000	1.86462200	0.27678100
H	1.81369600	3.29470600	-0.18209800

O	-4.17306100	-0.67273100	-0.11413300
H	-3.64424000	-0.55952100	0.70823300
H	-4.38983800	-1.61301500	-0.14099800
H	0.86574600	-0.28196300	-0.06441500
Br	2.24470400	-0.78985800	-0.09209900

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**W5-20B**

O	-0.87691700	-1.86949400	-0.21457100
H	-1.28969500	-1.47507300	-1.00005600
H	0.03969200	-1.53990600	-0.22312400
O	-3.13928300	-0.26775300	-1.30364100
H	-3.40534900	-0.50884300	-0.39675600
H	-3.92222400	-0.41128400	-1.84975300
O	-2.61826300	-0.64665300	1.41890500
H	-2.82763600	-1.04826300	2.27044700
H	-1.89991100	-1.19793500	1.01903800
H	1.50634700	0.95573800	-0.07781000
O	0.76007800	2.29599800	-0.18208500
H	-0.20392800	2.15248600	0.01766900
H	1.06904900	2.94296100	0.46685900
O	-1.84117000	1.83479500	0.25984500
H	-2.04128700	1.12648700	0.90072600
H	-2.27055000	1.50069200	-0.54566600
Br	2.19914100	-0.37920600	-0.01169100

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**W5-21B**

O	2.40206600	-1.01470800	-0.70527600
H	1.58884500	-1.49203800	-0.92780100
H	2.34400600	-0.90685600	0.26764500
O	-2.40178200	2.15861600	0.30255000
H	-2.89307100	2.72459300	-0.30691100
H	-2.60767700	1.25300600	0.01860100
H	-0.39309200	0.12741900	0.18236600
O	2.06210600	-0.24153800	1.97828000
H	1.70778200	-0.81820000	2.66715500
H	1.35992500	0.41406300	1.81582900
O	0.24807300	1.43862100	0.58655600
H	0.86325600	1.67590400	-0.15920200
H	-0.55012700	2.00149100	0.50619100
O	1.99490400	1.58134300	-1.41742100
H	2.81697000	2.08700400	-1.42336500
H	2.26522500	0.64000900	-1.27813800
Br	-1.16985700	-1.11671600	-0.20913900

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**W5-22B**

O	-3.34045100	-1.88201100	-0.05270900
O	-4.04560200	0.80059700	0.28041200
O	-1.30698000	1.44282700	0.57456500
O	-0.89630400	-0.83860600	-0.69846100
O	1.09500900	2.25206700	-0.62458000
H	-3.95078600	-2.41429500	-0.57660700
H	-3.75705500	-0.99607700	0.01358500
H	-3.15639700	1.20307400	0.36174400
H	-4.52520700	1.37391300	-0.32989800
H	-1.11386000	0.54172300	0.18959000
H	-1.09916600	1.36465800	1.51636000



H	-0.08430400	-1.30742300	-0.45565800
H	-1.65316200	-1.43838400	-0.52074300
H	1.85143100	0.79047600	-0.23368000
H	0.18783400	2.13333500	-0.26731500
H	0.97752600	2.34255300	-1.58026600
Br	2.40793600	-0.50835900	0.17283000

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**W5-23B**

O	-2.43592900	-1.58636000	-1.41376500
H	-3.19586900	-1.42967900	-1.98776900
H	-1.82027700	-0.84547000	-1.59677900
O	-1.43459400	2.99814800	-0.16764800
H	-1.60055500	3.89318600	0.15107600
H	-1.37233200	2.44888600	0.63273200
O	-0.57301400	0.49383800	-1.30661000
H	-0.71860000	1.40609000	-1.60730900
H	-0.76231900	0.57138600	-0.34093500
O	-0.95757100	0.65593900	1.41651500
H	-0.08558200	0.39507100	1.74713000
H	-1.54351400	-0.12618600	1.56235500
O	-2.65709000	-1.45743000	1.33211900
H	-2.65760700	-1.60656700	0.35894000
H	-2.51124300	-2.32877600	1.72057100
H	1.14563500	0.04629400	-0.79301700
Br	2.27393900	-0.32163800	0.03623200

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**W5-24B**

O	2.09598600	1.74489900	-0.17122600
H	2.16762800	1.23036800	-0.98958900
H	1.18368700	2.10944200	-0.17459200
O	2.76754600	-0.96724400	-1.31975800
H	3.14544900	-0.94200700	-0.42099900
H	3.43050500	-1.40653000	-1.86711100
O	2.59351600	-0.34134900	1.39956900
H	2.97574400	-0.17827600	2.26996700
H	2.41096000	0.54961000	0.99843500
O	-0.51293300	2.63091300	0.00258600
H	-1.08533800	1.84066500	0.00928400
H	-0.93692600	3.23143000	-0.62355700
H	-0.78160400	-1.07017500	0.11310900
O	0.50948400	-1.78920200	0.25440000
H	1.09415200	-1.33583600	0.89964300
H	1.03093300	-1.72363500	-0.56794200
Br	-2.12182800	-0.35797700	-0.02774900

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**W5-25B**

O	-2.38327800	-1.19179700	-0.46974300
H	-2.43380300	-0.83786800	0.44353600
H	-1.55846800	-1.69987200	-0.46885200
O	2.36879500	2.20631700	0.19631400
H	2.62174800	1.28190000	0.04344200
H	3.02905200	2.72858400	-0.27623600
O	-2.16724000	0.17217700	1.97313100
H	-1.53574500	0.83953500	1.64623600
H	-2.86015700	0.67513400	2.41849400
H	0.41457900	0.11860800	0.15739100

O	-0.30122500	1.49751000	0.33662400
H	-0.83331500	1.57983300	-0.49701800
H	0.48619200	2.07049500	0.24862300
O	-2.02028200	1.22002200	-1.68655000
H	-1.86410800	1.17547400	-2.63761900
H	-2.21164400	0.29161100	-1.40465300
Br	1.22204300	-1.12735000	-0.07061600

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**W5-26B**

H	1.24078300	0.90725400	-0.49915200
O	-3.76284200	0.45751300	0.27748500
H	-4.40348000	0.77614300	-0.37037200
H	-3.41848400	-0.38543700	-0.10016500
O	-2.62357100	-1.80418400	-0.73640000
H	-1.75132600	-2.02239500	-0.33950100
H	-3.05607100	-2.65599500	-0.86911600
O	-0.18994200	-2.40246900	0.41968000
H	-0.17048900	-2.46855700	1.38322200
H	0.54896800	-1.79909200	0.21670600
O	0.22274800	1.82287100	-1.04455300
H	0.59927600	2.69545800	-1.22619400
H	-0.48640300	1.96923800	-0.35804200
O	-1.70540900	2.15225300	0.75221700
H	-2.47187200	1.54614400	0.59657300
H	-1.49541700	2.05813500	1.68950300
Br	2.26676100	-0.06939400	0.07226000

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**W5-27B**

O	0.26495100	1.94574400	-0.05506500
H	1.23413100	1.68957800	-0.32561200
H	0.12417900	1.73645300	0.91208400
O	0.70210200	-1.88105700	1.02607900
H	-0.04973100	-1.56732400	0.47752400
H	0.56169100	-1.43288000	1.87235100
O	-0.58248100	0.82976800	2.18469900
H	-1.19864700	0.39046300	1.54917500
H	-1.15232100	1.22869300	2.85643000
O	2.58719600	1.30103500	-0.78688000
H	3.35285200	1.80055100	-0.47674700
H	2.79477500	0.33553800	-0.62566700
H	-0.38660800	1.25305200	-0.47909100
O	2.99104200	-1.24021600	-0.24308800
H	2.17219600	-1.53966900	0.22831400
H	3.12042100	-1.87831200	-0.95592000
Br	-1.66501200	-0.27595300	-0.62968000

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**W5-28B**

O	-1.36975300	-2.12720800	-0.46521200
O	0.38707700	-1.25343900	1.34142100
O	-0.61295000	1.41489900	1.02902300
O	-2.49349600	0.29210400	-0.70811400
O	-5.26931800	0.70431500	-0.05810200
H	-1.86276100	-1.27719400	-0.61567500
H	-1.01823100	-2.36558100	-1.33244900
H	-0.23454500	-1.68825000	0.69569100
H	0.54189100	-1.89603400	2.04517800

H	-0.26519700	0.56647900	1.36154200
H	0.15182600	1.80751200	0.58427200
H	-1.92590300	0.82650400	-0.11345000
H	-3.41094100	0.46762200	-0.43531000
H	-5.79249500	1.08114800	-0.77784300
H	-5.76979600	-0.07302800	0.22279300
H	1.73146600	-0.51498800	0.44625300
Br	2.64920600	0.30915600	-0.31980400

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**W5-29B**

O	-0.03773700	1.18161400	-1.70139100
H	-0.79227400	1.64542300	-1.12457400
H	-0.37225500	0.28394700	-1.95651100
O	-2.38664200	-1.84947900	0.51334800
H	-3.29919900	-1.99325900	0.23412000
H	-1.85928200	-1.86107800	-0.30672100
O	-0.42404800	-1.49389600	-1.55939800
H	0.31639900	-1.35892400	-0.91195200
H	-0.10598600	-2.18266700	-2.15962800
H	0.68987100	0.90797800	-1.00289400
O	-1.81464400	2.12246000	-0.22769800
H	-1.76809900	3.04481200	0.05598800
H	-1.68632800	1.55414000	0.60120900
O	-1.34699900	0.47047100	1.71880800
H	-1.78252700	-0.36688800	1.45551400
H	-0.39372100	0.27359000	1.61672000
Br	1.68954200	-0.09704100	0.38712500

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**W5-30B**

O	0.92880400	2.71525800	0.23117500
O	-0.65152700	-1.17124800	0.64915100
O	-1.33337100	1.15528600	-0.27434600
O	-4.05904500	0.90680600	-0.07721000
O	-3.30934200	-1.79393000	-0.20053400
H	1.28195400	3.36436600	-0.39105000
H	1.50137100	1.93762200	0.11394500
H	0.99249700	-0.93028700	0.20821100
H	-0.92391800	-0.23764400	0.38577600
H	-0.67009500	-1.18159000	1.61712600
H	-2.26966400	1.39623500	-0.13173100
H	-0.75917500	1.91969500	-0.08327600
H	-4.71539100	1.03449500	0.61809400
H	-3.92380300	-0.06396800	-0.12522100
H	-2.35480400	-1.77333600	0.01011500
H	-3.36538200	-2.24904300	-1.05019800
Br	2.36006500	-0.50611200	-0.10850500

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**W5-31B**

O	0.32800900	2.68637900	-0.10271600
H	0.66485000	3.14974800	-0.87985200
H	0.78135100	1.81174000	-0.10745500
O	1.31110000	0.12281400	0.04129500
H	1.89666400	-0.20940900	-0.67265000
H	0.50384500	-0.42048500	0.00370800
H	-2.11959500	0.40165200	0.00590500

O	3.56055800	-0.54785800	-1.39463000
H	3.95412100	-0.59125800	-0.50007300
H	3.83477500	-1.36284900	-1.83293800
O	-2.27476900	1.96605100	-0.01625600
H	-1.35006100	2.32275800	-0.05018700
H	-2.64403800	2.29200400	0.81635900
O	3.73847500	-0.44331900	1.38800500
H	2.80259000	-0.18377600	1.29127000
H	4.11463000	0.18710900	2.01427500
Br	-1.87846100	-1.07627900	0.01674400

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**W5-32B**

O	-0.08772300	1.76178300	-0.37123200
H	-0.03691100	2.13237900	-1.26347300
H	0.62076300	1.06734900	-0.33171600
O	1.65735900	-0.26363000	-0.05943100
H	2.39221400	-0.40758000	-0.68992600
H	1.11213200	-1.07977800	-0.05143600
O	-0.21947900	-2.27947200	0.15415500
H	-0.41212200	-2.98102500	-0.48113300
H	-1.03582500	-1.74721800	0.17912500
O	4.13950900	-0.07670500	-1.26065900
H	4.38969300	0.16341500	-0.34526300
H	4.80657300	-0.71286400	-1.54612100
H	-1.42445100	0.97247700	-0.16621000
O	3.93026700	0.41180900	1.47636000
H	2.99082000	0.22237000	1.28869400
H	3.92549600	1.22234200	2.00016800
Br	-2.64822400	0.13479600	0.05410700

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**W5-33B**

O	1.83636200	-1.22721600	-0.39622500
H	2.01470600	-0.85852400	0.53520600
H	2.02340400	-0.43461200	-1.00567000
O	-2.26245400	2.21439200	0.05808900
H	-2.27571800	1.24919000	-0.08144300
H	-3.12366800	2.41421400	0.44543400
O	2.11112200	0.02673100	1.86316500
H	1.51697000	0.77526200	1.62979500
H	1.70223800	-0.38467500	2.63738300
O	2.05651100	0.99550800	-1.68927800
H	2.87274200	1.49261900	-1.82710700
H	1.51443800	1.51697400	-1.05193600
O	0.46016500	1.66953400	0.41389900
H	-0.08539500	0.85530100	0.26206600
H	-0.24452800	2.33885600	0.48580800
H	0.79946500	-1.32046900	-0.40070200
Br	-1.15223700	-1.05930700	-0.10360100

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**W5-34B**

H	0.75494700	-0.77716000	-0.46304200
O	-2.62207200	-1.82428000	1.36034000
H	-2.94749300	-2.15315400	2.20664300
H	-2.62954500	-0.85440200	1.44209800
O	-0.80496800	-1.07360100	-0.72175400
H	-1.12643700	-1.88624000	-0.29398200

H	-1.20869100	-0.37570100	-0.14518700
O	-2.04770300	0.89871000	0.69559900
H	-2.41066700	1.25982700	-0.13311100
H	-1.31725900	1.49961800	0.95827100
O	0.30784400	2.19172600	1.37343600
H	0.97678400	1.58157900	1.01394700
H	0.59106800	3.06331900	1.06819500
O	-2.40218400	0.92880900	-2.10607300
H	-3.00356400	0.88944900	-2.85948600
H	-1.94848800	0.06900700	-2.09434600
Br	2.13777200	-0.32248700	-0.15749700

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**W5-35B**

O	0.69739500	2.34603200	0.00668600
H	0.87562900	2.87101900	-0.78564600
H	-0.26439600	2.12995700	-0.03431000
O	-3.08357800	-0.39201700	-1.92996600
H	-3.52776200	-0.89995000	-2.61906500
H	-2.48913900	-1.02424900	-1.48965400
O	-1.83518700	1.30555100	0.05487300
H	-2.51902200	1.40286400	-0.62664100
H	-1.53240800	0.38238600	-0.10146400
O	-1.15944700	-1.39276400	-0.06694100
H	-1.42113200	-1.43357600	0.87315600
H	-0.18744600	-1.42623900	-0.06743700
H	1.48237400	0.91586600	-0.04677100
O	-2.12036900	-0.41033600	2.35835000
H	-2.77795600	-0.45843200	3.06229500
H	-2.30412800	0.41793600	1.88203300
Br	2.13356800	-0.41512300	-0.09801500

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**W5-36B**

O	-3.10659300	2.10643400	0.71335500
H	-3.15505700	1.13328600	0.73088000
H	-4.02271800	2.40810000	0.73654200
O	-2.19462900	-0.59283600	0.21521200
H	-1.72666700	0.06091800	-0.36042700
H	-1.54636500	-0.78293300	0.91388300
H	1.31031000	-0.59109300	0.46753900
O	-1.26976400	-3.01754500	-0.81157300
H	-1.10294500	-3.04139800	-1.76236000
H	-1.81859700	-2.21704700	-0.66495100
O	-1.11921400	1.47790200	-1.21100500
H	-1.64608500	2.09672400	-0.67248600
H	-0.19736800	1.61867200	-0.94478000
O	0.33229400	-1.90743900	1.07552800
H	-0.06665600	-2.47263300	0.37100300
H	0.77724900	-2.51186800	1.68386600
Br	2.05880400	0.56477600	-0.01002400

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**W5-37B**

O	0.14178500	2.36895300	0.53426900
O	-1.80243100	0.71211100	1.17638000
O	1.77323100	0.58701900	-0.78359800
O	4.42955800	0.39933100	0.24459200

O	-2.37076200	2.72553200	-0.85956500
H	0.78114700	1.80872000	0.03647100
H	-0.40881400	2.78723100	-0.15065300
H	-1.02006700	1.33565800	1.09298800
H	-2.02358700	0.67678400	2.11665300
H	-1.21661900	-0.71627300	0.54194500
H	1.31802900	-0.26553600	-0.69795400
H	2.66975200	0.43716500	-0.43038300
H	5.11209300	0.69074900	-0.37451000
H	4.56470300	0.94925700	1.02792900
H	-2.56841000	1.95054100	-0.30659100
H	-2.72257400	2.50419100	-1.73080200
Br	-0.62447700	-1.90005900	-0.10347800

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**W5-38B**

H	-1.12011200	-0.31459200	-0.10513200
O	0.45948400	0.19925700	-0.24207300
H	0.26613700	1.15005500	-0.11233300
H	1.00977500	-0.07918800	0.51651700
O	4.25966500	0.90680200	0.15511800
H	3.90021700	0.38261300	0.89177500
H	5.12062900	1.21838300	0.45930200
O	2.87717000	-1.08043900	-1.39966100
H	3.51494700	-0.35473400	-1.27466400
H	2.03324000	-0.61543700	-1.53031400
O	-0.93013300	2.60296400	-0.09276000
H	-1.76553700	2.11520600	-0.00582800
H	-1.01502400	3.34923700	0.51415300
O	2.49549100	-1.03051500	1.28132600
H	2.66955200	-1.33779600	0.35781500
H	2.43696900	-1.82571800	1.82506500
Br	-2.58126300	-0.47064500	0.02423000

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**W5-39B**

O	1.56743200	2.34535300	0.09556600
H	0.65370300	1.99468700	0.01120400
H	1.70677100	2.88426100	-0.69490100
O	-0.68145400	0.74051100	-0.10225500
H	-0.13630200	-0.06185200	-0.06182100
H	-1.32904700	0.64703900	0.62359600
O	-3.35991900	-1.90598900	-0.03360100
H	-3.38828600	-1.36715900	0.77548700
H	-3.75279200	-2.75372200	0.20659500
O	-3.39561200	0.63554300	-1.35264600
H	-3.53285200	-0.32824700	-1.31778600
H	-2.42926400	0.71325300	-1.42796200
H	2.28030000	0.76689600	0.03797900
O	-3.10258100	0.57082000	1.34559300
H	-3.41832500	0.80804800	0.44039700
H	-3.52468700	1.19021200	1.95330100
Br	2.53279600	-0.67380900	-0.00478100

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**W5-40B**

O	-3.25372600	-0.42615500	-0.88514900
H	-2.37966000	-0.01469000	-0.77819400
H	-3.89855800	0.28158700	-0.70729900

O	1.06058800	1.26940800	1.77842300
H	0.31882500	0.77917800	1.35680700
H	0.83414800	2.20419700	1.68071800
O	-5.24293300	1.58028500	-0.36938800
H	-5.78453700	1.45606800	0.42123600
H	-5.88151600	1.73504200	-1.07797000
O	-0.51971600	-0.32339200	0.17825900
H	-0.94237900	-1.14851700	0.50567500
H	0.25839000	-0.61140200	-0.32436700
O	-2.31689000	-2.28349800	0.89861800
H	-2.36018900	-3.20442500	0.61345300
H	-2.88621100	-1.78743400	0.26933200
H	2.21267300	0.70377100	0.64529200
Br	2.93401200	0.03067000	-0.44030800

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**W5-41B**

O	4.09884200	-0.98000300	0.50719900
H	3.16940900	-1.02339700	0.79165600
H	4.62113700	-1.13926000	1.30267500
O	1.33797300	-0.15001300	0.33187100
H	1.84667100	0.32594100	-0.36674600
H	0.62118500	-0.63698800	-0.13262500
O	-1.79815100	2.37938600	-0.14030400
H	-2.03924300	1.50919900	-0.53017300
H	-1.44102200	2.89708400	-0.87405400
O	-0.54788700	0.96944300	1.64461700
H	-0.88450100	1.73596100	1.08160700
H	0.34709100	0.69621300	1.22979300
O	3.24737800	1.03614800	-1.19728600
H	3.86678400	0.43704400	-0.73444100
H	3.42126800	0.90164700	-2.13757300
H	-1.12814500	0.20678200	1.21387800
Br	-1.80302500	-0.91285500	-0.28607900

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