

Supplementary information

Hydrogen bond strengths in microhydrated clusters of HNO and HONO: Energetic insights via molecular tailoring approach

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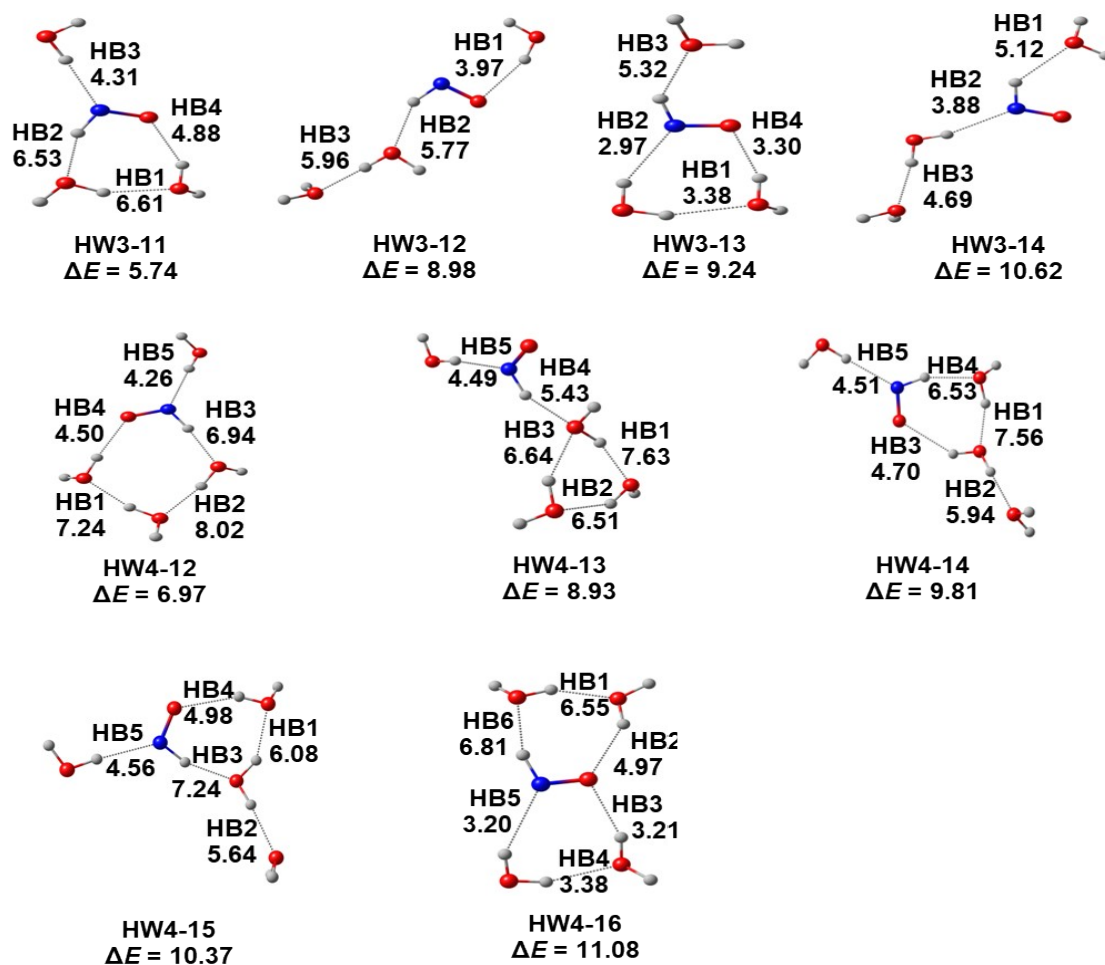


Fig. S1 The MTA-based energies of individual HBs and relative energies (ΔE) of various isomers (with ΔE values above 5 kcal/mol) in each category of $\text{HNO}(\text{H}_2\text{O})_{n=3-4}$. All energy values are in kcal/mol. Also see Fig. 3 and 4 in the main text.

Table S1 The relevant structural parameters *viz.* distance (in Å) and bond angle (in degree), the MTA-based HB energies in complex (E_{HB}^{MTA}), energy in dimer (E^{Dimer}), and cooperativity contribution (E^{Coop}) of all individual HBs in $\text{HNO}(\text{H}_2\text{O})_{n=1-4}$ complexes. All energy values are in kcal/mol.

Complex	HB labels	HB distance	HB angle	E_{HB}^{MTA}	E^{Dimer}	E^{Coop}
HW1-1	HB1	2.17	131	-	5.11	-
HW1-2	HB1	2.12	166	-	3.93	-
HW1-3	HB1	2.13	174	-	2.93	-
HW2-1	HB1	2.02	157	6.02	4.20	1.83
	HB2	2.07	155	5.15	3.32	1.83
	HB3	1.88	153	6.64	4.81	1.83
HW2-2	HB1	2.20	124	5.01	3.56	1.46
	HB2	2.10	144	5.35	3.89	1.46
	HB3	1.92	153	6.28	4.83	1.46
HW2-3	HB1	2.06	140	5.36	4.78	0.59
	HB2	1.91	178	5.68	5.10	0.59
HW2-4	HB1	2.09	173	4.39	3.86	0.53
	HB2	2.03	138	5.16	4.64	0.53
HW2-5	HB1	2.46	149	2.71	2.88	-0.17
	HB2	2.17	149	2.38	2.55	-0.17
	HB3	2.03	161	3.68	3.85	-0.17
HW2-6	HB1	2.10	136	3.67	3.20	0.48
	HB2	2.11	169	5.26	4.78	0.48
HW2-7	HB1	2.17	169	2.65	2.98	-0.33
	HB2	1.98	174	4.80	5.13	-0.33
HW3-1	HB1	1.97	162	6.16	3.85	2.31
	HB2	2.01	147	5.73	3.34	2.40
	HB3	1.82	168	7.72	4.96	2.76
	HB4	1.82	167	7.58	4.91	2.68
HW3-2	HB1	1.80	170	8.13	4.86	3.27
	HB2	1.81	165	7.64	4.85	2.79
	HB3	1.98	178	5.12	2.76	2.36
	HB4	1.95	172	6.53	3.69	2.84
HW3-3	HB1	1.84	154	7.67	4.71	2.96
	HB2	1.91	149	6.84	4.44	2.40
	HB3	2.19	134	6.03	4.10	1.92
	HB4	2.04	167	4.27	3.55	0.72
	HB5	2.23	144	1.77	1.62	0.16
HW3-4	HB1	1.87	153	7.29	4.81	2.47
	HB2	1.95	144	6.59	4.45	2.15
	HB3	1.96	147	6.89	4.87	2.02
	HB4	2.18	132	5.28	5.15	0.13
HW3-5	HB1	1.84	172	7.18	5.00	2.18
	HB2	1.84	172	7.28	5.10	2.18
	HB3	2.33	101	4.63	3.02	1.61
	HB4	2.03	152	4.13	2.53	1.61
HW3-6	HB1	1.85	154	7.65	4.83	2.82
	HB2	1.95	147	6.51	4.33	2.18

	HB3	2.05	144	6.47	4.68	1.79
	HB4	2.40	109	3.39	3.10	0.30
	HB5	2.80	105	0.20	0.55	-0.35
HW3-7	HB1	1.99	145	6.62	4.73	1.89
	HB2	1.94	148	6.72	4.50	2.22
	HB3	1.85	154	7.63	4.82	2.81
	HB4	2.11	171	3.90	3.68	0.21
HW3-8	HB1	1.80	161	7.52	4.79	2.73
	HB2	1.90	178	5.77	5.08	0.69
	HB3	2.17	148	4.91	3.27	1.64
	HB4	2.02	159	5.95	4.13	1.82
HW3-9	HB1	1.97	148	6.66	4.77	1.89
	HB2	1.94	148	6.75	4.49	2.26
	HB3	1.86	153	7.50	4.83	2.68
	HB4	2.09	175	3.02	2.92	0.10
HW3-10	HB1	1.95	149	6.15	4.83	1.33
	HB2	1.93	176	5.39	5.10	0.30
	HB3	1.95	159	6.67	4.01	2.66
	HB4	2.05	159	5.19	3.38	1.81
HW3-11	HB1	1.88	153	6.61	4.82	1.79
	HB2	1.96	157	6.53	3.99	2.53
	HB3	2.10	175	4.31	3.86	0.46
	HB4	2.15	150	4.88	3.31	1.57
HW3-12	HB1	2.11	162	3.97	3.18	0.79
	HB2	1.99	149	5.77	4.30	1.47
	HB3	1.89	179	5.96	5.03	0.93
HW3-13	HB1	2.04	158	3.38	3.61	-0.23
	HB2	2.39	151	2.97	2.74	0.23
	HB3	2.05	143	5.32	4.47	0.85
	HB4	2.09	156	3.30	3.02	0.27
HW3-14	HB1	2.11	135	5.12	4.81	0.31
	HB2	2.15	164	3.88	3.83	0.05
	HB3	1.99	173	4.69	5.13	-0.43
HW4-1	HB1	1.74	168	9.06	4.67	4.38
	HB2	1.77	165	8.62	4.76	3.85
	HB3	1.78	165	8.44	4.81	3.63
	HB4	1.89	161	7.34	4.86	2.48
	HB5	2.12	166	3.77	3.44	0.33
	HB6	2.27	141	0.74	1.17	-0.43
HW4-2	HB1	1.76	168	8.76	4.74	4.02
	HB2	1.77	166	8.55	4.77	3.78
	HB3	1.78	165	8.44	4.80	3.64
	HB4	1.91	161	7.34	4.85	2.48
	HB5	2.26	134	3.11	2.95	0.16
	HB6	2.34	129	1.06	1.33	-0.27
HW4-3	HB1	1.88	158	6.67	4.73	1.94
	HB2	1.75	161	8.50	4.32	4.19
	HB3	1.75	164	8.67	4.64	4.03
	HB4	1.90	157	6.02	4.19	1.82
	HB5	2.23	149	3.50	3.08	0.42

	HB6	2.26	137	3.15	2.67	0.48
HW4-4	HB1	1.77	175	8.23	4.83	3.40
	HB2	1.77	176	8.35	4.80	3.55
	HB3	1.78	174	8.05	4.82	3.22
	HB4	1.92	170	6.55	3.66	2.89
HW4-5	HB5	1.92	163	6.21	3.09	3.12
	HB1	2.10	145	2.18	2.42	-0.24
	HB2	1.98	140	5.71	4.21	1.50
	HB3	2.13	143	5.53	4.02	1.51
	HB4	1.80	155	8.19	4.71	3.48
	HB5	2.18	135	5.49	4.22	1.26
HW4-6	HB6	1.99	164	5.74	3.64	2.10
	HB7	2.03	174	3.62	2.49	1.13
	HB1	1.84	164	7.11	4.50	2.61
	HB2	1.81	166	7.91	4.89	3.02
	HB3	1.81	165	7.87	4.46	3.41
	HB4	1.75	169	8.85	4.73	4.12
	HB5	2.11	180	4.10	3.84	0.26
HW4-7	HB1	2.17	141	5.26	3.99	1.27
	HB2	1.96	142	5.77	4.23	1.53
	HB3	2.12	145	2.09	2.40	-0.31
	HB4	2.23	134	5.38	4.12	1.27
	HB5	1.79	156	8.29	4.74	3.55
	HB6	2.14	137	4.79	3.09	1.70
	HB7	2.06	159	4.36	3.01	1.35
HW4-8	HB1	1.81	164	7.83	4.90	2.93
	HB2	1.80	167	8.19	4.87	3.32
	HB3	1.79	164	8.19	4.35	3.84
	HB4	1.82	168	7.05	4.15	2.90
	HB5	2.78	118	0.26	0.97	-0.70
	HB6	2.27	147	3.24	3.01	0.23
HW4-9	HB1	1.96	152	3.44	2.64	0.80
	HB2	1.91	150	5.43	4.19	1.24
	HB3	2.23	136	5.82	3.81	2.01
	HB4	1.76	170	7.97	4.74	3.23
	HB5	1.94	164	6.10	3.45	2.65
	HB6	1.97	174	4.75	2.58	2.17
HW4-10	HB1	1.85	163	7.19	4.56	2.64
	HB2	1.80	167	8.01	4.91	3.10
	HB3	1.80	165	7.87	4.42	3.44
	HB4	1.76	168	8.64	4.73	3.91
	HB5	2.09	175	2.99	2.95	0.04
HW4-11	HB1	1.81	170	7.87	4.87	3.01
	HB2	1.79	168	8.15	4.79	3.36
	HB3	1.94	155	4.71	3.52	1.19
	HB4	2.31	134	4.42	2.78	1.64
	HB5	2.07	131	5.57	3.08	2.49
	HB6	2.09	149	3.34	2.60	0.74
HW4-12	HB1	1.82	165	7.24	4.88	2.36
	HB2	1.79	170	8.02	4.84	3.18

HW4-13	HB3	1.89	173	6.94	3.37	3.57
	HB4	2.02	176	4.50	2.88	1.62
	HB5	2.09	172	4.26	3.80	0.46
	HB1	1.84	156	7.63	4.74	2.89
	HB2	1.95	143	6.51	4.41	2.10
HW4-14	HB3	2.02	144	6.64	4.78	1.86
	HB4	2.05	142	5.43	4.51	0.92
	HB5	2.08	170	4.49	3.86	0.62
	HB1	1.80	161	7.56	4.79	2.77
	HB2	1.89	179	5.94	5.06	0.88
HW4-15	HB3	2.29	142	4.70	3.09	1.60
	HB4	1.95	159	6.53	3.92	2.60
	HB5	2.08	179	4.51	3.82	0.69
	HB1	1.95	148	6.08	4.82	1.26
	HB2	1.91	174	5.64	5.12	0.52
HW4-16	HB3	1.88	162	7.24	3.56	3.68
	HB4	2.13	154	4.98	3.45	1.53
	HB5	2.08	174	4.56	3.85	0.72
	HB1	1.87	154	6.55	4.82	1.74
	HB2	2.20	147	4.97	3.26	1.71
	HB3	2.09	156	3.21	2.76	0.44
	HB4	2.05	159	3.38	3.62	-0.24
HB5	2.42	149	3.20	2.94	0.26	
HB6	1.94	159	6.81	3.94	2.87	

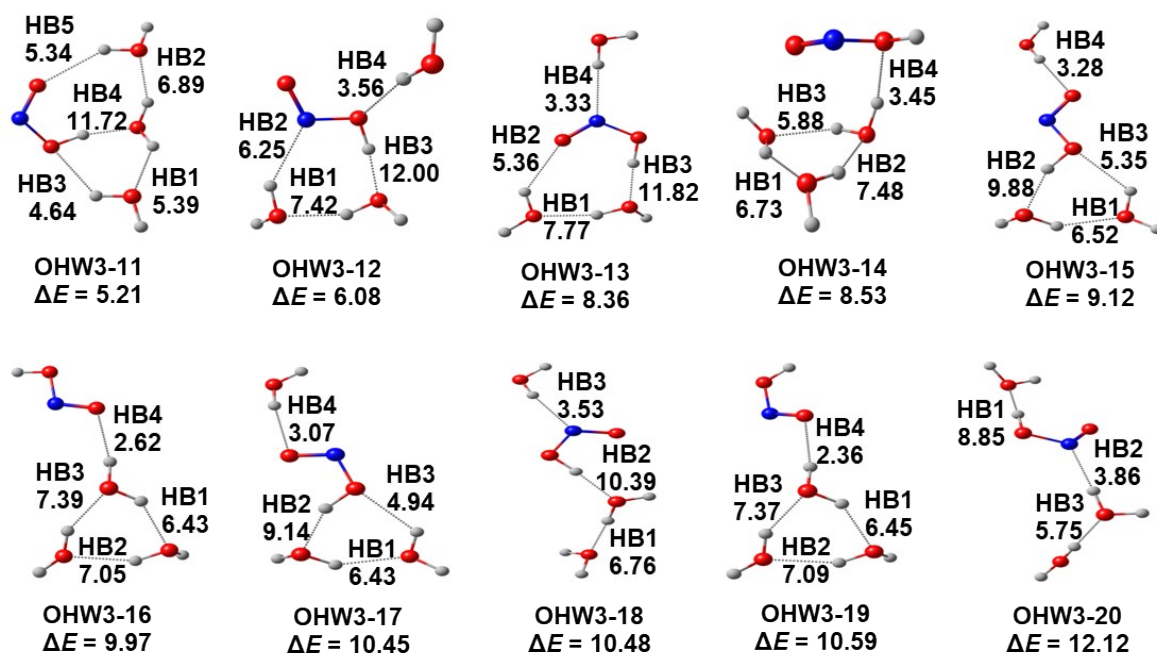


Fig. S2 The MTA-based energies of individual HBs and relative energies (ΔE) of various isomers (with ΔE values above 5 kcal/mol) of $\text{HONO}(\text{H}_2\text{O})_{n=3}$ category. All energy values are in kcal/mol. Also see Fig. 7 of the main text.

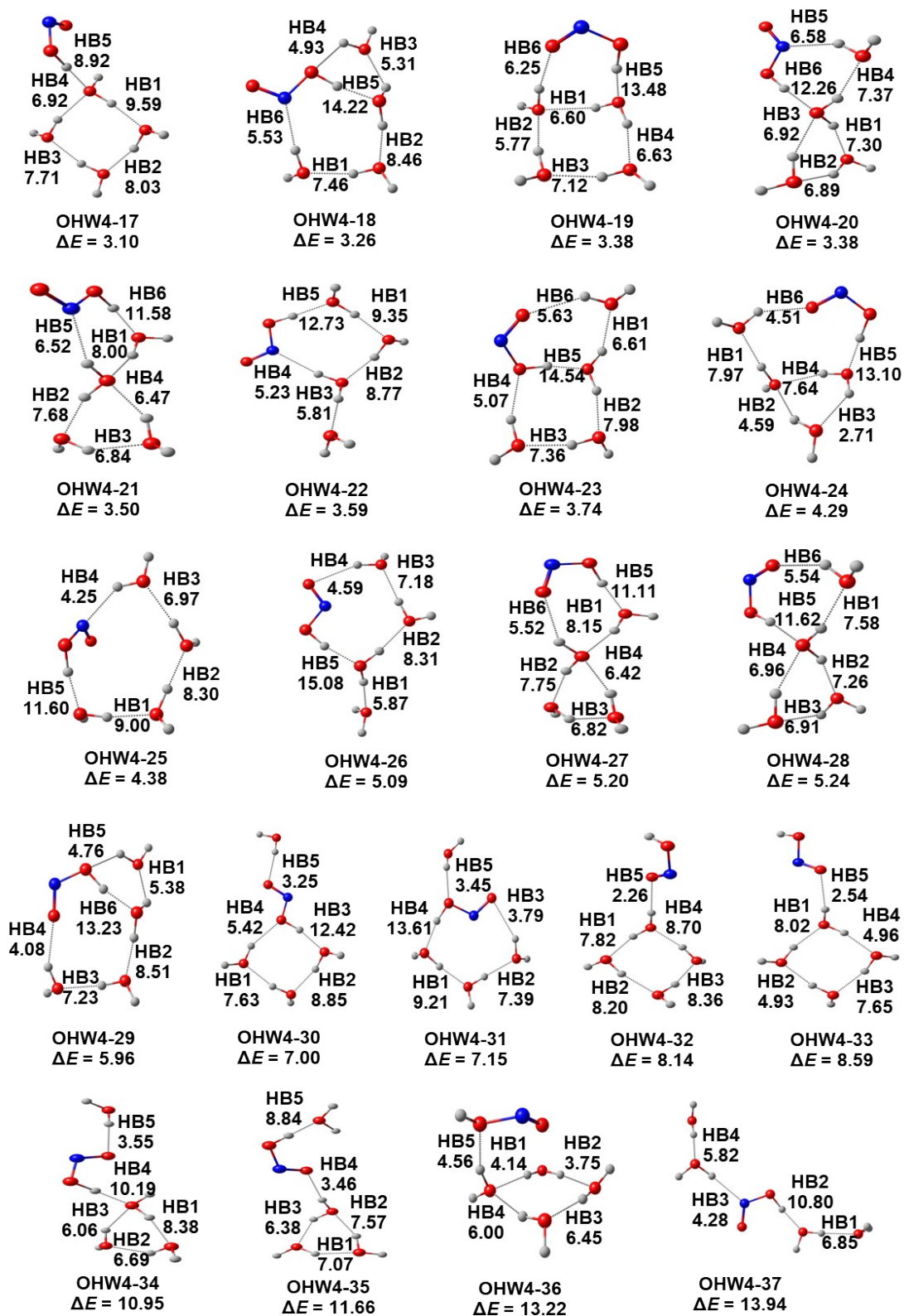


Fig. S3 The MTA-based energies of individual HBs and relative energies (ΔE) of various isomers (with ΔE values above 3 kcal/mol) of HONO(H₂O)_{n=4} category. All energy values are in kcal/mol. Also see Fig. 8 of the main text.

Table S2 The relevant structural parameters *viz.* distance (in Å) and bond angle (in degree), the MTA-based HB energies in complex (E_{HB}^{MTA}), energy in dimer (E^{Dimer}), and cooperativity contribution (E^{Coop}) of all individual HBs in HONO(H₂O)_{n=1-4} complexes. All energy values are in kcal/mol.

Complex	HB labels	HB distance	HB angle	E_{HB}^{MTA}	E^{Dimer}	E^{Coop}
OHW1-1	HB1	1.81	174	-	8.20	-
OHW1-2	HB1	1.81	178	-	7.88	-
OHW1-3	HB1	2.03	166	-	3.52	-
OHW1-4	HB1	2.05	160	-	3.17	-
OHW1-5	HB1	2.18	170	-	2.55	-
OHW1-6	HB1	2.25	179	-	2.56	-
OHW1-7	HB1	2.20	175	-	2.49	-
OHW2-1	HB1	1.83	154	7.47	4.75	2.72
	HB2	1.71	172	11.52	8.80	2.72
	HB3	2.18	148	6.51	3.79	2.72
OHW2-2	HB1	1.92	148	6.67	4.73	1.94
	HB2	1.78	153	8.82	6.88	1.94
	HB3	2.17	132	5.44	3.50	1.94
OHW2-3	HB1	1.84	157	7.19	4.50	2.69
	HB2	1.71	173	10.86	8.17	2.69
	HB3	2.15	145	5.39	2.70	2.69
OHW2-4	HB1	1.85	176	6.62	5.04	1.58
	HB2	1.72	178	9.98	8.40	1.58
OHW2-5	HB1	1.92	147	6.57	4.73	1.84
	HB2	1.80	149	8.17	6.33	1.84
	HB3	2.15	133	5.10	3.26	1.84
OHW2-6	HB1	1.86	177	6.50	5.06	1.44
	HB2	1.73	177	9.32	7.88	1.44
OHW2-7	HB1	2.11	170	3.53	2.86	0.67
	HB2	1.77	170	9.24	8.57	0.67
OHW2-8	HB1	2.20	172	3.21	2.60	0.61
	HB2	1.77	179	8.58	7.98	0.61
OHW2-9	HB1	1.96	175	4.90	5.14	-0.23
	HB2	2.26	155	2.10	2.33	-0.23
OHW2-10	HB1	1.97	176	4.85	5.13	-0.29
	HB2	2.30	169	2.08	2.37	-0.29
OHW2-11	HB1	1.96	175	4.92	5.13	-0.22
	HB2	2.23	154	2.00	2.22	-0.22
OHW3-1	HB1	1.74	172	9.06	4.65	4.42
	HB2	1.79	164	7.69	4.76	2.93
	HB3	2.03	173	5.57	2.99	2.59
	HB4	1.65	178	12.91	8.84	4.08
OHW3-2	HB1	1.81	165	7.76	4.62	3.13
	HB2	1.77	165	8.66	5.08	3.58
	HB3	1.67	165	10.84	7.45	3.39
	HB4	1.92	157	6.03	3.08	2.95
OHW3-3	HB1	1.76	172	9.02	4.83	4.20
	HB2	1.87	164	7.46	4.93	2.53

	HB3	2.18	173	4.29	2.15	2.13
	HB4	1.67	178	12.91	9.12	3.79
OHW3-4	HB1	1.82	165	7.66	4.89	2.77
	HB2	1.77	165	8.51	4.81	3.70
	HB3	1.68	162	10.51	7.02	3.49
	HB4	1.94	157	5.32	2.77	2.55
OHW3-5	HB1	1.76	179	9.03	4.77	4.26
	HB2	1.83	173	7.44	4.91	2.53
	HB3	2.03	142	4.10	1.84	2.27
	HB4	1.66	175	12.13	8.12	4.01
OHW3-6	HB1	1.77	157	8.54	4.64	3.89
	HB2	1.94	148	6.23	4.32	1.91
	HB3	2.23	133	5.92	4.24	1.68
	HB4	1.74	166	9.63	8.13	1.51
OHW3-7	HB1	1.90	151	7.00	4.81	2.19
	HB2	1.88	178	5.59	4.61	0.98
	HB3	1.63	173	13.49	8.96	4.54
	HB4	2.13	152	6.77	3.89	2.88
OHW3-8	HB1	1.76	160	8.48	4.59	3.88
	HB2	1.89	179	5.56	4.65	0.92
	HB3	2.31	142	6.62	3.72	2.89
	HB4	1.69	173	11.90	8.78	3.12
OHW3-9	HB1	2.16	130	5.50	4.19	1.31
	HB2	1.94	147	6.34	4.58	1.75
	HB3	1.79	158	8.68	4.68	4.00
	HB4	1.79	169	9.07	7.79	1.28
	HB5	2.75	109	3.03	1.31	1.72
OHW3-10	HB1	1.80	158	8.16	4.73	3.42
	HB2	1.92	144	6.73	4.62	2.11
	HB3	2.10	139	6.18	4.45	1.74
	HB4	1.76	178	8.92	8.08	0.84
OHW3-11	HB1	2.04	137	5.39	4.26	1.13
	HB2	1.88	154	6.89	4.84	2.05
	HB3	2.29	130	4.64	3.12	1.51
	HB4	1.62	164	11.72	7.30	4.42
	HB5	2.22	146	5.34	2.91	2.43
OHW3-12	HB1	1.84	154	7.42	4.74	2.68
	HB2	2.26	143	6.25	3.78	2.47
	HB3	1.66	174	12.00	8.50	3.50
	HB4	2.01	165	3.56	2.99	0.57
OHW3-13	HB1	1.81	164	7.77	4.84	2.93
	HB2	2.25	137	5.36	2.61	2.75
	HB3	1.67	175	11.82	8.22	3.60
	HB4	2.17	179	3.33	2.67	0.65
OHW3-14	HB1	1.96	148	6.73	4.84	1.89
	HB2	1.85	152	7.48	4.76	2.71
	HB3	2.02	144	5.88	4.74	1.14
	HB4	2.14	148	3.45	3.19	0.26
OHW3-15	HB1	1.92	146	6.52	4.61	1.91
	HB2	1.72	158	9.88	7.32	2.55

	HB3	2.28	127	5.35	3.48	1.87
	HB4	2.12	177	3.28	2.74	0.54
OHW3-16	HB1	1.98	144	6.43	4.81	1.61
	HB2	1.92	150	7.05	4.85	2.20
	HB3	1.87	152	7.39	4.81	2.58
	HB4	2.16	168	2.62	0.23	2.39
OHW3-17	HB1	1.92	146	6.43	4.60	1.83
	HB2	1.73	154	9.14	6.67	2.47
	HB3	2.29	128	4.94	3.20	1.73
	HB4	2.15	171	3.07	2.52	0.55
OHW3-18	HB1	1.84	177	6.76	5.02	1.73
	HB2	1.68	175	10.39	8.00	2.39
	HB3	2.17	171	3.53	2.62	0.90
OHW3-19	HB1	1.98	145	6.45	4.80	1.65
	HB2	1.91	150	7.09	4.84	2.25
	HB3	1.88	151	7.37	4.81	2.56
	HB4	2.15	170	2.36	0.18	2.18
OHW3-20	HB1	1.76	178	8.85	7.98	0.87
	HB2	2.10	174	3.86	2.59	1.28
	HB3	1.91	180	5.75	5.12	0.64
OHW4-1	HB1	1.72	174	9.35	4.58	4.77
	HB2	1.75	176	8.68	4.73	3.96
	HB3	1.78	174	8.07	4.79	3.28
	HB4	1.88	168	5.70	2.74	2.96
	HB5	1.62	174	12.30	7.72	4.57
OHW4-2	HB1	1.71	177	9.45	4.41	5.04
	HB2	1.75	173	8.60	4.75	3.85
	HB3	1.78	172	7.79	4.72	3.07
	HB4	2.02	169	5.13	2.64	2.49
	HB5	1.62	177	13.21	8.66	4.55
OHW4-3	HB1	1.71	169	9.75	4.47	5.28
	HB2	1.76	166	8.65	4.72	3.93
	HB3	1.80	165	8.00	4.88	3.12
	HB4	2.03	153	6.84	4.69	2.15
	HB5	1.76	160	8.98	7.59	1.39
	HB6	2.45	120	-0.72	-0.08	-0.64
OHW4-4	HB1	1.78	166	7.04	3.66	3.38
	HB2	1.83	161	7.30	4.56	2.74
	HB3	1.86	169	6.08	4.51	1.57
	HB4	2.27	132	6.07	3.89	2.17
	HB5	1.61	175	14.08	8.99	5.09
	HB6	1.98	165	6.67	3.51	3.16
OHW4-5	HB1	1.94	150	5.66	4.35	1.31
	HB2	1.71	164	9.47	4.10	5.37
	HB3	1.75	164	8.79	4.56	4.23
	HB4	1.86	161	6.74	4.68	2.06
	HB5	2.50	133	2.19	1.59	0.59
	HB6	1.79	175	9.46	8.22	1.23
OHW4-6	HB1	1.72	174	9.30	4.62	4.68
	HB2	1.75	174	8.62	4.74	3.89

	HB3	1.78	174	8.06	4.83	3.23
	HB4	1.86	169	5.45	2.57	2.88
	HB5	1.62	171	11.67	7.26	4.40
OHW4-7	HB1	1.73	176	9.22	4.11	5.11
	HB2	1.76	177	8.49	4.62	3.87
	HB3	1.82	176	7.28	4.49	2.79
	HB4	1.95	164	5.61	2.83	2.78
	HB5	1.62	173	13.86	8.99	4.86
OHW4-8	HB1	1.71	161	9.31	4.13	5.17
	HB2	1.99	153	5.77	4.56	1.21
	HB3	1.90	157	5.77	4.11	1.66
	HB4	1.77	162	8.43	4.48	3.95
	HB5	2.29	132	2.82	2.19	0.63
	HB6	1.76	166	9.17	7.72	1.45
OHW4-9	HB1	1.93	148	6.52	4.73	1.79
	HB2	1.81	160	7.94	4.89	3.05
	HB3	1.85	165	7.29	4.95	2.35
	HB4	1.99	154	5.20	2.85	2.34
	HB5	1.54	174	14.88	8.19	6.70
	HB6	2.26	145	6.34	4.03	2.31
OHW4-10	HB1	1.72	172	9.60	4.54	5.06
	HB2	1.78	159	7.94	4.19	3.75
	HB3	1.99	150	4.28	3.13	1.15
	HB4	2.13	152	4.04	2.80	1.24
	HB5	2.19	153	5.04	2.56	2.48
	HB6	1.61	175	14.12	8.98	5.14
OHW4-11	HB1	1.70	171	9.72	4.41	5.31
	HB2	1.79	163	8.06	4.37	3.68
	HB3	1.81	164	7.64	4.81	2.83
	HB4	1.90	161	6.91	4.74	2.17
	HB5	1.77	172	9.38	8.40	0.98
OHW4-12	HB1	1.71	169	9.62	4.51	5.12
	HB2	1.76	166	8.61	4.74	3.88
	HB3	1.80	165	8.03	4.87	3.16
	HB4	1.99	155	6.95	4.75	2.20
	HB5	2.46	120	-0.66	-0.02	-0.64
	HB6	1.80	154	8.03	6.86	1.17
OHW4-13	HB1	1.84	164	7.20	4.90	2.29
	HB2	1.92	154	5.97	4.55	1.43
	HB3	1.71	167	9.52	4.07	5.45
	HB4	1.75	167	8.89	4.69	4.19
	HB5	1.81	171	8.65	7.59	1.06
	HB6	2.61	109	1.09	0.62	0.47
OHW4-14	HB1	1.73	176	9.54	4.49	5.05
	HB2	1.77	176	8.52	4.71	3.81
	HB3	1.80	172	7.68	4.86	2.83
	HB4	1.92	156	5.44	2.21	3.23
	HB5	1.63	174	12.48	8.06	4.41
OHW4-15	HB1	2.02	139	2.83	1.83	1.00
	HB2	1.95	152	4.59	4.03	0.56

	HB3	2.04	154	7.51	4.51	3.00
	HB4	1.84	177	7.87	4.80	3.07
	HB5	2.10	155	4.84	2.30	2.54
	HB6	1.63	165	13.94	9.11	4.83
OHW4-16	HB1	1.92	152	5.76	4.08	1.68
	HB2	1.77	159	8.55	4.62	3.93
	HB3	2.44	126	5.43	3.70	1.73
	HB4	1.77	159	7.84	4.27	3.58
	HB5	1.70	174	10.15	7.88	2.27
	HB6	2.52	125	2.67	1.65	1.02
	HB7	2.52	122	0.01	0.96	-0.95
OHW4-17	HB1	1.71	170	9.59	4.47	5.12
	HB2	1.79	163	8.03	4.37	3.66
	HB3	1.81	164	7.71	4.82	2.89
	HB4	1.89	162	6.92	4.73	2.19
	HB5	1.77	178	8.92	8.11	0.81
OHW4-18	HB1	1.81	164	7.46	4.87	2.59
	HB2	1.77	169	8.46	4.86	3.60
	HB3	2.06	135	5.31	4.25	1.06
	HB4	2.31	128	4.93	3.36	1.58
	HB5	1.56	168	14.22	8.12	6.10
	HB6	2.05	173	5.53	3.16	2.36
OHW4-19	HB1	2.11	142	6.60	4.26	2.33
	HB2	1.88	169	5.77	4.52	1.25
	HB3	1.84	160	7.12	4.60	2.52
	HB4	1.80	164	6.63	3.62	3.01
	HB5	1.61	171	13.48	8.10	5.38
	HB6	1.94	167	6.25	2.66	3.60
OHW4-20	HB1	1.84	154	7.30	4.39	2.91
	HB2	1.93	144	6.89	4.74	2.15
	HB3	1.99	147	6.92	4.88	2.04
	HB4	1.84	155	7.37	4.77	2.60
	HB5	2.16	148	6.58	3.90	2.68
	HB6	1.68	174	12.26	8.87	3.39
OHW4-21	HB1	1.81	157	8.00	4.82	3.18
	HB2	1.84	155	7.68	4.80	2.87
	HB3	1.94	144	6.84	4.73	2.11
	HB4	2.00	145	6.47	4.51	1.96
	HB5	2.20	148	6.52	3.72	2.79
	HB6	1.70	171	11.58	8.78	2.80
OHW4-22	HB1	1.73	172	9.35	4.57	4.77
	HB2	1.73	166	8.77	4.57	4.20
	HB3	1.89	180	5.81	4.99	0.82
	HB4	2.09	171	5.23	3.03	2.20
	HB5	1.65	177	12.73	8.78	3.95
OHW4-23	HB1	1.89	154	6.61	4.54	2.07
	HB2	1.81	162	7.98	4.97	3.01
	HB3	1.84	165	7.36	4.94	2.43
	HB4	1.96	156	5.07	2.65	2.42
	HB5	1.54	168	14.54	7.53	7.01

OHW4-24	HB6	2.21	146	5.63	2.97	2.66
	HB1	1.79	173	7.97	4.81	3.16
	HB2	1.96	151	4.59	3.97	0.62
	HB3	2.01	141	2.71	1.86	0.84
	HB4	2.01	157	7.64	4.54	3.10
	HB5	1.62	177	13.10	8.10	5.01
OHW4-25	HB6	1.99	144	4.51	1.83	2.68
	HB1	1.74	171	9.00	4.54	4.46
	HB2	1.77	178	8.30	4.78	3.52
	HB3	1.83	174	6.97	4.50	2.47
	HB4	2.08	146	4.25	2.16	2.09
	HB5	1.63	165	11.60	7.44	4.16
OHW4-26	HB1	1.89	174	5.87	5.04	0.83
	HB2	1.81	173	8.31	5.01	3.30
	HB3	1.89	176	7.18	4.94	2.25
	HB4	2.17	155	4.59	2.18	2.40
	HB5	1.59	168	15.08	10.60	4.48
	HB6	2.18	145	5.52	2.66	2.87
OHW4-27	HB1	1.80	163	8.15	4.83	3.31
	HB2	1.83	155	7.75	4.80	2.95
	HB3	1.94	144	6.82	4.72	2.10
	HB4	2.01	144	6.42	4.51	1.91
	HB5	1.70	174	11.11	8.21	2.89
	HB6	2.18	145	5.52	2.66	2.87
OHW4-28	HB1	1.83	161	7.58	4.84	2.73
	HB2	1.85	153	7.26	4.43	2.84
	HB3	1.93	144	6.91	4.75	2.16
	HB4	1.98	148	6.96	4.88	2.08
	HB5	1.69	171	11.62	8.23	3.40
	HB6	2.14	145	5.54	2.77	2.77
OHW4-29	HB1	2.07	135	5.38	4.29	1.09
	HB2	1.78	175	8.51	4.95	3.56
	HB3	1.83	172	7.23	4.98	2.25
	HB4	2.06	150	4.08	1.95	2.14
	HB5	2.25	131	4.76	3.14	1.61
	HB6	1.57	164	13.23	7.16	6.07
OHW4-30	HB1	1.82	165	7.63	4.92	2.71
	HB2	1.76	165	8.85	4.74	4.11
	HB3	1.62	167	12.42	7.73	4.69
	HB4	1.96	154	5.42	3.05	2.36
	HB5	2.13	175	3.25	2.75	0.50
	HB6	1.57	164	13.23	7.16	6.07
OHW4-31	HB1	1.82	165	7.63	4.92	2.71
	HB2	1.76	165	8.85	4.74	4.11
	HB3	1.62	167	12.42	7.73	4.69
	HB4	1.96	154	5.42	3.05	2.36
	HB5	2.13	175	3.25	2.75	0.50
	HB6	1.57	164	13.23	7.16	6.07
OHW4-32	HB1	1.75	174	9.21	4.76	4.45
	HB2	1.86	176	7.39	4.95	2.44
	HB3	2.30	152	3.79	1.97	1.82
	HB4	1.62	167	13.61	8.83	4.79
	HB5	2.05	169	3.45	2.77	0.68
	HB6	1.57	164	13.23	7.16	6.07
OHW4-32	HB1	1.81	165	7.82	4.93	2.89
	HB2	1.79	166	8.20	4.89	3.31
	HB3	1.78	166	8.36	4.84	3.52
	HB4	1.77	167	8.70	4.79	3.91
	HB5	2.15	177	2.26	2.22	0.04

OHW4-33	HB1	1.78	165	8.02	4.34	3.68
	HB2	1.79	167	4.93	1.72	3.21
	HB3	1.82	165	7.65	4.51	3.13
	HB4	1.81	165	4.96	1.72	3.24
	HB5	2.18	166	2.54	2.50	0.04
OHW4-34	HB1	1.77	160	8.38	4.66	3.72
	HB2	1.92	144	6.69	4.60	2.08
	HB3	2.15	137	6.06	4.37	1.69
	HB4	1.71	178	10.19	8.32	1.88
	HB5	2.09	178	3.55	2.66	0.88
OHW4-35	HB1	1.92	150	7.07	4.84	2.23
	HB2	1.86	153	7.57	4.77	2.80
	HB3	1.99	145	6.38	4.43	1.95
	HB4	2.05	171	3.46	2.55	0.92
	HB5	1.77	178	8.84	2.53	6.31
OHW4-36	HB1	2.11	175	4.14	4.78	-0.64
	HB2	2.01	162	3.75	3.72	0.04
	HB3	1.88	167	6.45	5.09	1.36
	HB4	1.87	158	6.00	4.53	1.47
	HB5	1.94	154	4.56	3.35	1.21
OHW4-37	HB1	1.83	177	6.85	5.01	1.84
	HB2	1.67	176	10.80	9.03	1.76
	HB3	2.08	176	4.28	3.63	0.65
	HB4	1.91	177	5.82	5.04	0.78

Table S3 Coordinates of the MP2/6-311++G(d,p) optimized structures of HNO(H₂O)_{n=1-4} complexes.

HNO(H₂O)_{n=1-4}							
HW1-1			HW1-2				
N	1.219181000000	0.597893000000	0.003296000000	N	-0.834855000000	0.353859000000	-0.000268000000
H	0.254783000000	1.005552000000	0.056190000000	H	-1.167722000000	1.351398000000	0.000597000000
O	1.092249000000	-0.621609000000	0.004653000000	O	-1.807979000000	-0.383548000000	0.000133000000
H	-1.323637000000	-0.806103000000	0.012724000000	O	2.215067000000	0.021655000000	0.000141000000
O	-1.703158000000	0.074609000000	-0.057055000000	H	1.252942000000	-0.039854000000	-0.000675000000
H	-2.578134000000	-0.008696000000	0.327230000000	H	2.502053000000	-0.893416000000	-0.000240000000
HW1-3			HW2-1				
N	1.597373000000	-0.454623000000	0.044655000000	N	1.840599000000	0.371714000000	-0.005027000000
H	2.586977000000	-0.135439000000	-0.113803000000	H	1.011798000000	1.011129000000	-0.018815000000
O	0.874847000000	0.529742000000	-0.022271000000	O	1.408955000000	-0.779525000000	0.001398000000
H	-1.194769000000	0.045698000000	0.031802000000	H	-1.471996000000	2.159511000000	-0.415368000000
O	-2.123811000000	-0.194479000000	-0.039923000000	O	-0.936921000000	1.536520000000	0.080185000000
H	-2.582111000000	0.590001000000	0.266972000000	H	-1.421949000000	0.697657000000	0.031374000000
HW2-2			HW2-3				
N	1.175773000000	-0.039693000000	0.006886000000	N	2.382850000000	0.688302000000	0.006464000000
H	0.795059000000	0.935142000000	0.002530000000	H	1.364434000000	0.862586000000	0.175318000000
O	2.398977000000	-0.011397000000	-0.007794000000	O	2.498902000000	-0.512444000000	-0.221258000000
H	-2.026618000000	1.950974000000	-0.369337000000	O	-0.412864000000	-0.166522000000	0.374400000000
O	-1.351891000000	1.429367000000	0.068912000000	H	-1.357324000000	-0.118212000000	0.173637000000
H	-1.681324000000	0.518589000000	0.029670000000	H	-0.156538000000	-1.055643000000	0.119255000000
O	-1.441039000000	-1.379021000000	-0.083518000000	O	-3.230508000000	0.018024000000	-0.178264000000
H	-0.475465000000	-1.336467000000	-0.027906000000	H	-3.553388000000	0.597113000000	-0.873388000000
H	-1.690444000000	-2.101978000000	0.496042000000	H	-3.821381000000	0.183575000000	0.560899000000
HW2-4			HW2-5				
N	-0.143968000000	0.146036000000	0.009021000000	N	1.532672000000	-0.720056000000	-0.064295000000
H	0.613368000000	-0.574666000000	0.044636000000	H	2.465719000000	-1.175734000000	-0.223359000000
O	0.396135000000	1.246454000000	0.010915000000	O	1.720453000000	0.477559000000	0.098989000000
O	-3.115102000000	-0.553467000000	0.010297000000	H	-0.769632000000	-1.575514000000	-0.015922000000
H	-2.194663000000	-0.262572000000	-0.013470000000	O	-1.711692000000	-1.401662000000	0.051366000000
H	-3.610210000000	0.259153000000	-0.108341000000	H	-1.740189000000	-0.440834000000	-0.037353000000
O	2.691019000000	-0.636111000000	-0.055672000000	O	-1.129976000000	1.492644000000	-0.125246000000
H	3.421389000000	-1.168864000000	0.266738000000	H	-1.514022000000	2.199913000000	0.397788000000
H	3.001474000000	0.269685000000	0.022971000000	H	-0.200858000000	1.484231000000	0.128041000000
HW2-6			HW2-7				
N	0.113276000000	0.890772000000	0.024538000000	O	-0.748446000000	1.289304000000	0.216360000000
H	1.149343000000	1.033970000000	0.030276000000	H	-1.392969000000	0.582533000000	0.093218000000
O	-0.075546000000	-0.319323000000	0.113036000000	H	0.078646000000	0.897826000000	-0.076133000000
O	-3.128658000000	-0.276571000000	-0.047906000000	O	-2.871220000000	-0.712397000000	-0.114237000000
H	-2.176577000000	-0.411553000000	0.000761000000	H	-3.260214000000	-1.045295000000	0.698417000000
H	-3.206011000000	0.677127000000	-0.118334000000	H	-3.621595000000	-0.370141000000	-0.606637000000
H	2.512844000000	-1.073843000000	0.026219000000	O	2.115284000000	0.208783000000	-0.387114000000
O	2.849715000000	-0.183114000000	-0.102449000000	N	2.398654000000	-0.776696000000	0.278548000000
H	3.763376000000	-0.229040000000	0.187864000000	H	3.440612000000	-0.913576000000	0.221228000000
HW3-1			HW3-2				
N	-1.580631000000	-0.039484000000	-0.029369000000	N	-2.348606000000	0.465194000000	0.076247000000
H	-1.171528000000	0.922829000000	-0.028683000000	H	-1.492275000000	1.065654000000	0.044459000000
O	-2.805040000000	0.020775000000	-0.046039000000	O	-1.975790000000	-0.706959000000	0.046799000000
H	0.796709000000	2.783078000000	0.535845000000	O	0.246351000000	1.945093000000	-0.055491000000
O	0.499650000000	2.035538000000	0.013629000000	H	1.073401000000	1.430573000000	-0.005423000000
H	1.259349000000	1.424694000000	0.004671000000	H	0.460606000000	2.686881000000	-0.624814000000
O	2.408052000000	0.018793000000	-0.002129000000	O	0.696444000000	-1.936567000000	-0.034690000000
H	1.866512000000	-0.790715000000	0.033195000000	H	0.637401000000	-2.650810000000	-0.673109000000
H	3.030750000000	-0.141921000000	-0.714321000000	H	-0.193184000000	-1.556067000000	-0.011004000000
H	-0.292749000000	-1.532696000000	0.002920000000	H	3.015507000000	0.133897000000	0.775783000000
O	0.543657000000	-2.030074000000	0.003121000000	O	2.408061000000	0.230288000000	0.039244000000
H	0.404816000000	-2.749139000000	0.623296000000	H	1.938262000000	-0.621334000000	-0.006520000000

<p>HW3-3</p> <p>N 2.243336000000 0.607942000000 0.454359000000 H 1.356153000000 1.034303000000 0.097242000000 O 2.156831000000 -0.608164000000 0.298909000000 O -0.531268000000 1.438436000000 -0.681157000000 H -1.245494000000 1.189918000000 -0.066871000000 H -0.822928000000 2.261711000000 -1.079605000000 O -2.338785000000 -0.006622000000 0.804653000000 H -2.553474000000 -0.222068000000 1.714208000000 H -1.876464000000 -0.786336000000 0.452228000000 H -0.497744000000 -0.672718000000 -1.238698000000 O -0.584002000000 -1.501440000000 -0.750991000000 H 0.314389000000 -1.638081000000 -0.430343000000</p>	<p>HW3-4</p> <p>N -2.968732000000 0.122629000000 0.651074000000 H -1.972244000000 0.093823000000 0.977931000000 O -2.951516000000 -0.096896000000 -0.555378000000 O -0.077844000000 -0.066210000000 -0.091870000000 H 0.595824000000 -0.766182000000 -0.048227000000 H -0.618204000000 -0.285884000000 -0.857307000000 O 2.367366000000 -1.374854000000 0.013356000000 H 2.867542000000 -1.902230000000 0.639337000000 H 2.749303000000 -0.485132000000 -0.066777000000 H 1.374433000000 1.251895000000 -0.092502000000 O 2.330258000000 1.413933000000 -0.074269000000 H 2.438362000000 2.227524000000 0.421769000000</p>
<p>HW3-5</p> <p>N 0.371875000000 -1.518360000000 0.636799000000 H -1.847111000000 -0.555460000000 -0.118531000000 O -2.204680000000 0.341485000000 -0.076698000000 H -2.885240000000 0.361468000000 -0.753372000000 H -0.808870000000 1.537291000000 0.052290000000 O 0.010234000000 2.056947000000 0.124080000000 H -0.096452000000 2.552800000000 0.938772000000 H 1.489396000000 0.989986000000 -0.098424000000 O 2.186650000000 0.323784000000 -0.228683000000 H 2.738037000000 0.696112000000 -0.919109000000 H 1.366657000000 -1.759306000000 0.431827000000 O -0.312146000000 -1.871512000000 -0.317581000000</p>	<p>HW3-6</p> <p>O 0.534878000000 -0.599026000000 1.548349000000 H 1.014105000000 -1.006078000000 2.273266000000 H 0.914142000000 -0.994346000000 0.742247000000 N -1.871909000000 0.324760000000 0.198573000000 H -1.785384000000 -0.252578000000 1.068168000000 O -1.869343000000 -0.433800000000 -0.762582000000 H 1.087864000000 -1.278472000000 -1.772110000000 O 1.537435000000 -0.932445000000 -0.997793000000 H 1.440274000000 0.031627000000 -1.064143000000 O 0.980361000000 1.692914000000 -0.160622000000 H 0.803238000000 1.237337000000 0.674620000000 H 0.162474000000 2.168049000000 -0.330880000000</p>
<p>HW3-7</p> <p>O 0.258389000000 -0.219746000000 0.933550000000 H -0.648172000000 -0.166755000000 0.607398000000 H 0.653921000000 0.634692000000 0.707846000000 N -2.535055000000 -0.284210000000 -0.326927000000 H -2.723803000000 -0.890539000000 -1.165325000000 O -3.560708000000 0.309070000000 -0.033545000000 H 2.860797000000 2.122463000000 -0.036984000000 O 2.145384000000 1.522810000000 -0.256451000000 H 2.576257000000 0.669001000000 -0.420114000000 O 2.461968000000 -1.270433000000 -0.352812000000 H 1.628173000000 -1.176709000000 0.142438000000 H 2.957945000000 -1.936284000000 0.127298000000</p>	<p>HW3-8</p> <p>N 2.585753000000 -0.783306000000 -0.325028000000 O 1.620045000000 -1.411986000000 0.104518000000 H 2.307265000000 0.225679000000 -0.356531000000 O 1.122443000000 1.855709000000 -0.237276000000 H 0.310057000000 1.459335000000 0.127739000000 H 1.227679000000 2.679138000000 0.243044000000 O -0.847680000000 0.230389000000 0.763395000000 H -0.301742000000 -0.556139000000 0.653779000000 H -1.704180000000 -0.002304000000 0.377729000000 O -3.403601000000 -0.415411000000 -0.355351000000 H -4.180434000000 -0.376263000000 0.208421000000 H -3.688575000000 -0.015916000000 -1.181265000000</p>
<p>HW3-9</p> <p>O -0.200967000000 -0.091355000000 0.923338000000 H 0.686059000000 -0.294246000000 0.608936000000 H -0.752165000000 -0.821138000000 0.604662000000 N 3.185367000000 0.498280000000 -0.318008000000 H 4.161055000000 0.291567000000 -0.651717000000 O 2.648035000000 -0.569143000000 -0.057463000000 H -3.205471000000 -1.767954000000 -0.172589000000 O -2.388762000000 -1.312669000000 -0.385381000000 H -2.639283000000 -0.378970000000 -0.470493000000 O -2.147738000000 1.482007000000 -0.252491000000 H -1.340952000000 1.201693000000 0.215086000000 H -2.491361000000 2.210372000000 0.268153000000</p>	<p>HW3-10</p> <p>N 1.725125000000 -1.635006000000 -0.014730000000 O 2.423022000000 -0.634863000000 -0.180135000000 H 0.748044000000 -1.299413000000 0.157723000000 O -0.722177000000 -0.067318000000 0.500208000000 H -0.400469000000 0.828549000000 0.329563000000 H -1.650475000000 -0.064270000000 0.233598000000 O 1.067728000000 2.014389000000 -0.140250000000 H 1.706853000000 1.290140000000 -0.169141000000 H 1.511577000000 2.709072000000 0.350737000000 O -3.525320000000 -0.175176000000 -0.209713000000 H -3.818995000000 -0.594487000000 -1.022436000000 H -4.118434000000 -0.520804000000 0.462186000000</p>
<p>HW3-11</p> <p>N -0.813028000000 -0.048566000000 0.029159000000 H -0.135411000000 0.749122000000 0.010119000000 O -0.164611000000 -1.092311000000 0.044842000000 H 1.974077000000 -1.245660000000 -0.025819000000 O 2.839500000000 -0.829922000000 -0.121153000000 H 3.427007000000 -1.354570000000 0.427401000000 H -2.907715000000 0.076453000000 0.000762000000 O -3.863695000000 0.204955000000 -0.039346000000 H -4.211582000000 -0.687711000000 0.001744000000 H 2.277790000000 0.955816000000 0.008957000000 O 1.602774000000 1.648339000000 0.086849000000 H 1.955284000000 2.398025000000 -0.396813000000</p>	<p>HW3-12</p> <p>N -1.101956000000 0.539373000000 -0.331469000000 H -0.062884000000 0.530858000000 -0.444820000000 O -1.404125000000 -0.536222000000 0.182583000000 O -4.373359000000 0.143742000000 0.186923000000 H -3.497474000000 -0.250993000000 0.256099000000 H -4.185519000000 0.990709000000 -0.223229000000 H 1.532391000000 -1.326070000000 0.091856000000 O 1.651711000000 -0.471441000000 -0.328360000000 H 2.563928000000 -0.224966000000 -0.118501000000 H 4.975047000000 0.360983000000 -0.469870000000 O 4.353207000000 0.259670000000 0.255449000000 H 4.568729000000 0.977882000000 0.855978000000</p>
<p>HW3-13</p> <p>N 0.587654000000 0.490555000000 -0.207125000000 H 1.577792000000 0.812930000000 -0.119046000000 O 0.609358000000 -0.735276000000 -0.132979000000 H -1.535073000000 1.589586000000 -0.130738000000 O -2.476417000000 1.593353000000 0.063242000000 H -2.657341000000 0.650233000000 0.160909000000</p>	<p>HW3-14</p> <p>N 1.011917000000 0.112931000000 0.053270000000 H 1.793189000000 -0.566329000000 -0.102524000000 O 1.516932000000 1.211168000000 0.255479000000 O -1.790801000000 -1.166577000000 0.287515000000 H -1.008608000000 -0.615902000000 0.175944000000 H -2.525042000000 -0.571151000000 0.098527000000</p>

O	-2.300917000000	-1.362324000000	0.164090000000	O	3.894761000000	-0.411426000000	-0.293580000000
H	-2.721115000000	-1.976450000000	-0.441878000000	H	4.693870000000	-0.879339000000	-0.041713000000
H	-1.363362000000	-1.410955000000	-0.056664000000	H	4.048542000000	0.494742000000	-0.013311000000
O	3.511008000000	0.153002000000	0.067858000000	O	-4.190377000000	0.455671000000	-0.256050000000
H	3.553389000000	-0.793067000000	0.229607000000	H	-4.775855000000	0.561571000000	0.497902000000
H	4.287881000000	0.503807000000	0.510006000000	H	-4.753644000000	0.075204000000	-0.934623000000
HW4-1				HW4-2			
H	-0.638465000000	1.527972000000	0.429369000000	H	1.587629000000	1.509608000000	-0.044869000000
O	0.181889000000	1.380930000000	0.947562000000	O	2.382134000000	1.295582000000	-0.574406000000
H	-2.979547000000	-1.880322000000	-0.104202000000	H	0.058926000000	-2.031022000000	1.718312000000
H	0.131085000000	2.012160000000	1.669614000000	H	3.075208000000	1.855312000000	-0.218316000000
O	-2.316391000000	-1.303575000000	-0.488943000000	O	-0.049563000000	-1.392111000000	1.009858000000
H	-1.488925000000	-1.516273000000	-0.012766000000	H	0.722958000000	-1.538811000000	0.425138000000
H	-2.342874000000	0.463901000000	-0.534108000000	H	0.033182000000	0.506509000000	1.192586000000
O	-2.128999000000	1.416556000000	-0.467484000000	O	0.125117000000	1.445510000000	0.962897000000
H	-2.288905000000	1.769337000000	-1.345325000000	H	-0.738749000000	1.651632000000	0.588673000000
H	0.880064000000	-1.662494000000	0.497021000000	H	2.252908000000	-1.759281000000	-1.478914000000
O	0.035464000000	-1.442195000000	0.903602000000	O	2.157628000000	-1.424678000000	-0.584784000000
H	0.142654000000	-0.501319000000	1.118690000000	H	2.378295000000	-0.473418000000	-0.646687000000
N	2.740222000000	0.539977000000	-0.673230000000	N	-2.390429000000	0.199161000000	-0.221400000000
O	2.663436000000	-0.673301000000	-0.496377000000	O	-3.451348000000	0.027820000000	-0.808193000000
H	1.920164000000	0.979892000000	-0.192551000000	H	-1.949089000000	-0.731639000000	-0.029099000000
HW4-3				HW4-4			
H	-1.079360000000	1.512949000000	-0.687292000000	H	-0.492679000000	3.005169000000	-0.710131000000
O	-1.272416000000	1.998832000000	0.131555000000	O	-0.198426000000	2.374223000000	-0.049515000000
H	-2.206054000000	-2.338131000000	0.119487000000	H	-0.871687000000	1.668240000000	-0.059209000000
H	-0.988624000000	2.899909000000	-0.034280000000	O	-0.322905000000	-2.360495000000	0.088620000000
O	-1.395018000000	-1.862134000000	-0.069875000000	H	-0.279684000000	-3.113568000000	0.681174000000
H	-1.203978000000	-1.342149000000	0.740715000000	H	0.606410000000	-2.077046000000	-0.014663000000
H	-1.007381000000	-0.704985000000	-1.330641000000	O	2.330575000000	1.311465000000	0.162499000000
O	-0.617746000000	0.065742000000	-1.795235000000	H	1.460578000000	1.743178000000	0.061334000000
H	-0.838966000000	-0.063152000000	-2.720400000000	H	2.708662000000	1.715540000000	0.946436000000
H	0.330975000000	-0.101925000000	1.798575000000	H	2.773069000000	-1.571081000000	-0.963421000000
O	-0.631238000000	-0.124945000000	1.866021000000	O	2.242638000000	-1.409400000000	-0.180390000000
H	-0.893018000000	0.732974000000	1.494086000000	H	2.310891000000	-0.444755000000	-0.036636000000
N	1.886183000000	-0.063048000000	0.157796000000	N	-1.951837000000	0.077256000000	-0.009612000000
O	3.083608000000	-0.087443000000	-0.100595000000	H	-1.545472000000	-0.884086000000	0.063463000000
H	1.345598000000	-0.074571000000	-0.739781000000	O	-3.177785000000	0.011410000000	-0.008844000000
HW4-5				HW4-6			
N	2.871292000000	-0.506994000000	0.061402000000	O	-0.296570000000	-0.512180000000	-1.005479000000
H	1.995915000000	-1.071199000000	0.170327000000	H	-1.181735000000	-0.496140000000	-0.622200000000
O	2.525940000000	0.650485000000	-0.172454000000	H	0.023387000000	0.404445000000	-0.926435000000
O	0.102180000000	-1.660799000000	0.281547000000	N	-3.120758000000	-0.465064000000	-0.198137000000
H	-0.446275000000	-1.286864000000	0.982780000000	H	-3.778285000000	-1.271083000000	0.353205000000
H	-0.468385000000	-1.548069000000	-0.489052000000	O	-3.666922000000	0.562498000000	0.567146000000
O	-0.279242000000	1.701509000000	-0.260904000000	H	0.767382000000	2.669021000000	-0.060386000000
H	-0.663404000000	1.253266000000	-1.024402000000	O	1.041448000000	1.897890000000	-0.560745000000
H	0.643798000000	1.413802000000	-0.265324000000	H	1.795925000000	1.535553000000	-0.059369000000
H	-2.282432000000	0.630166000000	2.160198000000	O	2.980731000000	0.489909000000	0.813175000000
O	-1.864733000000	0.243505000000	1.387660000000	H	3.930303000000	0.478223000000	0.678520000000
H	-1.286548000000	0.940883000000	1.016443000000	H	2.690707000000	-0.423150000000	0.621939000000
O	-2.033928000000	-0.418112000000	-1.317474000000	O	1.763630000000	-1.886941000000	-0.115557000000
H	-2.420115000000	-0.276285000000	-0.439456000000	H	0.965965000000	-1.495861000000	-0.300254000000
H	-2.773325000000	-0.639444000000	-1.888330000000	H	2.053093000000	-2.554979000000	-0.509205000000
HW4-7				HW4-8			
N	2.224448000000	0.064201000000	-0.059860000000	N	-2.982265000000	0.546614000000	-0.262800000000
H	1.838843000000	-0.883821000000	0.158134000000	H	-3.999850000000	0.805908000000	-0.205983000000
O	3.448895000000	0.034748000000	-0.056438000000	O	-2.902547000000	-0.639107000000	-0.545991000000
O	-0.091920000000	-1.772920000000	0.353436000000	H	-0.512593000000	-1.907177000000	0.059886000000
H	-0.623355000000	-1.353035000000	1.040748000000	O	0.065441000000	-1.493242000000	0.705329000000
H	-0.646421000000	-1.635547000000	-0.424588000000	H	0.958624000000	-1.578913000000	0.322195000000
O	-0.244222000000	1.718363000000	-0.292883000000	O	2.581808000000	-1.246689000000	-0.416575000000
H	-0.634471000000	1.287363000000	-1.062877000000	H	3.410790000000	-1.508101000000	-0.010424000000
H	0.666980000000	1.386532000000	-0.282614000000	H	2.627348000000	-0.272076000000	-0.459569000000
H	-2.339330000000	0.808153000000	2.090512000000	H	-1.002821000000	1.439823000000	0.407296000000
O	-1.919192000000	0.357698000000	1.354710000000	O	-0.140063000000	1.277505000000	0.801977000000
H	-1.294024000000	1.005536000000	0.967970000000	H	-0.128649000000	0.304244000000	0.883086000000
O	-2.096244000000	-0.377741000000	-1.326204000000	O	2.353958000000	1.495890000000	-0.318064000000
H	-2.460590000000	-0.177140000000	-0.449994000000	H	2.402617000000	2.147938000000	-1.019599000000
H	-2.857304000000	-0.568636000000	-1.879228000000	H	1.451611000000	1.587202000000	0.049306000000

Table S4 Coordinates of the MP2/6-311++G(d,p) optimized structures of HONO(H₂O)_{n=1-4} complexes.

HONO(H ₂ O) _{n=1-4}						
OHW1-1			OHW1-2			
O	-2.363326000000	-0.154433000000	O	-2.017735000000	-0.066979000000	-0.070440000000
H	-2.405589000000	-1.106765000000	H	-1.904262000000	-1.014583000000	0.050127000000
H	-2.998880000000	0.024709000000	H	-2.812637000000	0.153065000000	0.422373000000
N	0.906509000000	-0.393657000000	N	1.410749000000	0.045910000000	0.011679000000
O	0.243916000000	0.820315000000	O	0.531313000000	1.084575000000	-0.001106000000
H	-0.694447000000	0.539032000000	H	-0.380157000000	0.699567000000	-0.015486000000
O	2.088579000000	-0.253553000000	O	0.889149000000	-1.037523000000	0.004200000000
OHW1-3			OHW1-4			
O	-2.480166000000	-0.225627000000	O	-2.695230000000	-0.205130000000	-0.203207000000
H	-1.584923000000	0.023868000000	H	-3.233791000000	-0.254614000000	0.588830000000
H	-2.770025000000	-0.786453000000	H	-1.815849000000	-0.001060000000	0.130026000000
N	1.426979000000	0.183579000000	N	1.193728000000	-0.300156000000	0.434388000000
O	0.261963000000	0.863354000000	O	0.148143000000	0.598945000000	0.162690000000
H	0.334170000000	1.740240000000	H	0.409366000000	1.073909000000	-0.651914000000
O	1.472194000000	-0.920565000000	O	2.082609000000	-0.233458000000	-0.347940000000
OHW1-5			OHW1-6			
O	-2.819760000000	-0.260715000000	O	2.660478000000	-0.079470000000	0.000080000000
H	-3.399913000000	0.503108000000	H	2.878687000000	0.855168000000	-0.000974000000
H	-1.939466000000	0.125501000000	H	1.698805000000	-0.084145000000	0.000442000000
N	0.859386000000	-0.352868000000	N	-0.550009000000	-0.137309000000	0.000382000000
O	2.219007000000	-0.021067000000	O	-1.202593000000	1.076724000000	0.000000000000
H	2.641378000000	-0.892968000000	H	-2.157262000000	0.860451000000	-0.000593000000
O	0.186040000000	0.623586000000	O	-1.278928000000	-1.081043000000	-0.000202000000
OHW1-7			OHW2-1			
O	2.863315000000	-0.038340000000	O	1.706551000000	-1.240237000000	-0.069217000000
H	2.873368000000	-0.977860000000	H	1.971244000000	-0.303914000000	-0.040348000000
H	1.934159000000	0.195162000000	H	2.244711000000	-1.676427000000	0.595423000000
N	-0.855854000000	-0.408366000000	N	-1.111537000000	0.237065000000	0.014790000000
O	-2.202816000000	-0.210595000000	O	-0.980991000000	-1.115573000000	-0.041984000000
H	-2.324824000000	0.759417000000	H	0.001572000000	-1.247313000000	-0.041879000000
O	-0.221964000000	0.609164000000	O	-2.254828000000	0.590863000000	0.026236000000
OHW2-2			OHW2-3			
O	-2.060432000000	-1.316120000000	O	-0.884260000000	1.608469000000	-0.083197000000
H	-1.113463000000	-1.454132000000	H	-1.558120000000	0.911161000000	-0.009291000000
H	-2.478458000000	-2.008627000000	H	-1.210616000000	2.343468000000	0.440407000000
N	1.789502000000	0.434212000000	N	1.772382000000	-0.619480000000	0.020786000000
O	0.537067000000	-0.074982000000	O	1.671768000000	0.719665000000	0.029187000000
H	-0.072803000000	0.695862000000	H	0.707502000000	0.981958000000	-0.006024000000
O	2.624764000000	-0.408426000000	O	0.713862000000	-1.200628000000	-0.029777000000
O	-1.685520000000	1.439349000000	O	-2.254960000000	-0.790652000000	-0.045351000000
H	-2.158566000000	0.598062000000	H	-1.438302000000	-1.301903000000	-0.021257000000
H	-2.030257000000	2.010783000000	H	-2.878418000000	-1.293161000000	0.483762000000
OHW2-4			OHW2-5			
O	1.183497000000	1.143863000000	O	-1.119623000000	1.589801000000	0.148256000000
H	1.188245000000	1.578105000000	H	-1.237023000000	2.290736000000	-0.496793000000
H	1.935007000000	0.529707000000	H	-1.838871000000	0.960593000000	-0.019905000000
N	-1.858102000000	-0.064189000000	N	1.819959000000	-0.686041000000	0.007972000000
O	-1.168835000000	0.121501000000	O	0.478023000000	-0.586232000000	0.303385000000
H	-0.319029000000	0.514885000000	H	0.204065000000	0.367698000000	0.240537000000
O	-2.932538000000	-0.550632000000	O	2.337955000000	0.365743000000	-0.224592000000
O	3.308613000000	-0.702445000000	O	-2.364454000000	-0.878960000000	-0.221000000000
H	3.092665000000	-1.638551000000	H	-3.006365000000	-1.426339000000	0.236907000000
H	3.983925000000	-0.633121000000	H	-1.516733000000	-1.313218000000	-0.064945000000
OHW2-6			OHW2-7			
O	-0.853755000000	-0.628746000000	O	-2.835592000000	1.050906000000	-0.064784000000
H	-0.675841000000	-1.500863000000	H	-3.473388000000	1.291593000000	0.612578000000
H	-1.735675000000	-0.391602000000	H	-2.313913000000	1.847793000000	-0.199750000000
N	2.338511000000	0.346568000000	N	-0.010061000000	-0.390590000000	-0.021579000000
O	1.275964000000	1.038211000000	O	-1.161121000000	-1.121756000000	0.019289000000
H	0.516715000000	0.400602000000	H	-1.845306000000	-0.416313000000	0.002184000000
O	2.124483000000	-0.825085000000	O	0.964172000000	-1.087134000000	-0.006564000000
O	-3.409762000000	0.148224000000	O	3.171537000000	1.043484000000	0.025988000000

H -3.479933000000	0.866751000000	-0.969724000000	H 2.559974000000	0.300078000000	0.005339000000
H -4.090279000000	0.338310000000	0.315646000000	H 4.031086000000	0.626971000000	-0.060734000000
OHW2-8			OHW2-9		
O -3.034204000000	-0.057031000000	0.028424000000	O -4.045627000000	-0.404534000000	0.062575000000
H -3.066297000000	0.887103000000	0.209212000000	H -4.580932000000	-0.379434000000	-0.734585000000
H -3.760311000000	-0.432731000000	0.533537000000	H -4.624702000000	-0.051610000000	0.742836000000
N 0.389763000000	0.074548000000	-0.098264000000	N 2.061731000000	0.201786000000	0.261623000000
O -0.434889000000	-0.993957000000	-0.101586000000	O 3.383854000000	-0.090314000000	-0.125254000000
H -1.365683000000	-0.653165000000	-0.050787000000	H 3.860879000000	0.693700000000	0.184303000000
O -0.167321000000	1.140911000000	-0.041126000000	O 1.327168000000	-0.670364000000	-0.055149000000
O 3.526465000000	-0.188733000000	0.136833000000	O -1.422947000000	0.880416000000	-0.127327000000
H 2.569466000000	-0.201414000000	0.029948000000	H -0.764376000000	0.193160000000	-0.004529000000
H 3.774075000000	0.668843000000	-0.214419000000	H -2.262574000000	0.410059000000	-0.058149000000
OHW2-10			OHW2-11		
O -3.420269000000	-0.629461000000	0.381367000000	O 3.793419000000	-0.650878000000	0.099179000000
H -4.077802000000	-0.249393000000	0.969511000000	H 4.569855000000	-0.211851000000	0.455639000000
H -3.940803000000	-1.049529000000	-0.308012000000	H 4.123222000000	-1.114268000000	-0.674879000000
N 1.513951000000	-0.099334000000	-0.003072000000	N -1.904329000000	-0.553738000000	-0.035655000000
O 2.551478000000	0.524085000000	0.652764000000	O -3.233352000000	-0.347702000000	-0.311664000000
H 3.337685000000	-0.033788000000	0.483286000000	H -3.447092000000	0.526495000000	0.073801000000
O 1.832528000000	-1.100605000000	-0.569569000000	O -1.405152000000	0.340871000000	0.582382000000
O -1.383945000000	1.268202000000	-0.544222000000	O 1.484421000000	1.092691000000	-0.322152000000
H -0.537055000000	0.915475000000	-0.260674000000	H 0.754357000000	0.711383000000	0.170159000000
H -2.018022000000	0.614797000000	-0.225327000000	H 2.215266000000	0.484549000000	-0.157096000000
OHW3-1			OHW3-2		
O 0.968315000000	-1.888798000000	0.076788000000	H 0.846514000000	2.700972000000	-0.745390000000
H 1.682143000000	-1.221460000000	-0.002340000000	O 0.919393000000	2.001440000000	-0.092171000000
H 1.236586000000	-2.454771000000	0.804325000000	H 0.107824000000	1.481410000000	-0.196954000000
N -1.563694000000	0.190286000000	0.002610000000	H 1.208995000000	-2.575128000000	-0.724189000000
O -1.564510000000	-1.155001000000	-0.102475000000	O 0.938527000000	-1.917301000000	-0.079772000000
H -0.601651000000	-1.407027000000	-0.038211000000	H 1.721081000000	-1.344095000000	0.051861000000
O -2.666213000000	0.663417000000	-0.034493000000	H 2.280760000000	0.822659000000	0.103216000000
O 2.770709000000	0.131413000000	-0.070233000000	O 2.828285000000	0.023546000000	0.216146000000
H 2.204629000000	0.922847000000	-0.008413000000	H 3.356264000000	0.196861000000	0.998592000000
H 3.355693000000	0.301854000000	-0.811772000000	N -2.170242000000	-0.497922000000	0.227433000000
O 0.798366000000	2.032709000000	0.046136000000	O -0.967332000000	-0.105262000000	-0.365725000000
H 0.625423000000	2.757892000000	0.650895000000	O -2.964213000000	0.384656000000	0.220879000000
H -0.010294000000	1.498734000000	0.061469000000	H -0.367028000000	-0.893856000000	-0.274023000000
OHW3-3			OHW3-4		
O -2.078923000000	1.201274000000	0.007345000000	H 1.526188000000	2.601360000000	-0.602284000000
H -2.547614000000	1.659496000000	0.708507000000	O 1.544616000000	1.857317000000	0.003729000000
H -1.186291000000	1.605796000000	-0.005830000000	H 0.612845000000	1.644513000000	0.163689000000
N -0.179472000000	-1.108363000000	0.034846000000	H 0.079001000000	-2.528755000000	-0.408493000000
O -1.494670000000	-1.374189000000	-0.074255000000	O 0.278819000000	-1.839414000000	0.229110000000
H -1.872563000000	-0.453567000000	-0.026515000000	H 1.202375000000	-1.571897000000	0.047629000000
O 0.507194000000	-2.097493000000	-0.012999000000	H 2.432174000000	0.286018000000	-0.205138000000
O 2.521903000000	0.220355000000	-0.013395000000	O 2.690484000000	-0.653056000000	-0.244727000000
H 2.157403000000	-0.673255000000	0.000482000000	H 3.468236000000	-0.716095000000	0.313944000000
H 3.274555000000	0.182595000000	0.581489000000	N -2.219377000000	0.661351000000	-0.018752000000
O 0.479115000000	2.193368000000	-0.011224000000	O -0.930859000000	0.510286000000	0.445691000000
H 1.165047000000	1.504043000000	0.033346000000	O -2.724978000000	-0.361938000000	-0.374730000000
H 0.788816000000	2.786920000000	-0.699176000000	H -0.649836000000	-0.450163000000	0.349345000000
OHW3-5			OHW3-6		
O -0.693658000000	1.978541000000	-0.008663000000	O -1.153679000000	1.568032000000	-0.092749000000
H 0.261413000000	1.761236000000	-0.014314000000	H -1.473940000000	0.881243000000	-0.714849000000
H -0.781320000000	2.692324000000	0.627317000000	H -1.536711000000	2.396821000000	-0.389365000000
N -1.730838000000	-1.254505000000	-0.017991000000	O -1.862841000000	-0.749942000000	-1.287189000000
O -2.379344000000	-0.087358000000	0.030999000000	H -1.258710000000	-1.212174000000	-1.873742000000
H -1.704473000000	0.659378000000	0.009460000000	H -1.731443000000	-1.168776000000	-0.421293000000
O -0.527257000000	-1.142328000000	-0.099856000000	O -1.409497000000	-0.936398000000	1.477692000000
O 1.975241000000	1.347546000000	0.002009000000	H -0.670507000000	-1.222172000000	2.020802000000
H 2.158924000000	0.392327000000	0.049534000000	H -1.356315000000	0.026551000000	1.499682000000
H 2.542396000000	1.661211000000	-0.706189000000	N 1.587348000000	-0.120577000000	-0.452445000000
O 2.308848000000	-1.426082000000	0.015150000000	O 1.380147000000	0.837004000000	0.520389000000
H 1.406007000000	-1.765142000000	-0.009964000000	O 2.595519000000	-0.729852000000	-0.268469000000
H 2.762281000000	-1.982345000000	0.652980000000	H 0.519000000000	1.231794000000	0.248486000000

OHW3-7			OHW3-8		
O	1.132686000000	0.038179000000	O	-0.425043000000	2.178839000000
H	1.959418000000	-0.178534000000	H	-0.507717000000	2.945466000000
H	0.935763000000	0.956999000000	H	0.342925000000	1.680411000000
N	-1.838254000000	-0.268754000000	N	-1.526764000000	-0.785044000000
O	-1.091298000000	-1.278506000000	O	-2.261986000000	0.247494000000
H	-0.212855000000	-0.838595000000	H	-1.639822000000	1.019348000000
O	-2.947975000000	-0.611040000000	O	-2.129112000000	-1.820189000000
O	-0.214901000000	2.278056000000	O	1.301521000000	0.344870000000
H	-0.960340000000	1.670691000000	H	0.658984000000	-0.370379000000
H	-0.601951000000	3.081578000000	H	2.116546000000	-0.007147000000
O	3.570497000000	-0.651274000000	O	3.716786000000	-0.654261000000
H	4.418729000000	-0.487145000000	H	3.810995000000	-0.862386000000
H	3.736951000000	-0.527036000000	H	4.288111000000	-1.284034000000
OHW3-9			OHW3-10		
H	-1.168218000000	-0.434197000000	O	0.351915000000	-0.237362000000
O	-0.656920000000	-1.264772000000	H	-0.029428000000	-0.649178000000
H	-0.885987000000	-1.812889000000	H	1.072028000000	-0.835431000000
H	-1.093573000000	-1.158753000000	N	-2.941806000000	0.125100000000
O	-1.293296000000	-0.398861000000	O	-1.829857000000	0.345611000000
H	-1.581595000000	-0.772595000000	H	-1.039883000000	0.119399000000
H	-1.923170000000	0.857250000000	O	-2.714795000000	-0.272821000000
O	-1.982367000000	1.072911000000	O	2.718873000000	-1.341811000000
H	-1.434634000000	1.857643000000	H	2.991052000000	-1.732949000000
N	2.046627000000	0.516111000000	H	3.087546000000	-0.444518000000
O	1.871631000000	-0.797005000000	O	2.684591000000	1.409043000000
O	1.156290000000	1.230138000000	H	1.788657000000	1.285878000000
H	0.998091000000	-0.888525000000	H	3.036853000000	2.159820000000
OHW3-11			OHW3-12		
O	0.247245000000	-1.280551000000	O	-1.291143000000	-1.789820000000
H	-0.550692000000	-1.643038000000	H	-1.179629000000	-2.574597000000
H	0.998897000000	-1.611367000000	H	-2.034277000000	-1.301924000000
N	-0.260887000000	1.979450000000	N	-0.003920000000	1.111795000000
O	0.714998000000	1.256111000000	O	0.642980000000	0.009087000000
H	0.376597000000	0.322860000000	H	-0.044523000000	-0.712102000000
O	-1.311521000000	1.396430000000	O	0.699562000000	2.075596000000
O	2.606257000000	-0.809342000000	O	-2.839007000000	0.198626000000
H	2.495810000000	0.132973000000	H	-2.145229000000	0.854802000000
H	3.554275000000	-0.930992000000	H	-3.660448000000	0.655116000000
O	-2.212725000000	-1.524095000000	O	3.131989000000	-0.953537000000
H	-3.079859000000	-1.868060000000	H	3.915450000000	-0.484653000000
H	-2.322852000000	-0.566956000000	H	2.421045000000	-0.538816000000
OHW3-13			OHW3-14		
O	-2.159469000000	1.365213000000	O	-2.151217000000	0.856856000000
H	-2.588232000000	0.491585000000	H	-1.983177000000	0.829833000000
H	-2.646377000000	1.924312000000	H	-1.871510000000	1.735048000000
N	0.957271000000	-0.031989000000	N	1.844034000000	0.617234000000
O	0.510324000000	1.229875000000	O	2.065432000000	-0.631250000000
H	-0.494791000000	1.228193000000	H	2.684832000000	-1.089341000000
O	0.098085000000	-0.880924000000	O	1.087328000000	1.295191000000
O	4.067114000000	-0.433635000000	O	-1.252973000000	-0.147876000000
H	3.110230000000	-0.323675000000	H	-1.080713000000	-0.898817000000
H	4.390844000000	0.467807000000	H	-1.712491000000	-0.524698000000
O	-2.894586000000	-1.287263000000	O	-0.740526000000	-1.621152000000
H	-3.436778000000	-1.852629000000	H	-1.197105000000	-0.904148000000
H	-2.007528000000	-1.657791000000	H	0.187570000000	-1.482669000000
OHW3-15			OHW3-16		
O	-3.141415000000	-1.164136000000	O	-3.309408000000	-1.188616000000
H	-2.269468000000	-1.462041000000	H	-3.427356000000	-0.231616000000
H	-3.747640000000	-1.827680000000	H	-3.625014000000	-1.573107000000
N	0.772352000000	0.279519000000	N	2.566925000000	0.313763000000
O	-0.501561000000	-0.165754000000	O	3.929640000000	0.146831000000
H	-1.074067000000	0.628119000000	H	4.238561000000	1.062696000000
O	1.575102000000	-0.596436000000	O	2.026238000000	-0.736120000000
O	-2.510011000000	1.509931000000	O	-2.769727000000	1.558865000000
H	-3.055518000000	0.745256000000	H	-1.976844000000	1.201258000000
H	-2.633790000000	2.150882000000	H	-3.088556000000	2.239499000000
O	4.432890000000	0.198479000000	O	-0.937513000000	-0.218071000000
H	3.544678000000	-0.032906000000	H	-1.542393000000	-0.891681000000
H	4.989302000000	-0.414940000000	H	-0.060720000000	-0.506509000000

OHW3-17			OHW3-18				
O	-2.076322000000	1.525451000000	0.034721000000	O	1.972901000000	0.783319000000	0.327405000000
H	-2.009885000000	2.202828000000	-0.642550000000	H	1.951034000000	1.537492000000	-0.267380000000
H	-2.751167000000	0.903403000000	-0.279828000000	H	2.754712000000	0.270256000000	0.064467000000
N	0.846352000000	-0.548153000000	0.429414000000	N	-1.383755000000	0.241093000000	0.101782000000
O	-0.496710000000	-0.542318000000	0.610988000000	O	-0.383987000000	-0.455102000000	0.671125000000
H	-0.847825000000	0.377141000000	0.429508000000	H	0.469813000000	0.048751000000	0.527850000000
O	1.299837000000	0.526422000000	0.131230000000	O	-1.049471000000	1.276308000000	-0.419814000000
O	-3.216191000000	-0.947353000000	-0.520099000000	O	-4.289031000000	-0.879672000000	-0.206375000000
H	-3.977477000000	-1.478891000000	-0.276104000000	H	-3.382000000000	-0.602129000000	-0.035919000000
H	-2.459195000000	-1.423093000000	-0.159799000000	H	-4.732582000000	-0.054896000000	-0.413964000000
O	4.288661000000	-0.066019000000	-0.473568000000	O	4.206315000000	-0.767728000000	-0.380721000000
H	4.335850000000	-0.933220000000	-0.066009000000	H	4.894698000000	-0.918071000000	0.272686000000
H	3.391035000000	0.219445000000	-0.277299000000	H	4.076790000000	-1.626054000000	-0.793171000000
OHW3-19			OHW3-20				
O	-3.232350000000	-1.277021000000	-0.338042000000	O	-3.699551000000	-0.807179000000	-0.126081000000
H	-3.425087000000	-0.330433000000	-0.436763000000	H	-3.913223000000	-0.280872000000	-0.902167000000
H	-3.518640000000	-1.672094000000	-1.163648000000	H	-4.532694000000	-0.920351000000	0.339093000000
N	2.592876000000	0.337423000000	-0.306927000000	N	-0.569417000000	0.559977000000	0.062401000000
O	3.957026000000	0.259460000000	-0.294815000000	O	-1.211351000000	-0.256965000000	0.920062000000
H	4.171244000000	-0.573677000000	0.173494000000	H	-2.114995000000	-0.433777000000	0.547378000000
O	2.059410000000	-0.593654000000	0.227758000000	O	-1.209854000000	0.889113000000	-0.903151000000
O	-2.908372000000	1.497947000000	-0.212586000000	O	2.435338000000	1.024370000000	0.422289000000
H	-2.083846000000	1.213279000000	0.217640000000	H	1.477454000000	0.913906000000	0.365963000000
H	-3.267467000000	2.170903000000	0.369047000000	H	2.599973000000	1.857078000000	-0.026331000000
O	-0.936794000000	-0.133000000000	0.855536000000	O	4.005204000000	-1.231693000000	-0.436324000000
H	-1.494440000000	-0.843418000000	0.504791000000	H	3.474271000000	-0.477096000000	-0.144721000000
H	-0.043257000000	-0.356376000000	0.581121000000	H	4.436843000000	-1.519887000000	0.369625000000
OHW4-1			OHW4-2				
O	0.253468000000	-2.234857000000	-0.147229000000	O	0.102421000000	-2.147328000000	0.532009000000
H	1.187164000000	-1.934775000000	-0.093664000000	H	0.974004000000	-1.879248000000	0.167342000000
H	0.158536000000	-2.886699000000	0.551143000000	H	0.285330000000	-2.481992000000	1.412381000000
N	-2.558638000000	-0.526392000000	0.292375000000	N	-1.996010000000	0.257671000000	-0.076434000000
O	-1.383780000000	-0.198710000000	-0.374623000000	O	-2.186091000000	-1.072362000000	-0.144451000000
H	-0.807106000000	-1.010159000000	-0.270867000000	H	-1.304101000000	-1.457461000000	0.122824000000
O	-3.338978000000	0.370860000000	0.271071000000	O	-2.975230000000	0.888991000000	-0.371784000000
O	2.605736000000	1.458236000000	0.291116000000	O	2.794316000000	1.324417000000	-0.147006000000
H	2.841520000000	1.915300000000	1.101270000000	H	3.374614000000	1.723878000000	0.504620000000
H	1.718784000000	1.799969000000	0.067135000000	H	1.913134000000	1.696055000000	0.046535000000
O	2.760860000000	-1.251218000000	0.026189000000	O	2.504924000000	-1.369488000000	-0.400062000000
H	3.426586000000	-1.409293000000	-0.646630000000	H	2.843805000000	-1.625618000000	-1.260390000000
H	2.756246000000	-0.279477000000	0.146451000000	H	2.683364000000	-0.409512000000	-0.329754000000
O	0.032581000000	2.252350000000	-0.266262000000	O	0.237937000000	2.155164000000	0.456698000000
H	-0.246893000000	2.828120000000	-0.981587000000	H	-0.198094000000	2.938764000000	0.112442000000
H	-0.563470000000	1.488469000000	-0.321983000000	H	-0.426196000000	1.456280000000	0.355812000000
OHW4-3			OHW4-4				
O	-0.301779000000	1.146672000000	1.180493000000	O	0.367891000000	-1.425999000000	1.008269000000
H	-0.271715000000	1.809519000000	1.874976000000	H	1.186064000000	-1.526872000000	0.482595000000
H	-1.011341000000	1.439950000000	0.563087000000	H	0.535862000000	-0.633060000000	1.530064000000
N	2.851102000000	0.434742000000	-0.295339000000	N	-2.057151000000	0.142082000000	-0.206727000000
O	1.724821000000	-0.281303000000	0.099603000000	O	-1.893927000000	-1.191167000000	-0.270555000000
H	1.117970000000	0.409659000000	0.450865000000	H	-1.020357000000	-1.335212000000	0.205716000000
O	3.688070000000	-0.279075000000	-0.744018000000	O	-3.064465000000	0.526947000000	-0.734638000000
O	-2.318089000000	1.633374000000	-0.514770000000	O	0.150957000000	1.562773000000	1.097842000000
H	-2.675015000000	0.739182000000	-0.692819000000	H	-0.668805000000	1.238140000000	0.687207000000
H	-2.246269000000	2.047997000000	-1.377439000000	H	-0.118314000000	2.311370000000	1.636655000000
O	-2.949427000000	-0.996029000000	-0.816289000000	O	2.695198000000	-1.269379000000	-0.419603000000
H	-2.246704000000	-1.401816000000	-0.272761000000	H	2.714778000000	-0.327837000000	-0.667571000000
H	-3.748190000000	-1.477940000000	-0.591953000000	H	3.074391000000	-1.743682000000	-1.161750000000
O	-0.866996000000	-1.699147000000	0.841252000000	O	2.356853000000	1.467042000000	-0.654422000000
H	-0.680835000000	-0.841653000000	1.248663000000	H	2.195192000000	2.043061000000	-1.404609000000
H	-0.008412000000	-1.964028000000	0.494582000000	H	1.601189000000	1.617788000000	-0.061966000000
OHW4-5			OHW4-6				
O	-0.762741000000	-0.072741000000	2.139985000000	O	-0.408880000000	-1.942242000000	-0.400971000000
H	-1.158615000000	0.049611000000	3.005275000000	H	0.562366000000	-1.956122000000	-0.256785000000
H	-0.941859000000	0.744594000000	1.652287000000	H	-0.766773000000	-2.596926000000	0.203732000000
O	-0.989729000000	1.711130000000	-0.028938000000	N	-2.607626000000	0.644420000000	0.182899000000
H	-1.199299000000	2.622733000000	-0.249117000000	O	-1.386052000000	0.493996000000	-0.438539000000
H	-1.565908000000	1.163789000000	-0.611990000000	H	-1.100145000000	-0.475117000000	-0.396297000000
O	-2.277316000000	-0.123481000000	-1.478746000000	O	-3.070663000000	-0.380660000000	0.588929000000
H	-3.201058000000	-0.350247000000	-1.604432000000	O	2.897025000000	0.812911000000	0.431099000000
H	-1.878843000000	-0.893796000000	-1.018154000000	H	3.197972000000	1.161782000000	1.272901000000
O	-0.943832000000	-1.913717000000	0.044537000000	H	2.170304000000	1.408393000000	0.164760000000

H -0.90061200000	-1.44440000000	0.89505900000	O 2.25609300000	-1.80948900000	0.03177900000
H -0.01918700000	-1.95889900000	-0.21875900000	H 2.90063000000	-2.14245400000	-0.59645300000
N 1.80948300000	-0.26336600000	-0.31522700000	H 2.53533400000	-0.88764100000	0.20682700000
O 1.71084000000	1.10441400000	-0.22926600000	O 0.72941000000	-0.35332400000	-0.27494700000
O 2.94486700000	-0.62511300000	-0.38121600000	H 0.69068200000	2.94354000000	-1.03088800000
H 0.74229500000	1.26622800000	-0.17442500000	H -0.07245100000	1.81088100000	-0.34689900000
OHW4-7			OHW4-8		
O 2.71274400000	0.27107000000	0.23600400000	O -0.71264000000	-0.41580800000	1.63666700000
H 3.57937000000	0.44845800000	-0.13532100000	H -1.23955900000	-1.05282800000	1.10085100000
H 2.15973500000	1.04584800000	-0.00721600000	H -0.67681700000	-0.78776400000	2.52167100000
N 0.12159200000	-1.40546500000	0.01193600000	N 2.53963400000	-0.25434100000	0.36374600000
O 1.34399900000	-1.94906700000	0.05365900000	O 1.30991100000	0.22660400000	-0.08223800000
H 1.93283300000	-1.14154000000	0.10592400000	H 0.68910300000	-0.03422600000	0.63723300000
O -0.75161700000	-2.23869000000	-0.04881600000	O 3.40603900000	-0.02991100000	-0.41707700000
O 1.09176500000	2.35112000000	-0.37150300000	O -1.77514600000	1.95390600000	0.38202500000
H 1.02148500000	2.77214600000	-1.23087100000	H -1.46321600000	1.33141400000	1.05435800000
H 0.16273500000	2.24038700000	-0.08399500000	H -1.43209500000	2.80664000000	0.65828200000
O -1.53227000000	2.12273600000	0.37764500000	O -2.07196100000	-1.75999300000	-0.22095800000
H -2.02368400000	1.30459200000	0.18244400000	H -1.81719500000	-1.14068200000	-0.93765900000
O -1.78561000000	2.35031800000	1.27460700000	H -2.01735100000	-2.63669900000	-0.60669100000
H -2.84965800000	-0.25497200000	-0.24611500000	O -1.17724500000	0.26963300000	-1.79322900000
H -2.28744300000	-1.04082500000	-0.17975800000	H -1.43692400000	1.01953500000	-1.23269800000
H -3.73027000000	-0.55870600000	-0.01636000000	H -0.21504400000	0.31955200000	-1.78308400000
OHW4-9			OHW4-10		
O 0.22930300000	1.53536800000	0.88066400000	O 2.50782200000	-0.91091900000	0.09524400000
H 1.09200700000	1.62662400000	0.43385300000	H 2.51700400000	0.04736300000	-0.12221500000
H -0.41240500000	2.03815900000	0.35628200000	H 3.10559700000	-1.00840000000	0.83986900000
N -1.56668600000	-0.93906300000	0.04355300000	N -0.65561600000	-1.18807300000	0.13964700000
O -0.38988700000	-0.94178300000	0.73171500000	O 0.22077000000	-2.14812500000	-0.17496700000
H -0.17446300000	0.04841800000	0.85260100000	H 1.10784800000	-1.70515300000	-0.03026300000
O -1.93614700000	-2.04076600000	-0.24356500000	O -1.80172100000	-1.52559000000	-0.03121700000
O -2.05929100000	2.04104900000	-0.64527100000	O 2.32539100000	1.73871600000	-0.37551900000
H -2.30343900000	1.11238000000	-0.55003500000	H 1.41701100000	1.97619400000	-0.10053600000
H -2.88568100000	2.52316100000	-0.56863900000	H 2.47197700000	2.19924200000	-1.20425200000
O 2.65393800000	1.18190700000	-0.36933600000	O -0.18779600000	1.81555800000	0.65158000000
H 2.65047400000	0.21071500000	-0.42779800000	H -1.07139900000	1.98275300000	0.29210200000
H 3.52167300000	1.40292200000	-0.02465500000	H -0.22215800000	0.86128800000	0.78933300000
O 2.23231700000	-1.58252700000	-0.28831100000	O -2.83753900000	1.29091300000	-0.31111600000
H 1.32886600000	-1.66372700000	0.04900600000	H -3.72914300000	1.54743000000	-0.06574500000
H 2.30790100000	-2.27118700000	-0.95266100000	H -2.82283400000	0.33137100000	-0.20786000000
OHW4-11			OHW4-12		
H 0.31107800000	0.37698000000	1.62041700000	O 0.00445800000	-0.87028300000	-1.17131400000
O -0.00137700000	0.14076700000	0.74144300000	H 0.20101200000	-1.45008800000	-1.91158600000
H -0.64165200000	0.85466100000	0.51119900000	H -0.69203400000	-1.33360500000	-0.65202800000
H -4.33776200000	-0.24042500000	-1.15009600000	N 2.97542300000	0.41748900000	0.59542700000
O -3.81966400000	-0.03019900000	-0.37044500000	O 1.69051600000	0.74411100000	0.23942100000
H -3.25674800000	-0.81287400000	-0.22634600000	H 1.28766900000	-0.03228800000	-0.23035500000
H -2.70710300000	1.34351300000	-0.12254900000	O 3.29850800000	-0.68797500000	0.26805600000
O -1.93202600000	1.88832900000	0.11992800000	O -2.03632000000	-1.83840600000	0.27911500000
H -1.88867000000	2.57934700000	-0.54457900000	H -2.55433800000	-1.03544100000	0.49175200000
H -1.11065700000	-1.36560600000	0.41226600000	H -1.97251700000	-2.31900000000	1.10745000000
O -1.85284200000	-1.90789100000	0.09852500000	O -3.12819700000	0.61605200000	0.72438800000
H -1.81617500000	-2.71023300000	0.62341400000	H -2.45341500000	1.17388000000	0.29126400000
N 3.17853600000	0.07443400000	0.24485100000	H -3.97027000000	0.98308400000	0.44728700000
O 2.27324100000	-0.15185200000	-0.77098900000	O -1.04375500000	1.77912900000	-0.64361200000
O 4.30556400000	-0.00063700000	-0.13562700000	H -0.67793800000	0.99991500000	-1.08662700000
H 1.41477800000	-0.05454000000	-0.30035500000	H -0.27779900000	2.15008700000	-0.19358000000
OHW4-13			OHW4-14		
O -1.90508900000	-1.51934000000	-0.19826400000	O -1.82061500000	1.76926100000	0.01946200000
H -1.31720800000	-2.10252700000	-0.68619100000	H -0.85917300000	1.94484900000	-0.07553300000
H -1.41909400000	-1.34825400000	0.62761400000	H -2.12234900000	2.40290800000	0.67453500000
O -0.41492000000	-0.58108500000	1.96934100000	N -1.69991800000	-1.61196000000	0.01359800000
H -0.58711600000	-0.57539100000	2.91346000000	O -2.67693400000	-0.71855100000	0.12601400000
H -0.26450700000	0.34647100000	1.73064600000	H -2.28416500000	0.21274000000	0.08294800000
O -0.02958100000	1.79950600000	0.49989100000	O -0.59742500000	-1.12137600000	-0.12964900000
H 0.01145400000	2.75161800000	0.62211800000	O 0.81178500000	2.36675800000	-0.21166600000
O -0.77176500000	1.64873600000	-0.13164800000	H 1.51566800000	1.71600000000	-0.01833800000
H -1.99052700000	1.02292500000	-1.15231100000	H 1.11853900000	2.81629500000	-1.00215700000
H -2.04676800000	0.07230200000	-0.91348400000	O 2.84876700000	0.58419900000	0.24089300000
H -2.90234300000	1.31365800000	-1.22397600000	H 2.65379200000	-0.36228900000	0.11220400000
N 2.18106600000	-0.72391700000	-0.63227400000	H 3.36319700000	0.61533900000	1.05042400000
O 2.38072500000	0.49990300000	-0.07364500000	O 2.06859300000	-2.05250600000	-0.05337100000

O	1.026613000000	-0.967348000000	-0.864372000000	H	1.104710000000	-1.999568000000	-0.128591000000
H	1.492116000000	0.924308000000	0.042251000000	H	2.335832000000	-2.684824000000	-0.724137000000
OHW4-15				OHW4-16			
O	-1.356274000000	-1.449790000000	-0.802482000000	O	-0.487280000000	-0.929405000000	-1.683227000000
H	-2.053682000000	-1.362634000000	-0.135699000000	H	-1.288784000000	-0.395614000000	-1.710084000000
H	-1.220452000000	-0.522022000000	-1.049328000000	H	0.211435000000	-0.303564000000	-1.899495000000
N	1.382510000000	-0.699761000000	0.055783000000	N	2.032377000000	0.276317000000	-0.256245000000
O	1.050623000000	-1.996585000000	0.054819000000	O	1.308716000000	0.591110000000	0.877504000000
H	0.100692000000	-1.943773000000	-0.265741000000	H	0.567732000000	1.142102000000	0.520711000000
O	2.512202000000	-0.497143000000	0.432968000000	O	2.981853000000	-0.399167000000	-0.005928000000
O	-1.112810000000	1.479248000000	-0.680501000000	O	-2.730839000000	0.099139000000	0.193004000000
H	-0.212378000000	1.741908000000	-0.410797000000	H	-2.216559000000	-0.595427000000	0.656136000000
H	-1.360860000000	2.132804000000	-1.339628000000	H	-3.630211000000	0.022844000000	0.518406000000
O	-2.980691000000	0.076068000000	0.932385000000	O	-0.871408000000	-1.696362000000	1.005022000000
H	-2.405618000000	0.777867000000	0.592766000000	H	-0.537576000000	-1.669807000000	0.092775000000
H	-3.170815000000	0.320951000000	1.839808000000	H	-0.126863000000	-1.372734000000	1.522169000000
O	1.490710000000	2.295712000000	0.005423000000	O	-0.778997000000	1.947296000000	-0.133454000000
H	2.071885000000	1.542603000000	0.176861000000	H	-1.611787000000	1.464502000000	0.034089000000
H	1.743573000000	2.950550000000	0.660389000000	H	-0.970383000000	2.872592000000	0.035635000000
OHW4-17				OHW4-18			
H	0.591606000000	-0.474635000000	-1.326210000000	O	-0.013668000000	-1.603910000000	-0.788210000000
O	0.182645000000	-0.229020000000	-0.489857000000	H	0.915440000000	-1.679385000000	-0.493616000000
H	-0.508603000000	-0.914096000000	-0.334948000000	H	-0.542927000000	-2.128618000000	-0.173463000000
H	-4.310470000000	0.380548000000	0.892746000000	N	-0.585995000000	1.552709000000	-0.160578000000
O	-3.721303000000	0.334530000000	0.177027000000	O	-1.369574000000	0.568148000000	-0.653780000000
H	-3.106752000000	0.885277000000	0.088776000000	H	-0.745671000000	-0.223683000000	-0.765374000000
H	-2.659063000000	-1.298409000000	0.058715000000	O	-1.191769000000	2.561428000000	0.074325000000
O	-1.891109000000	-1.884530000000	-0.092318000000	O	2.581616000000	-1.479944000000	0.071155000000
H	-1.962887000000	-2.572831000000	0.572480000000	H	2.665769000000	-0.528447000000	0.260885000000
H	-0.884242000000	1.319980000000	-0.297801000000	H	3.343053000000	-1.691517000000	-0.473250000000
O	-1.628403000000	1.909313000000	-0.090291000000	O	2.354070000000	1.249875000000	0.445932000000
H	-1.498647000000	2.680253000000	-0.646594000000	H	2.540681000000	1.787607000000	1.219093000000
N	3.478199000000	0.077441000000	0.310766000000	H	1.423960000000	1.430066000000	0.243832000000
O	2.396603000000	0.071792000000	1.131907000000	O	-2.328557000000	-1.859653000000	0.825690000000
O	3.211909000000	-0.063196000000	-0.854916000000	H	-3.148153000000	-2.333040000000	0.984810000000
H	1.588935000000	-0.050671000000	0.565058000000	H	-2.607132000000	-0.989496000000	0.520232000000
OHW4-19				OHW4-20			
O	0.026701000000	-1.089334000000	1.140422000000	O	-0.712273000000	0.210006000000	-0.097890000000
H	0.826243000000	-1.451392000000	0.712196000000	H	-1.349662000000	0.266973000000	0.638107000000
H	0.316529000000	-0.225873000000	1.458562000000	H	-0.328416000000	1.099994000000	-0.186743000000
N	-2.680711000000	-0.042801000000	-0.683586000000	N	2.430441000000	-0.347292000000	0.062559000000
O	-2.158617000000	-1.201476000000	-0.297960000000	O	1.474536000000	-1.310129000000	0.121672000000
H	-1.316130000000	-1.059293000000	0.251167000000	H	0.626065000000	-0.792152000000	0.073931000000
O	-2.074260000000	0.942626000000	-0.311749000000	O	3.541198000000	-0.792523000000	0.169688000000
O	0.416453000000	1.796401000000	0.878458000000	O	1.049323000000	2.326496000000	-0.223612000000
H	-0.465544000000	1.646695000000	0.507295000000	H	1.787721000000	1.705596000000	-0.162222000000
H	0.344875000000	2.618568000000	1.370779000000	H	1.333039000000	2.994353000000	-0.852029000000
O	2.407524000000	-1.633866000000	-0.119746000000	O	-2.984213000000	-0.028176000000	1.440677000000
H	2.602329000000	-0.770851000000	-0.524640000000	H	-3.433640000000	-0.279857000000	0.618641000000
H	2.733167000000	-2.291546000000	-0.736935000000	H	-3.602238000000	0.538023000000	1.907359000000
O	2.556135000000	1.048263000000	-0.827653000000	O	-3.187765000000	-0.577038000000	-1.276259000000
H	2.486737000000	1.510797000000	-1.665499000000	H	-2.240448000000	-0.377442000000	-1.232980000000
H	1.845290000000	1.421600000000	-0.282003000000	H	-3.251967000000	-1.353540000000	-1.836193000000
OHW4-21				OHW4-22			
O	-1.026862000000	2.181264000000	-0.273706000000	O	-2.130811000000	1.551523000000	0.550199000000
H	-0.894872000000	2.947633000000	0.288855000000	H	-2.305738000000	1.906606000000	1.424668000000
H	-0.209032000000	1.654593000000	-0.194822000000	H	-1.348713000000	2.049948000000	0.227675000000
N	-2.118617000000	-0.769102000000	0.082669000000	N	-0.986231000000	-1.450259000000	-0.141415000000
O	-2.938986000000	0.312655000000	-0.014210000000	O	-2.241497000000	-1.069413000000	0.189678000000
H	-2.302715000000	1.067790000000	-0.103223000000	H	-2.172004000000	-0.083251000000	0.316655000000
O	-2.721325000000	-1.795874000000	0.202903000000	O	-0.891326000000	-2.633164000000	-0.316863000000
O	0.800825000000	0.160509000000	-0.000321000000	O	0.145447000000	2.721388000000	-0.314971000000
H	0.057533000000	-0.457233000000	-0.010582000000	H	0.717265000000	1.940733000000	-0.474720000000
H	1.414697000000	-0.152060000000	-0.690637000000	H	0.215036000000	3.246628000000	-1.115059000000
O	3.046957000000	-0.685697000000	-1.344489000000	O	3.744861000000	-0.616916000000	0.604299000000
H	3.607103000000	-0.314346000000	-2.029260000000	H	4.303558000000	-0.057418000000	1.149756000000
H	3.520979000000	-0.531881000000	-0.512318000000	H	4.362351000000	-1.156042000000	0.103299000000
O	3.316052000000	0.014340000000	1.334090000000	O	1.401354000000	0.366000000000	-0.698213000000
H	2.352851000000	0.087401000000	1.261482000000	H	0.715554000000	-0.288100000000	-0.509115000000
H	3.470488000000	-0.415756000000	2.177673000000	H	2.192092000000	0.037373000000	-0.246282000000

OHW4-23			OHW4-24				
O	0.21946600000	1.19851400000	0.85879000000	O	0.25945200000	-1.63596400000	0.76912400000
H	0.98983200000	1.60757800000	0.43462700000	H	0.64505100000	-0.77122300000	0.97669600000
H	-0.57477600000	1.60534300000	0.46500100000	H	0.91010800000	-1.98780200000	0.14343400000
N	0.89834200000	-2.00321800000	-0.06317500000	N	-2.50821400000	-0.11004400000	-0.31864300000
O	-0.08884700000	-1.32369400000	0.56117500000	O	-2.21538700000	-1.38760700000	-0.09235600000
H	0.16133100000	-0.33206600000	0.68908600000	H	-1.26595900000	-1.45256700000	0.25948200000
O	1.88960600000	-1.35148000000	-0.28052700000	O	-1.62579500000	0.66220500000	-0.00153700000
O	-2.21200700000	1.80931100000	-0.28802200000	O	1.86499800000	0.81190300000	0.73538500000
H	-2.92196200000	2.30928200000	0.12034800000	H	1.34651800000	1.54714900000	0.35420200000
H	-2.56060700000	0.90377900000	-0.36614500000	H	2.31449800000	1.20400700000	1.48836500000
O	-2.79681800000	-0.91692300000	-0.29852300000	O	0.21317200000	2.79923800000	-0.23765000000
H	-3.12370500000	-1.50160500000	-0.98588400000	H	-0.65227000000	2.37337900000	-0.28956100000
H	-1.96051300000	-1.31364200000	-0.01402500000	H	0.28640600000	3.30877700000	-1.04816900000
O	2.71082400000	1.59481300000	-0.34073000000	O	2.50223300000	-1.40278300000	-0.93131900000
H	2.81449600000	0.64887100000	-0.48975600000	H	3.40371500000	-1.67304600000	-1.11587300000
H	3.10972300000	2.01065800000	-1.10832900000	H	2.58004300000	-0.55430200000	-0.47124400000
OHW4-25			OHW4-26				
O	-2.53954800000	-0.49078000000	-0.18791200000	O	-1.55757800000	-0.01129100000	-0.77969300000
H	-2.93141700000	-0.67377100000	0.66973000000	H	-2.36604700000	0.10952500000	-0.26107600000
H	-2.31158800000	0.46288300000	-0.15982000000	H	-1.02330900000	0.79255700000	-0.63260500000
N	0.58654000000	-1.70579000000	0.12598600000	N	1.11217300000	-1.06549400000	0.02687100000
O	-0.23656700000	-1.50669400000	-0.91239900000	O	0.14109100000	-1.90918700000	-0.34329100000
H	-1.15474500000	-1.26462500000	-0.56379700000	H	-0.61061300000	-1.26075300000	-0.52340100000
O	0.05712300000	-1.72592000000	1.21128200000	O	2.15401700000	-1.61980200000	0.28649400000
O	-1.64166400000	2.06358700000	-0.09387400000	O	0.15078000000	2.13902800000	-0.32216100000
H	-1.80429900000	2.70937100000	-0.78481100000	H	1.04106800000	1.85740400000	-0.05040500000
H	-0.67770200000	2.10668600000	0.06128600000	H	0.31360600000	2.81153100000	-0.98726500000
O	1.06142600000	2.18499300000	0.40218700000	O	-4.01631000000	0.18897500000	0.66165700000
H	1.69662800000	1.52738100000	0.06837200000	H	-4.80191500000	-0.11652000000	0.20077100000
H	1.33779400000	2.34630000000	1.30700500000	H	-4.10655800000	-0.16922800000	1.54844300000
O	2.76216300000	0.15523000000	-0.50583600000	O	2.82156300000	1.37686000000	0.36845700000
H	3.70084300000	-0.01259500000	-0.39761300000	H	2.89200600000	0.41591200000	0.42916400000
H	2.33525200000	-0.70441900000	-0.38984000000	H	3.32804300000	1.70136300000	1.11657900000
OHW4-27			OHW4-28				
O	-1.10894000000	1.77775600000	-0.50233600000	O	-0.52041700000	0.28652300000	-0.06255700000
H	-0.96035900000	2.64130200000	-0.11043000000	H	-1.18473700000	0.37216700000	0.64577600000
H	-0.28220100000	1.27868800000	-0.36066000000	H	-0.09943300000	1.16066700000	-0.14192700000
N	-3.04224500000	-0.98202500000	0.26351100000	N	2.57451700000	-1.27833200000	-0.13178000000
O	-3.31623300000	0.31064800000	0.01968500000	O	1.29466300000	-1.67703800000	0.18249000000
H	-2.46412800000	0.80413600000	-0.16080300000	H	0.68565600000	-0.88056400000	0.12037600000
O	-1.86829300000	-1.26424400000	0.20863800000	O	2.72482700000	-0.08298100000	0.02513600000
O	0.88566000000	-0.04697000000	-0.01697100000	O	1.17778700000	2.46383700000	-0.19811300000
H	0.24388300000	-0.76507500000	0.02530700000	H	1.97073500000	1.91673200000	-0.16428700000
H	1.55652500000	-0.33326300000	-0.66489100000	H	1.36992100000	3.14060800000	-0.85146400000
O	3.25920200000	-0.67697800000	-1.24924200000	O	-2.85951600000	0.09798300000	1.38950100000
H	3.76376000000	-0.29644100000	-1.97130300000	H	-3.27028400000	-0.18078000000	0.55594300000
H	3.69092500000	-0.36239400000	-0.43963200000	H	-3.50208200000	0.67132800000	1.81214900000
O	3.36866000000	0.34779700000	1.33393400000	O	-2.94493900000	-0.53655100000	-1.31579200000
H	2.40696200000	0.25917900000	1.26241000000	H	-2.00372200000	-0.31998600000	-1.23372700000
H	3.57990400000	0.06397500000	2.22576400000	H	-2.96691300000	-1.34603400000	-1.83060800000
OHW4-29			OHW4-30				
O	-0.74049600000	-1.24381500000	-0.84846300000	H	1.96833600000	2.71305700000	-0.66488700000
H	0.14408600000	-1.56761600000	-0.58883700000	O	1.93342700000	1.99753400000	-0.02588700000
H	-1.37250800000	-1.65974600000	-0.24783000000	H	1.10489600000	1.53571700000	-0.21877200000
N	-0.56197200000	2.07003300000	-0.06661300000	H	2.06362600000	-2.58263300000	-0.68208000000
O	-1.49300900000	1.18641300000	-0.45686700000	O	1.77236500000	-1.90957400000	-0.06278100000
H	-1.04982200000	0.29159300000	-0.68507000000	H	2.56954100000	-1.38168800000	0.15111600000
O	0.57000400000	1.65170600000	-0.14566900000	H	3.21739000000	0.75034800000	0.29249100000
O	-2.96854500000	-1.00703300000	0.90042300000	O	3.70943400000	-0.07767000000	0.44177300000
H	-3.89139400000	-1.22154400000	1.05289000000	H	4.17379000000	0.05706900000	1.27080800000
H	-2.97132900000	-0.06993200000	0.67814900000	N	-1.27002700000	-0.44598000000	-0.12342500000
O	3.12322000000	0.38159200000	0.54004300000	O	-0.01010600000	-0.05626700000	-0.50459700000
H	3.54934000000	0.61261300000	1.36886600000	O	-2.05016200000	0.45572200000	-0.21010400000
H	2.47157100000	1.07785200000	0.39956000000	H	0.56798000000	-0.86194500000	-0.36546800000
O	1.80332700000	-2.00043200000	-0.10799700000	O	-5.02064400000	-0.14124700000	0.41125500000
H	2.36972400000	-2.47670300000	-0.71912100000	H	-4.08224800000	-0.00848700000	0.24556300000
H	2.32812600000	-1.22481700000	0.15592500000	H	-5.36762900000	0.75244200000	0.43792400000

OHW4-31			OHW4-32		
O 0.614406000000	2.397554000000	-0.093746000000	O 1.747460000000	1.940549000000	0.362110000000
H 0.568138000000	3.013386000000	0.641536000000	H 2.373279000000	1.486091000000	-0.234725000000
H 1.424973000000	1.868426000000	0.065179000000	H 2.289025000000	2.566726000000	0.846987000000
N -0.328781000000	-0.442759000000	-0.371241000000	N -2.820024000000	-0.212014000000	-0.530494000000
O -1.188938000000	0.580771000000	-0.597241000000	O -4.115228000000	0.082810000000	-0.854250000000
H -0.602416000000	1.373602000000	-0.413714000000	H -4.522905000000	0.424399000000	-0.031901000000
O -0.842236000000	-1.520093000000	-0.515144000000	O -2.554501000000	0.014153000000	0.616385000000
O 2.769297000000	0.779260000000	0.344556000000	O 2.194671000000	-1.907945000000	-0.004385000000
H 2.559919000000	-0.171211000000	0.335846000000	H 1.499642000000	-1.454388000000	0.515382000000
H 3.576491000000	0.848788000000	-0.170330000000	H 2.587014000000	-2.533317000000	0.608255000000
O -3.801183000000	-0.036298000000	0.734323000000	O 0.449056000000	-0.299662000000	1.342643000000
H -4.087521000000	-0.839585000000	0.294842000000	H 0.819540000000	0.570809000000	1.106210000000
H -3.031342000000	0.226982000000	0.219181000000	H -0.488870000000	-0.224880000000	1.145145000000
O 2.217661000000	-1.999379000000	0.218837000000	O 3.371503000000	0.297126000000	-1.132012000000
H 1.298290000000	-2.189964000000	0.000842000000	H 3.376901000000	0.201164000000	-2.086605000000
H 2.442886000000	-2.645632000000	0.892631000000	H 3.062852000000	-0.568747000000	-0.799227000000
OHW4-33			OHW4-34		
H 4.810758000000	0.400982000000	0.408312000000	O 1.099379000000	-0.457326000000	0.193272000000
O 4.114045000000	0.151870000000	-0.202345000000	H 0.590651000000	-1.212385000000	0.505042000000
H 3.476431000000	0.891236000000	-0.156568000000	H 1.856005000000	-0.838197000000	-0.298807000000
H -0.555640000000	-0.310082000000	0.088733000000	N -1.901887000000	0.846883000000	-0.656907000000
O 0.288436000000	-0.082378000000	0.487417000000	O -0.659104000000	1.260626000000	-0.944797000000
H 0.867806000000	-0.847285000000	0.315584000000	H -0.013777000000	0.611182000000	-0.542841000000
H 1.309867000000	1.345422000000	0.174915000000	O -1.946842000000	-0.175954000000	-0.010739000000
O 2.054498000000	1.957914000000	0.009846000000	O 3.532940000000	-1.162335000000	-0.779877000000
H 1.747354000000	2.526705000000	-0.698991000000	H 3.934405000000	-0.513687000000	-0.180468000000
H 3.044260000000	-1.314569000000	-0.105751000000	H 3.953030000000	-1.018417000000	-1.630828000000
O 2.279737000000	-1.919776000000	-0.065992000000	O -4.854261000000	-0.756643000000	0.709514000000
H 2.587014000000	-2.669150000000	0.447759000000	H -5.323853000000	-0.071803000000	0.229221000000
N -3.321517000000	0.320029000000	0.100910000000	H -3.933133000000	-0.594548000000	0.480918000000
O -4.687648000000	0.041116000000	-0.026971000000	O 3.551982000000	0.796552000000	1.172559000000
O -2.667064000000	-0.531543000000	-0.401995000000	H 2.604408000000	0.634403000000	1.264891000000
H -5.093246000000	0.798918000000	0.419957000000	H 3.852717000000	1.035917000000	2.051762000000
OHW4-35			OHW4-36		
O 3.781445000000	-1.071059000000	-0.871259000000	H 1.232210000000	1.535664000000	0.328459000000
H 4.094627000000	-0.488610000000	-0.160406000000	O 0.383478000000	1.823860000000	0.695593000000
H 4.038317000000	-1.952414000000	-0.593572000000	H 0.480898000000	2.764139000000	0.865645000000
N -1.648265000000	-1.007479000000	0.533070000000	H -2.167828000000	-2.041975000000	-0.546248000000
O -2.976331000000	-1.142029000000	0.691243000000	O -2.431312000000	-1.243954000000	-0.083441000000
H -3.414556000000	-0.363602000000	0.256934000000	H -1.775221000000	-1.155819000000	0.625657000000
O -1.324971000000	-0.012367000000	-0.072920000000	H -2.272571000000	0.540988000000	-0.989719000000
O 3.802494000000	0.975203000000	1.045461000000	O -1.955940000000	1.417804000000	-1.244566000000
H 2.917451000000	1.099430000000	0.659381000000	H -1.188845000000	1.533638000000	-0.675742000000
H 4.197612000000	1.849154000000	1.034754000000	H -0.251546000000	0.345823000000	1.650303000000
H 1.564807000000	0.673707000000	-0.548416000000	O -0.452717000000	-0.585846000000	1.835953000000
H 2.044819000000	-0.092086000000	-0.896691000000	H 0.627745000000	-0.615546000000	2.779397000000
H 0.672244000000	0.355392000000	-0.378060000000	N 1.833196000000	-1.127036000000	-0.527537000000
O -4.173818000000	1.008896000000	-0.561670000000	O 2.492420000000	0.200535000000	-0.301295000000
H -4.900464000000	1.557290000000	-0.253704000000	O 0.762962000000	-0.981387000000	-0.953992000000
H -3.501208000000	1.628991000000	-0.859641000000	H 3.347147000000	-0.065759000000	0.068986000000
OHW4-37					
O -2.868319000000	0.284229000000	-0.678430000000			
H -3.081660000000	1.220719000000	-0.695220000000			
H -3.646155000000	-0.154494000000	-0.295781000000			
N 0.410920000000	0.733227000000	0.074293000000			
O -0.379815000000	-0.350131000000	0.061584000000			
H -1.301059000000	-0.064960000000	-0.214205000000			
O -0.132538000000	1.769282000000	-0.222291000000			
O 3.360741000000	0.483364000000	0.775605000000			
H 2.419212000000	0.514073000000	0.558180000000			
H 3.638436000000	1.401030000000	0.724759000000			
O 5.088083000000	-1.393889000000	-0.554562000000			
H 4.480619000000	-0.769449000000	-0.132788000000			
H 5.305934000000	-1.997896000000	0.157186000000			
O -5.082859000000	-1.056381000000	0.401392000000			
H -5.543426000000	-1.693688000000	-0.151125000000			
H -5.030688000000	-1.479713000000	1.262551000000			