Electronic Supplementary Information

Hydration Shell Model for Expeditious and Reliable Individual Hydrogen Bond Energies in Large Water Clusters

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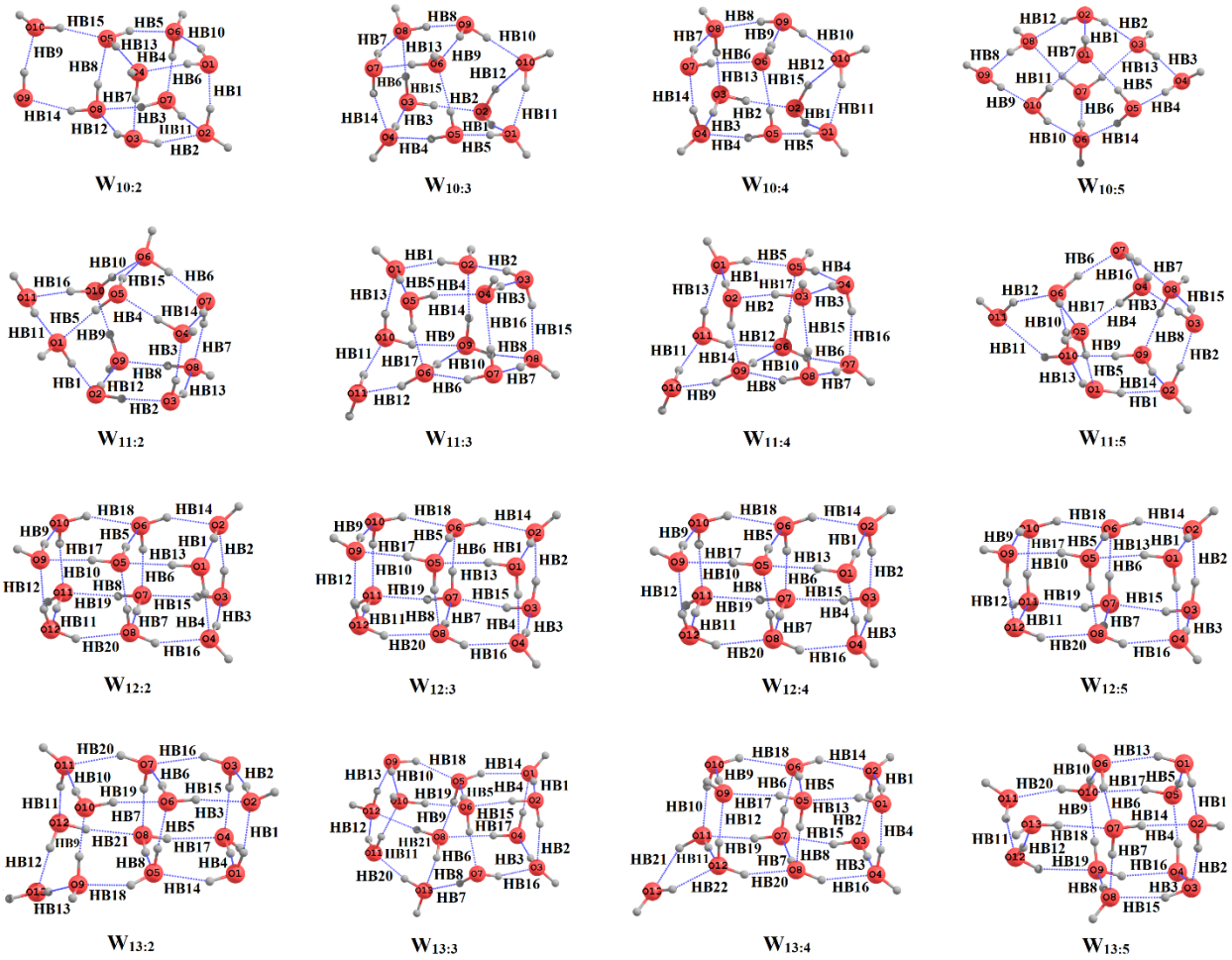

Fig. S1 The MTA-MP2/aDZ-optimized geometries of higher energy conformers of water clusters (W_n, n = 10-13).

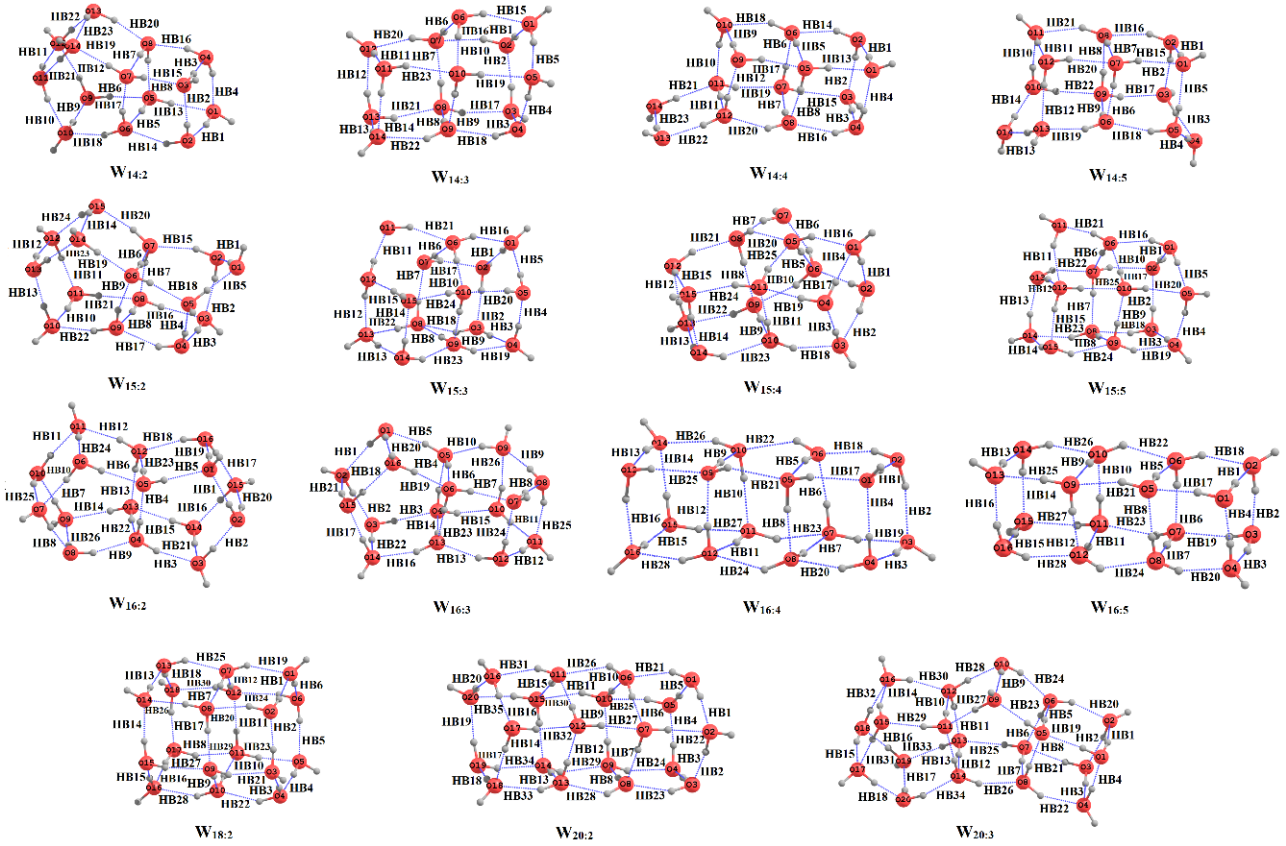

Fig. S2 The MTA-MP2/aDZ-optimized geometries of higher energy conformers of water clusters (W_n, n = 14-16, 18 and 20).

Table S1 Single point energies (in a.u.) of various species in the MTA (actual and shell-1) calculation of $W_{10:1}$ at MP2/aTZ level of theory. See text for details.

Species	Energy
$W_{10:1}$ ($E_{W_{10:1}}$)	-763.445748
Fragment F1 (E_{F1})	-687.078369
Fragment F2 (E_{F2})	-687.078231
Fragment F3 (E_{F3})	-610.728746
$W_{10:1}$ ($E_{shell-1}$)	-458.0223891
Fragment F1' ($E_{F1'}$)	-381.6668051
Fragment F2' ($E_{F2'}$)	-381.6695901
Fragment F3' ($E_{F3'}$)	-305.3247461

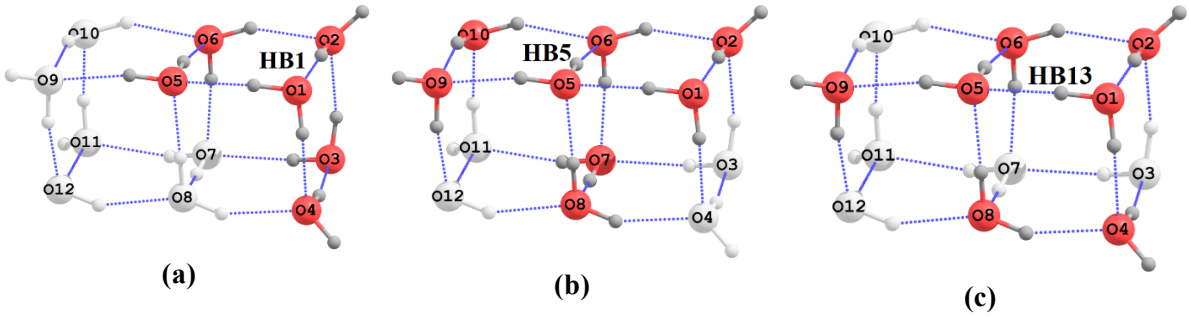

Fig. S3 Various shell-1 model for estimation of hydrogen bond energy (a) HB1(O2-H…O1) (b) HB5 (O5-H…O6) and (c) HB13 (O1-H…O5) in $W_{12:1}$ cluster.

Formulas

1. **Root mean square deviation (RMSD)**

$$\text{RMSD} = \sqrt{\frac{\sum_{i=1}^{N}(xi-yi)^2}{N}}$$

2. **Mean Absolute Error (MAE)**

$$\text{MAE} = \frac{\sum_{i=1}^{N}|xi-yi|}{N}$$

3. **Maximum Absolute Error ($|\Delta E_{max}|$)**

$$|\Delta E_{max}| = Maximum\ of\ |xi - yi|$$

4. **Standard Deviation (Sε)**

$$\text{Sum of Squares of Error (SSE)} = \sum_{i=1}^{N}(xi - yi)^2$$

$$S\varepsilon = \sqrt{\frac{SSE}{N-K-1}}$$

Where,

x_i = HB energy by Shell-1 model

y_i = HB energy by actual MTA-based method

N = Number of HB energy

Table S2 Hydrogen bond energies (kcal/mol) in higher energy $W_{10:n}$, n=2-5 clusters calculated using the actual MTA-based method and the shell-1 model at MP2/aTZ level of theory.

HB label	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
$W_{10:2}$									
HB1[#]	10.01	10.86	4.77	6.09	HB9	7.95	7.18	5.07	2.11
HB2	7.02	7.34	4.93	2.41	HB10	7.02	7.32	4.90	2.42
HB3	11.06	11.58	4.50	7.08	HB11	7.00	7.31	4.91	2.40
HB4	7.04	7.34	4.91	2.43	HB12	7.83	7.96	4.72	3.24
HB5	7.93	8.08	4.82	3.26	HB13	7.93	8.02	4.83	3.19
HB6	11.00	11.59	4.53	7.06	HB14	5.21	5.14	3.10	2.04
HB7	7.87	8.04	4.74	3.30	HB15	7.01	7.06	4.37	2.69
HB8	8.67	9.47	5.05	4.42					
$W_{10:3}$									
HB1[#]	7.33	7.48	4.77	2.71	HB9	7.27	7.05	5.13	1.92
HB2[#]	6.68	6.58	4.18	2.40	HB10	5.47	5.08	4.38	0.70
HB3[#]	11.28	10.42	4.30	6.12	HB11	7.05	6.31	4.33	1.98
HB4[#]	7.70	6.81	4.91	1.90	HB12	-0.06	0.16	1.25	-1.09
HB5[#]	11.54	11.08	4.16	6.92	HB13	4.33	4.47	4.20	0.27
HB6	10.53	9.96	4.52	5.44	HB14	3.26	3.69	3.41	0.28
HB7	7.36	6.75	4.92	1.83	HB15	3.76	3.84	3.56	0.28
HB8	10.48	10.41	4.59	5.82					
$W_{10:4}$									
HB1	7.22	6.54	4.69	1.85	HB9[#]	10.79	10.35	4.47	5.88
HB2	6.61	6.21	4.21	2.00	HB10	6.81	6.04	5.18	0.86
HB3	7.04	7.02	5.12	1.90	HB11	7.05	6.41	4.33	2.08
HB4	4.04	3.96	3.61	0.35	HB12	0.11	0.49	1.39	-0.90
HB5[#]	11.48	11.18	4.19	6.99	HB13	11.08	10.73	4.37	6.36
HB6	3.19	3.74	3.44	0.30	HB14	10.30	9.92	4.59	5.33
HB7	7.47	6.81	4.92	1.89	HB15[#]	7.43	6.70	4.89	1.81
HB8	4.90	4.84	4.24	0.60					
$W_{10:5}$									
HB1	10.63	10.24	4.61	5.63	HB8	9.91	9.03	4.21	4.82
HB2	7.08	6.64	4.86	1.78	HB9	9.92	9.16	4.33	4.83
HB3	9.91	9.03	4.21	4.82	HB10	6.72	6.35	4.67	1.68
HB4	9.92	9.16	4.33	4.83	HB11	6.83	6.50	4.87	1.63
HB5	6.83	6.50	4.87	1.63	HB12	7.08	6.64	4.86	1.78
HB6	10.53	10.21	4.64	5.57	HB13	7.05	6.65	4.94	1.71
HB7	7.05	6.65	4.94	1.71	HB14	6.72	6.35	4.67	1.68

[#] The shell-1 model for these HBs contains seven water molecules.

Table S3 Hydrogen bond energies (kcal/mol) in higher energy $W_{11:n}$, n=2-5 clusters calculated using the actual MTA-based method and the shell-1 model at MP2/aTZ level.

HB label	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
$W_{11:2}$									
HB1[#]	11.81	11.60	3.92	7.68	HB9[#]	11.74	11.43	3.93	7.50
HB2	6.58	6.50	3.55	2.95	HB10	7.36	6.62	5.02	1.60
HB3	6.85	6.80	5.03	1.77	HB11	7.52	6.86	4.78	2.08
HB4	10.60	11.02	4.61	6.41	HB12	7.31	6.46	4.96	1.50
HB5	7.08	6.42	4.92	1.50	HB13	6.27	6.05	4.95	1.10
HB6	10.63	11.07	4.49	6.58	HB14	7.50	7.55	4.96	2.59
HB7	6.99	6.79	5.04	1.75	HB15	7.22	7.37	5.15	2.22
HB8	8.06	7.61	4.37	3.24	HB16	6.40	5.75	4.28	1.47
$W_{11:3}$									
HB1	8.48	7.97	4.24	3.73	HB10	8.32	8.60	5.06	3.54
HB2	6.57	6.51	4.92	1.59	HB11	8.16	7.63	4.89	2.74
HB3	10.05	10.66	4.71	5.95	HB12	5.28	5.12	3.08	2.04
HB4	6.87	6.50	4.74	1.76	HB13	6.28	5.70	4.81	0.89
HB5[#]	11.95	11.58	3.97	7.61	HB14	7.18	6.94	5.05	1.89
HB6	7.59	7.64	4.51	3.13	HB15	7.35	7.45	5.03	2.42
HB7	10.77	11.42	4.53	6.89	HB16	7.01	7.33	4.95	2.38
HB8	7.47	7.81	4.66	3.15	HB17	8.17	7.53	4.54	2.99
HB9	2.87	3.23	2.60	0.63					
$W_{11:4}$									
HB1[#]	6.16	6.35	4.77	1.58	HB10	8.31	8.24	5.06	3.18
HB2[#]	11.01	10.36	4.34	6.02	HB11	8.19	7.37	4.87	2.50
HB3[#]	7.78	6.78	4.88	1.90	HB12	3.06	2.79	2.68	0.11
HB4[#]	11.60	10.55	4.04	6.51	HB13	4.44	4.06	4.11	-0.05
HB5[#]	7.47	7.11	4.33	2.78	HB14	4.72	4.69	3.59	1.10
HB6	7.50	6.90	4.68	2.22	HB15	3.11	3.69	3.54	0.15
HB7	10.70	9.76	4.48	5.28	HB16	3.14	3.50	3.46	0.04
HB8	7.70	6.78	4.52	2.26	HB17	3.29	3.50	3.68	-0.18
HB9	5.26	4.96	3.06	1.90					
$W_{11:5}$									
HB1	7.47	7.03	4.93	2.10	HB10	10.08	9.95	4.60	5.35
HB2	10.49	11.01	4.61	6.40	HB11	1.03	0.95	0.79	0.16
HB3	6.82	6.74	5.04	1.70	HB12	5.20	4.93	4.14	0.79
HB4	8.05	7.83	4.42	3.41	HB13	7.88	7.81	4.72	3.09
HB5	11.77	11.36	4.22	7.14	HB14	7.17	7.47	4.97	2.50
HB6	7.24	7.21	3.32	3.89	HB15	7.55	7.56	4.96	2.60
HB7	7.16	6.85	5.00	1.85	HB16	6.34	6.14	4.95	1.19
HB8	10.87	11.10	4.50	6.60	HB17	7.52	7.52	4.86	2.66
HB9	7.68	7.17	4.69	2.48					

[#] The shell-1 model for these HBs contains seven water molecules.

Table S4 Hydrogen bond energies (kcal/mol) in higher energy $W_{12:n}$, n=2-5 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{12:2}$				
HB1	11.11	4.77	6.34	HB11	9.68	4.73	4.94
HB2	7.43	5.01	2.42	HB12	6.67	5.02	1.66
HB3	11.11	4.77	6.34	HB13	7.28	4.46	2.82
HB4	7.43	5.01	2.42	HB14	7.32	4.51	2.81
HB5	9.15	4.79	4.36	HB15	7.28	4.46	2.82
HB6	8.68	4.77	3.91	HB16	7.32	4.51	2.81
HB7	9.15	4.79	4.36	HB17	3.68	2.95	0.73
HB8	8.68	4.77	3.91	HB18	3.83	2.90	0.93
HB9	9.68	4.73	4.94	HB19	3.68	2.95	0.73
HB10	6.67	5.02	1.66	HB20	3.83	2.90	0.93
			$W_{12:3}$				
HB1	9.67	4.73	4.94	HB11	11.11	4.76	6.35
HB2	6.68	5.02	1.66	HB12	7.45	5.02	2.43
HB3	9.67	4.73	4.94	HB13	3.82	2.89	0.93
HB4	6.68	5.02	1.66	HB14	3.70	2.95	0.74
HB5	9.17	4.79	4.37	HB15	3.82	2.89	0.93
HB6	8.69	4.76	3.93	HB16	3.70	2.95	0.74
HB7	9.17	4.79	4.37	HB17	7.32	4.51	2.81
HB8	8.69	4.76	3.93	HB18	7.27	4.45	2.82
HB9	11.11	4.76	6.35	HB19	7.32	4.51	2.81
HB10	7.45	5.02	2.43	HB20	7.27	4.45	2.82
			$W_{12:4}$				
HB1	6.67	5.02	1.66	HB11	9.66	4.74	4.92
HB2	9.66	4.74	4.92	HB12	6.67	5.02	1.66
HB3	6.67	5.02	1.66	HB13	3.82	2.89	0.92
HB4	9.66	4.74	4.92	HB14	3.77	2.93	0.84
HB5	7.90	4.79	3.11	HB15	3.82	2.89	0.92
HB6	7.90	4.79	3.11	HB16	3.77	2.93	0.84
HB7	7.90	4.79	3.11	HB17	3.77	2.93	0.83
HB8	7.90	4.79	3.11	HB18	3.82	2.89	0.92
HB9	9.65	4.74	4.92	HB19	3.77	2.93	0.83
HB10	6.67	5.02	1.66	HB20	3.82	2.89	0.92
			$W_{12:5}$				
HB1	9.66	4.73	4.92	HB11	6.68	5.02	1.66
HB2	6.68	5.02	1.66	HB12	9.66	4.73	4.92
HB3	9.66	4.73	4.92	HB13	3.82	2.89	0.92
HB4	6.68	5.02	1.66	HB14	3.76	2.93	0.83
HB5	7.90	4.79	3.11	HB15	3.82	2.89	0.92
HB6	7.90	4.79	3.11	HB16	3.76	2.93	0.83
HB7	7.90	4.79	3.11	HB17	3.76	2.93	0.83
HB8	7.90	4.79	3.11	HB18	3.82	2.89	0.92
HB9	6.68	5.02	1.66	HB19	3.76	2.93	0.83
HB10	9.66	4.73	4.92	HB20	3.82	2.89	0.92

Table S5 Hydrogen bond energies (kcal/mol) in higher energy $W_{13:n}$, n=2-5 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{13:2}$				
HB1	6.72	5.03	1.69	HB12	6.38	4.76	1.62
HB2	9.49	4.81	4.67	HB13	6.30	4.54	1.76
HB3	6.77	5.05	1.72	HB14	3.66	3.10	0.56
HB4	9.57	4.77	4.81	HB15	3.66	3.03	0.63
HB5	8.12	4.84	3.27	HB16	3.44	2.88	0.57
HB6	7.78	4.67	3.11	HB17	3.72	3.18	0.55
HB7	7.85	4.69	3.16	HB18	3.72	3.31	0.40
HB8	8.13	4.83	3.30	HB19	3.31	2.90	0.41
HB9	9.13	4.52	4.61	HB20	3.16	2.86	0.30
HB10	6.30	5.03	1.26	HB21	4.30	3.68	0.62
HB11	9.22	4.49	4.73				
			$W_{13:3}$				
HB1	11.26	4.47	6.78	HB12	3.26	3.26	0.00
HB2	6.55	4.79	1.76	HB13	9.55	4.57	4.97
HB3	10.01	4.83	5.18	HB14	7.67	4.81	2.86
HB4	7.80	4.95	2.85	HB15	4.94	2.69	2.26
HB5	6.27	3.79	2.48	HB16	4.98	4.26	0.72
HB6	6.42	3.70	2.72	HB17	5.60	4.19	1.41
HB7	5.57	4.81	0.76	HB18	6.82	4.62	2.20
HB8	5.06	3.87	1.19	HB19	8.30	4.38	3.92
HB9	9.10	4.72	4.38	HB20	9.51	4.25	5.27
HB10	4.00	3.63	0.37	HB21	6.79	4.71	2.08
HB11	6.14	5.02	1.11				
			$W_{13:4}$				
HB1	7.53	5.03	2.50	HB12	8.22	4.98	3.24
HB2	10.94	4.82	6.12	HB13	7.05	4.49	2.56
HB3	7.54	5.02	2.52	HB14	7.05	4.57	2.48
HB4	10.91	4.83	6.09	HB15	7.06	4.52	2.53
HB5	9.88	4.78	5.10	HB16	7.03	4.57	2.46
HB6	10.02	4.77	5.24	HB17	7.01	4.53	2.48
HB7	9.99	4.73	5.26	HB18	7.01	4.47	2.54
HB8	9.94	4.76	5.18	HB19	7.14	4.36	2.78
HB9	11.02	4.75	6.27	HB20	7.59	4.48	3.12
HB10	7.78	4.81	2.98	HB21	0.93	0.73	0.20
HB11	9.96	4.98	4.98	HB22	4.98	4.18	0.80
			$W_{13:5}$				
HB1	5.98	5.01	0.97	HB11	8.00	4.92	0.97
HB2	9.17	4.61	4.56	HB12	5.46	4.62	4.56
HB3	5.93	4.96	0.98	HB13	2.71	3.42	0.98
HB4	9.06	4.48	4.59	HB14	3.56	3.25	4.59
HB5	5.80	3.75	2.06	HB15	3.40	3.43	2.06
HB6	8.30	4.88	3.42	HB16	3.17	3.09	3.42
HB7	6.81	4.76	2.05	HB17	2.58	3.07	2.05
HB8	9.14	4.12	5.01	HB18	5.51	3.94	5.01
HB9	8.20	4.60	3.60	HB19	5.39	3.74	3.60
HB10	5.31	4.52	0.79	HB20	6.50	4.24	0.79

Table S6 Hydrogen bond energies (kcal/mol) in higher energy $W_{14:n}$, n=2-5 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{14:2}$				
HB1	9.24	4.97	4.28	HB13	3.43	3.07	0.35
HB2	6.79	4.98	1.81	HB14	3.78	3.10	0.68
HB3	11.84	4.20	7.63	HB15	7.04	4.34	2.70
HB4	6.67	4.88	1.79	HB16	5.85	3.23	2.62
HB5	8.12	4.83	3.30	HB17	6.83	4.72	2.11
HB6	6.24	4.30	1.94	HB18	6.97	4.83	2.14
HB7	8.08	4.95	3.13	HB19	6.39	4.33	2.06
HB8	5.26	3.22	2.04	HB20	5.06	2.97	2.09
HB9	9.88	4.70	5.18	HB21	10.65	4.41	6.24
HB10	4.26	3.60	0.65	HB22	10.47	4.37	6.10
HB11	7.01	4.91	2.10	HB23	6.63	4.76	1.87
HB12	5.09	4.29	0.79				
			$W_{14:3}$				
HB1	6.12	5.17	0.95	HB13	9.61	4.73	4.88
HB2	8.72	4.71	4.01	HB14	7.04	5.12	1.92
HB3	6.10	5.06	1.05	HB15	2.71	3.46	-0.74
HB4	9.01	4.45	4.56	HB16	2.52	2.46	0.06
HB5	6.79	4.34	2.45	HB17	3.01	2.93	0.08
HB6	7.44	4.11	3.32	HB18	3.34	2.92	0.42
HB7	7.34	4.54	2.80	HB19	1.93	2.70	-0.76
HB8	7.25	4.66	2.59	HB20	4.02	3.50	0.52
HB9	7.26	4.80	2.47	HB21	3.70	3.12	0.58
HB10	4.33	3.70	0.63	HB22	3.39	2.96	0.42
HB11	9.66	4.87	4.79	HB23	3.34	2.99	0.34
HB12	6.56	4.89	1.68				
			$W_{14:4}$				
HB1	10.97	4.81	6.16	HB13	7.13	4.60	2.53
HB2	7.54	5.03	2.52	HB14	7.12	4.52	2.60
HB3	10.86	4.84	6.02	HB15	6.95	4.56	2.39
HB4	7.55	5.03	2.52	HB16	6.98	4.46	2.52
HB5	10.03	4.71	5.32	HB17	6.87	4.50	2.37
HB6	9.91	4.75	5.16	HB18	6.91	4.55	2.35
HB7	9.82	4.83	4.98	HB19	7.33	4.24	3.09
HB8	9.84	4.71	5.13	HB20	7.47	4.39	3.08
HB9	7.21	5.05	2.15	HB21	7.73	4.56	3.18
HB10	10.13	5.10	5.03	HB22	7.39	4.43	2.96
HB11	10.25	4.55	5.70	HB23	8.35	5.17	3.18
HB12	9.44	4.95	4.49				
			$W_{14:5}$				
HB1	10.38	4.81	5.57	HB12	6.14	5.05	1.09
HB2	6.92	5.05	1.87	HB13	8.55	4.28	4.27
HB3	8.95	4.32	4.64	HB14	8.60	4.40	4.19
HB4	8.96	4.40	4.56	HB15	6.95	4.45	2.50
HB5	6.71	4.91	1.80	HB16	7.04	4.46	2.58
HB6	8.78	4.78	4.01	HB17	6.89	4.69	2.19
HB7	9.09	4.71	4.38	HB18	6.66	4.68	1.97
HB8	8.81	4.77	4.05	HB19	4.68	3.94	0.73
HB9	8.89	4.91	3.98	HB20	3.39	2.88	0.51
HB10	5.93	4.93	1.01	HB21	3.44	3.07	0.37
HB11	8.92	4.79	4.14	HB22	3.95	3.29	0.66

Table S7 Hydrogen bond energies (kcal/mol) in higher energy $W_{15:n}$, n=2-5 clusters calculated using the shell-1 model at MP2/aTZ level..

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{15:2}$				
HB1	8.62	4.42	4.20	HB13	10.54	4.61	5.93
HB2	5.93	4.88	1.06	HB14	6.79	4.96	1.82
HB3	9.01	4.76	4.25	HB15	4.01	3.41	0.60
HB4	6.12	5.02	1.10	HB16	3.58	3.07	0.51
HB5	8.55	4.32	4.23	HB17	3.86	3.17	0.69
HB6	9.51	4.56	4.95	HB18	4.68	3.98	0.71
HB7	7.86	4.87	3.00	HB19	8.65	4.54	4.10
HB8	7.98	4.86	3.12	HB20	7.75	4.06	3.69
HB9	8.08	5.01	3.07	HB21	4.18	3.19	0.99
HB10	7.05	5.08	1.97	HB22	4.90	3.84	1.06
HB11	10.42	4.64	5.78	HB23	6.42	5.02	1.40
HB12	7.54	5.00	2.55	HB24	6.44	5.02	1.42
			$W_{15:3}$				
HB1	7.85	4.53	3.32	HB13	11.15	4.72	6.44
HB2	10.61	4.53	6.08	HB14	7.47	4.92	2.55
HB3	7.23	5.00	2.23	HB15	10.59	4.52	6.07
HB4	10.65	4.25	6.40	HB16	6.08	4.55	1.53
HB5	7.13	5.11	2.01	HB17	6.05	4.50	1.56
HB6	5.95	3.74	2.21	HB18	7.13	4.88	2.25
HB7	9.50	4.69	4.81	HB19	7.48	4.26	3.23
HB8	9.76	4.60	5.17	HB20	7.22	4.46	2.76
HB9	9.50	4.64	4.85	HB21	6.55	4.36	2.19
HB10	9.28	4.56	4.73	HB22	7.44	4.90	2.54
HB11	5.83	4.30	1.53	HB23	7.56	4.64	2.92
HB12	7.18	5.15	2.03	HB24	6.81	4.56	2.25
			$W_{15:4}$				
HB1	10.12	4.65	5.46	HB14	11.04	4.81	6.23
HB2	6.98	5.12	1.86	HB15	7.13	5.01	2.12
HB3	9.63	4.80	4.83	HB16	3.81	2.94	0.87
HB4	6.68	4.99	1.69	HB17	5.31	3.83	1.49
HB5	7.73	4.97	2.76	HB18	3.86	3.30	0.56
HB6	6.26	3.58	2.69	HB19	3.98	3.32	0.66
HB7	7.44	4.95	2.49	HB20	4.39	2.70	1.68
HB8	7.82	4.40	3.42	HB21	5.88	4.03	1.85
HB9	8.60	4.65	3.94	HB22	7.61	4.70	2.92
HB10	6.18	3.61	2.57	HB23	6.58	4.61	1.97
HB11	8.32	4.50	3.83	HB24	6.80	5.15	1.65
HB12	11.28	4.65	6.64	HB25	7.70	5.01	2.69
HB13	7.61	5.03	2.58				
			$W_{15:5}$				
HB1	10.64	4.68	5.96	HB14	7.31	5.02	2.28
HB2	7.17	5.03	2.14	HB15	8.11	3.72	4.39
HB3	10.80	4.50	6.30	HB16	7.38	4.66	2.72
HB4	7.82	4.49	3.33	HB17	7.31	4.62	2.69
HB5	6.98	5.12	1.87	HB18	7.48	4.60	2.88
HB6	9.27	4.86	4.41	HB19	6.63	4.49	2.14
HB7	9.50	4.81	4.68	HB20	5.95	4.32	1.63
HB8	9.65	4.67	4.98	HB21	6.27	4.33	1.93
HB9	7.38	3.70	3.68	HB22	6.10	3.99	2.12
HB10	9.53	4.60	4.93	HB23	7.08	4.57	2.51
HB11	6.32	4.03	2.29	HB24	6.00	4.37	1.63
HB12	7.13	4.55	2.58	HB25	6.04	4.04	2.00
HB13	10.62	4.84	5.78				

Table S8 Hydrogen bond energies (kcal/mol) in higher energy $W_{16:n}$, n=2-5 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{16:2}$				
HB1	4.15	3.57	0.58	HB14	6.65	4.73	1.92
HB2	10.22	4.57	5.65	HB15	4.06	3.35	0.71
HB3	4.67	3.99	0.68	HB16	10.21	4.60	5.61
HB4	7.24	4.22	3.02	HB17	4.75	4.21	0.54
HB5	3.56	3.30	0.26	HB18	4.54	4.00	0.53
HB6	7.01	4.94	2.07	HB19	8.62	4.78	3.84
HB7	5.10	4.27	0.84	HB20	7.01	4.99	2.02
HB8	10.60	4.61	5.99	HB21	7.06	5.03	2.03
HB9	6.73	4.78	1.95	HB22	8.94	4.80	4.14
HB10	10.47	4.61	5.85	HB23	9.31	4.87	4.43
HB11	4.23	3.59	0.63	HB24	9.82	4.79	5.03
HB12	7.08	4.99	2.09	HB25	6.99	4.98	2.02
HB13	7.43	4.25	3.18	HB26	7.66	5.02	2.64
			$W_{16:3}$				
HB1	6.58	5.04	1.54	HB14	9.89	4.31	5.58
HB2	10.83	4.66	6.16	HB15	6.63	3.47	3.16
HB3	7.08	4.74	2.34	HB16	7.20	4.78	2.43
HB4	8.95	4.75	4.20	HB17	10.91	4.62	6.29
HB5	6.46	3.53	2.94	HB18	6.63	5.03	1.59
HB6	9.01	4.76	4.25	HB19	8.08	4.50	3.58
HB7	7.07	4.82	2.25	HB20	5.83	4.92	0.92
HB8	10.86	4.65	6.21	HB21	7.54	4.98	2.56
HB9	6.58	5.03	1.55	HB22	7.60	5.03	2.58
HB10	7.84	4.47	3.37	HB23	10.00	4.59	5.41
HB11	6.64	5.04	1.60	HB24	7.61	5.02	2.60
HB12	10.89	4.63	6.26	HB25	7.55	4.98	2.58
HB13	7.31	4.80	2.51	HB26	5.81	4.90	0.91
			$W_{16:4}$				
HB1	11.02	4.79	6.23	HB15	11.02	4.79	6.23
HB2	7.49	5.01	2.48	HB16	7.49	5.01	2.48
HB3	11.02	4.79	6.23	HB17	7.17	4.69	2.48
HB4	7.49	5.01	2.48	HB18	7.17	4.62	2.56
HB5	10.24	4.80	5.45	HB19	7.17	4.69	2.48
HB6	9.48	4.89	4.60	HB20	7.17	4.62	2.56
HB7	10.24	4.80	5.45	HB21	6.69	4.13	2.56
HB8	9.48	4.89	4.60	HB22	6.69	4.13	2.56
HB9	10.24	4.80	5.45	HB23	6.69	4.13	2.56
HB10	9.48	4.89	4.60	HB24	6.69	4.58	2.11
HB11	10.24	4.80	5.45	HB25	7.17	4.62	2.56
HB12	9.48	4.89	4.60	HB26	7.17	4.69	2.48
HB13	11.02	4.79	6.23	HB27	7.17	4.62	2.56
HB14	7.49	5.01	2.48	HB28	7.17	4.69	2.48
			$W_{16:5}$				
HB1	6.72	5.02	1.71	HB15	11.03	4.79	6.24
HB2	9.63	4.77	4.86	HB16	7.49	5.01	2.48
HB3	6.72	5.02	1.71	HB17	3.66	3.12	0.54
HB4	9.63	4.77	4.86	HB18	3.64	3.20	0.44
HB5	8.99	4.78	4.21	HB19	3.66	3.12	0.54
HB6	8.68	4.91	3.77	HB20	3.64	3.20	0.44
HB7	8.99	4.78	4.21	HB21	6.62	4.11	2.51
HB8	8.68	4.91	3.77	HB22	6.60	4.12	2.48
HB9	10.25	4.79	5.46	HB23	6.62	4.11	2.51
HB10	9.47	4.89	4.57	HB24	6.60	4.12	2.48
HB11	10.25	4.79	5.46	HB25	7.17	4.69	2.48
HB12	9.47	4.89	4.57	HB26	7.18	4.62	2.56
HB13	11.03	4.79	6.24	HB27	7.17	4.69	2.48
HB14	7.49	5.01	2.48	HB28	7.18	4.62	2.56

Table S9 Hydrogen bond energies (kcal/mol) in higher energy $W_{18:n}$, n=2 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{18:2}$				
HB1	7.01	4.99	2.02	HB16	7.01	4.99	2.02
HB2	10.53	4.61	5.92	HB17	10.53	4.61	5.92
HB3	7.01	4.99	2.02	HB18	7.01	4.99	2.02
HB4	10.53	4.61	5.92	HB19	7.48	4.65	2.83
HB5	7.01	4.99	2.02	HB20	7.34	4.51	2.83
HB6	10.53	4.61	5.92	HB21	7.48	4.65	2.83
HB7	9.63	4.54	5.09	HB22	7.34	4.51	2.83
HB8	9.63	4.54	5.09	HB23	7.48	4.65	2.83
HB9	9.63	4.54	5.09	HB24	7.34	4.51	2.83
HB10	9.63	4.54	5.09	HB25	7.34	4.51	2.83
HB11	9.63	4.54	5.09	HB26	7.48	4.65	2.83
HB12	9.63	4.54	5.09	HB27	7.34	4.51	2.83
HB13	10.53	4.61	5.92	HB28	7.48	4.65	2.83
HB14	7.01	4.99	2.02	HB29	7.34	4.51	2.83
HB15	10.53	4.61	5.92	HB30	7.48	4.65	2.83

Table S10 Hydrogen bond energies (kcal/mol) in higher energy $W_{20:n}$, n=2-3 clusters calculated using the shell-1 model at MP2/aTZ level.

HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$	HB label	$E_{HB}^{shell-1}$	E_{HB}^{dimer}	$E_{coop.}$
			$W_{20:2}$				
HB1	6.04	5.10	0.94	HB19	6.97	5.10	1.86
HB2	9.11	4.65	4.46	HB20	7.85	4.48	3.37
HB3	6.11	5.04	1.07	HB21	2.49	3.03	-0.53
HB4	9.16	4.47	4.69	HB22	3.40	3.19	0.21
HB5	5.69	3.82	1.88	HB23	3.22	3.05	0.18
HB6	8.66	4.64	4.02	HB24	3.23	3.12	0.11
HB7	8.27	4.83	3.45	HB25	2.48	3.06	-0.58
HB8	8.48	4.70	3.78	HB26	5.78	3.92	1.87
HB9	8.13	4.89	3.24	HB27	6.96	4.18	2.78
HB10	6.64	4.06	2.58	HB28	6.97	4.16	2.81
HB11	9.98	4.66	5.32	HB29	6.92	4.16	2.75
HB12	9.32	4.83	4.50	HB30	6.24	4.04	2.21
HB13	10.04	4.72	5.32	HB31	6.83	4.68	2.15
HB14	9.11	4.86	4.25	HB32	7.46	4.64	2.83
HB15	7.13	3.70	3.43	HB33	7.43	4.74	2.70
HB16	10.90	4.47	6.43	HB34	7.44	4.64	2.80
HB17	7.17	5.02	2.16	HB35	6.17	4.66	1.51
HB18	10.77	4.67	6.10				
			$W_{20:3}$				
HB1	6.62	4.99	1.63	HB18	10.86	4.64	6.22
HB2	9.68	4.73	4.95	HB19	4.10	3.14	0.95
HB3	6.74	5.01	1.72	HB20	4.02	3.22	0.80
HB4	9.64	4.73	4.91	HB21	3.70	3.16	0.54
HB5	8.91	4.83	4.08	HB22	3.72	3.19	0.53
HB6	8.19	4.81	3.37	HB23	6.62	4.69	1.93
HB7	8.21	4.94	3.27	HB24	6.60	4.67	1.92
HB8	8.36	4.79	3.57	HB25	3.97	2.88	1.09
HB9	6.69	4.95	1.74	HB26	4.72	3.45	1.28
HB10	9.17	4.59	4.58	HB27	8.23	4.59	3.65
HB11	8.95	4.82	4.13	HB28	7.62	4.40	3.22
HB12	8.74	5.00	3.74	HB29	6.30	3.46	2.83
HB13	8.95	4.83	4.11	HB30	7.81	4.57	3.24
HB14	5.80	4.89	0.92	HB31	6.59	5.04	1.55
HB15	7.53	4.97	2.56	HB32	6.60	5.04	1.56
HB16	10.86	4.62	6.24	HB33	6.91	4.69	2.22
HB17	7.57	5.03	2.53	HB34	7.05	4.80	2.25

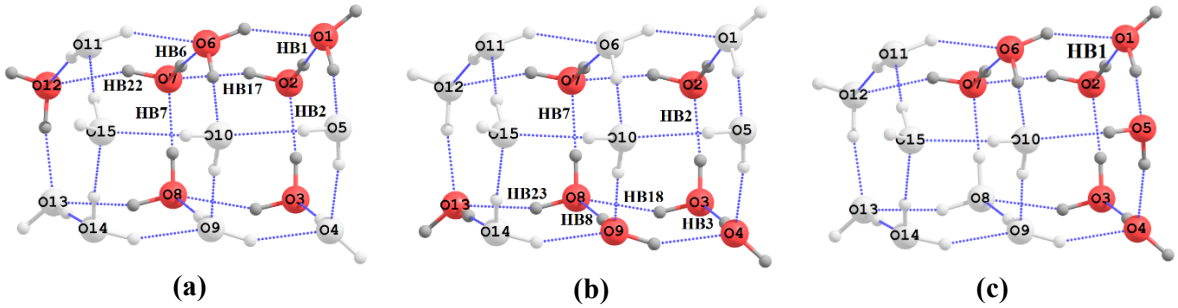

Fig. S4 Various shell-1 model for estimation of hydrogen bond energy (a) HB17(O2-H…O7) and (b) HB18 (O3-H…O8) and (c) HB1 (O2-H…O1) in $W_{15:1}$ cluster.

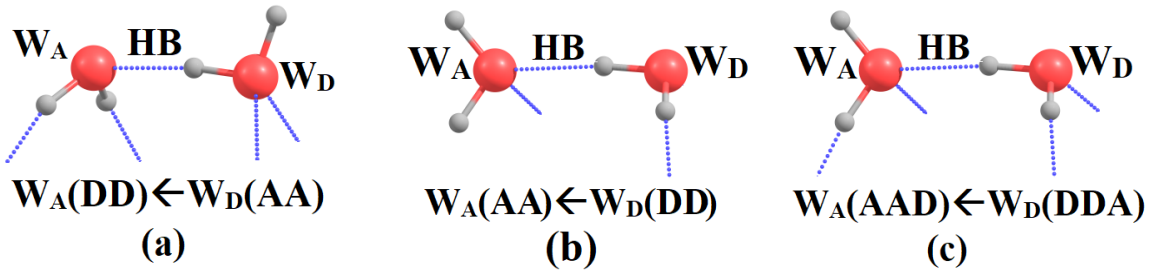

Fig. S5 Structural features corresponding to (a) the strong (b) weak HBs in small clusters and (c) the weak HBs in larger water clusters.

Table S11 Correlation parameters for the comparison of HB bond energies by the actual MTA-based method and the shell-1 or shell-2 models.

Cluster	RMSD	MAE	$\|\Delta E_{max}\|$	R^2	Sε
$W_{10:1}$	0.261	0.205	0.49	0.98	0.280
$W_{11:1}$	0.364	0.278	0.75	0.98	0.388
$W_{12:1}$	0.615	0.554	0.88	0.99	0.648
$W_{13:1}$	0.384	0.325	0.99	0.97	0.404
$W_{14:1}$	0.405	0.365	0.73	0.94	0.425
$W_{15:1}$	0.496	0.396	1.03	0.98	0.517
$W_{16:1}$	0.451	0.333	1.07	0.94	0.470
$W_{10:1}$ -$W_{11:1}$	0.320	0.243	0.75	0.98	0.331
$W_{12:1}$ -$W_{16:1}$	0.482	0.407	1.07	0.95	0.487
$(NH_3)_{8:n}$	0.216	0.200	0.37	0.96	0.226
$(HF)_n(H_2O)_m$	0.835	0.736	1.75	0.99	1.007
$(HF)_4(H_2O)_8$					
(shell-1)	0.863	0.678	1.31	0.99	0.910
(shell-2)	0.118	0.094	0.19	0.99	0.124

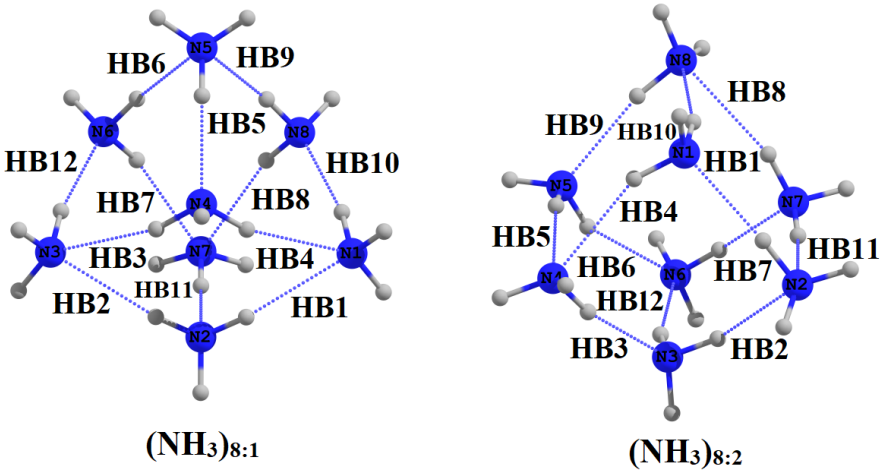

Fig. S6 The MP2/aDZ-optimized geometries of the two lowest energy conformers of ammonia octamer clusters.

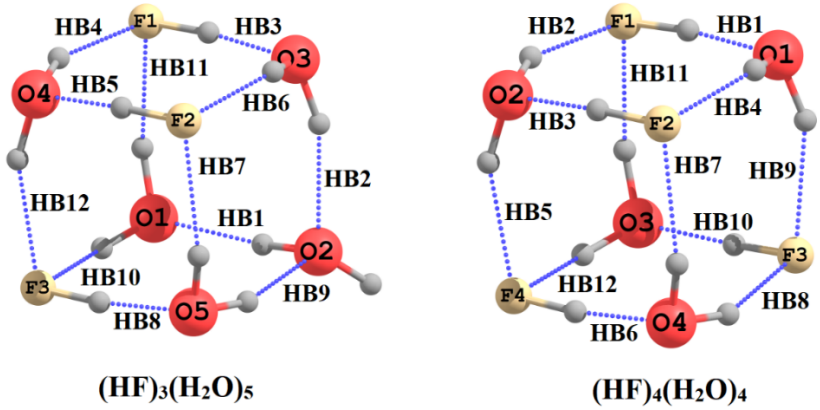

Fig. S7 The MP2/aDZ-optimized geometries of the two lowest energy conformers of HF-H_2O octamer clusters.

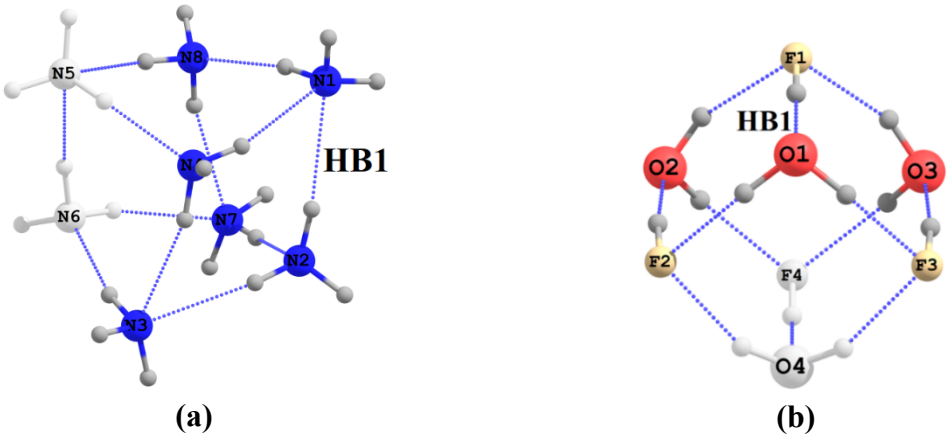

Fig. S8 Various shell-1 model for estimation of energy of hydrogen bond HB1 in (a) $(NH_3)_{8:1}$ and (b) $(HF)_4(H_2O)_4$ clusters. See Figs. S6-S7 and text for details

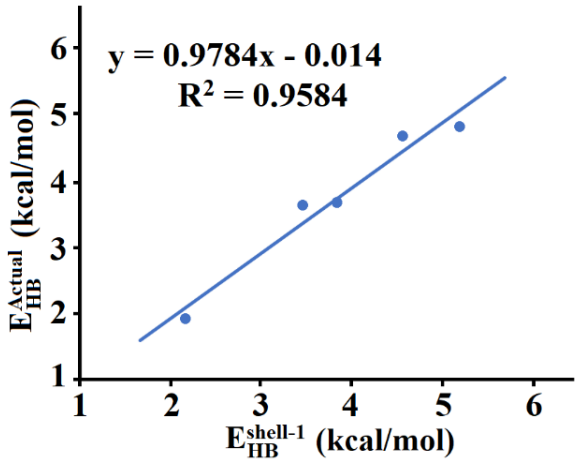

Fig. S9 Correlation plot between the HB energy, in $(NH_3)_{8:1}$ and $(NH_3)_{8:2}$ clusters, estimated by the actual MTA-based method and the shell-1 model.

Table S12 Hydrogen bond energies (kcal/mol) in $(NH_3)_{8:1}$ and $(NH_3)_{8:2}$ clusters calculated using the actual and shell-1 model at MP2/aTZ level.

HB label	Distance (Å)	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	ΔE_{HB}	E_{HB}^{dimer}	$E_{coop.}$
			$(NH_3)_{8:1}$			
HB1	2.30	3.68	3.83	-0.15	3.04	0.79
HB2	2.30	3.68	3.83	-0.15	3.04	0.79
HB3	2.30	3.68	3.83	-0.15	3.04	0.79
HB4	2.30	3.68	3.83	-0.15	3.04	0.79
HB5	2.10	4.82	5.19	-0.37	3.07	2.12
HB6	2.30	3.68	3.83	-0.15	3.04	0.79
HB7	2.30	3.68	3.83	-0.15	3.04	0.79
HB8	2.30	3.68	3.83	-0.15	3.04	0.79
HB9	2.30	3.68	3.83	-0.15	3.04	0.79
HB10	2.10	4.82	5.19	-0.37	3.07	2.12
HB11	2.10	4.82	5.19	-0.37	3.07	2.12
HB12	2.10	4.82	5.19	-0.37	3.07	2.12
			$(NH_3)_{8:2}$			
HB1	2.11	4.68	4.56	0.12	3.03	1.53
HB2	2.30	3.64	3.45	0.19	3.11	0.34
HB3	2.11	4.68	4.56	0.12	3.03	1.53
HB4	2.30	3.64	3.45	0.19	3.11	0.34
HB5	2.30	1.93	2.15	-0.22	2.11	0.04
HB6	2.30	3.64	3.45	0.19	3.11	0.34
HB7	2.11	4.68	4.56	0.12	3.03	1.53
HB8	2.30	3.64	3.45	0.19	3.11	0.34
HB9	2.11	4.68	4.56	0.12	3.03	1.53
HB10	2.30	1.93	2.15	-0.22	2.11	0.04
HB11	2.30	1.93	2.15	-0.22	2.11	0.04
HB12	2.30	1.93	2.15	-0.22	2.11	0.04

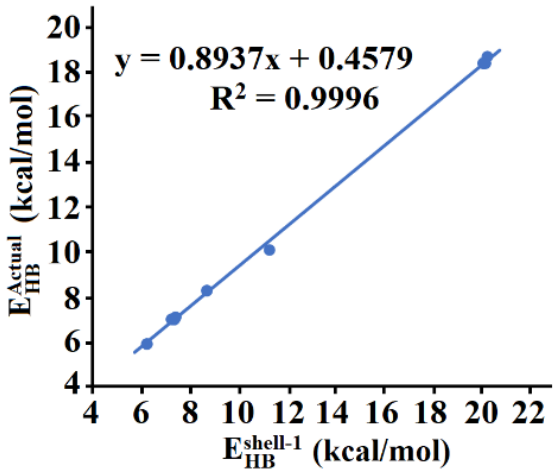

Fig. S10 Correlation plot between the HB energy, in $(HF)_3(H_2O)_5$ and $(HF)_4(H_2O)_4$ clusters, estimated by the actual MTA-based method versus the shell-1 model.

Table S13 Hydrogen bond energies (kcal/mol) in $(HF)_3(H_2O)_5$ and $(HF)_4(H_2O)_4$ clusters calculated using the actual and shell-1 model at MP2/aTZ level.

HB label	Distance (Å)	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	ΔE_{HB}	E_{HB}^{dimer}	$E_{coop.}$
			$(HF)_3(H_2O)_5$			
HB1	1.69	10.1	11.25	-1.15	4.6	6.65
HB2	1.85	8.3	8.67	-0.37	4.9	3.77
HB3	1.47	18.4	20.15	-1.75	9.8	10.35
HB4	1.87	7.1	7.38	-0.28	2.6	4.78
HB5	1.47	18.7	20.23	-1.53	9.8	10.43
HB6	1.91	7.0	7.20	-0.2	2.7	4.50
HB7	1.91	7.0	7.20	-0.2	2.7	4.50
HB8	1.47	18.4	20.15	-1.75	9.8	10.35
HB9	1.85	8.3	8.67	-0.37	4.9	3.77
HB10	1.97	5.9	6.19	-0.29	2.9	3.29
HB11	1.96	5.9	6.19	-0.29	2.9	3.29
HB12	1.87	7.1	7.38	-0.28	2.6	4.78
			$(HF)_4(H_2O)_4$			
HB1	1.47	18.4	20.06	-1.66	9.8	10.26
HB2	1.90	7.0	7.32	-0.32	2.7	4.62
HB3	1.47	18.4	20.06	-1.66	9.8	10.26
HB4	1.90	7.0	7.32	-0.32	2.7	4.62
HB5	1.90	7.0	7.32	-0.32	2.7	4.62
HB6	1.47	18.4	20.06	-1.66	9.8	10.26
HB7	1.90	7.0	7.32	-0.32	2.7	4.62
HB8	1.90	7.0	7.32	-0.32	2.7	4.62
HB9	1.90	7.0	7.32	-0.32	2.7	4.62
HB10	1.47	18.4	20.06	-1.66	9.8	10.26
HB11	1.90	7.0	7.32	-0.32	2.7	4.62
HB12	1.90	7.0	7.32	-0.32	2.7	4.62

Table S14 Hydrogen bond energies (kcal/mol) in $(HF)_4(H_2O)_8$ cluster calculated using the actual, shell-1 and shell-2 model at MP2/aTZ level.

HB label	E_{HB}^{Actual}	$E_{HB}^{shell-1}$	$E_{HB}^{shell-2}$	$\Delta E_{HB}^{Actual-shell-1}$	$\Delta E_{HB}^{Actual-shell-2}$	E_{HB}^{dimer}	$E_{coop.}^{Actual}$	$E_{coop.}^{shell-1}$	$E_{coop.}^{shell-2}$
				$(HF)_4(H_2O)_8$					
HB1	18.04	19.34	17.96	-1.30	0.08	9.80	8.24	9.54	8.16
HB2	6.93	7.19	6.77	-0.26	0.16	2.76	4.17	4.43	4.01
HB3	18.04	19.34	17.96	-1.30	0.08	9.80	8.24	9.54	8.16
HB4	6.93	7.19	6.77	-0.26	0.16	2.76	4.17	4.43	4.01
HB5	8.87	10.18	8.87	-1.31	0.00	4.86	4.01	5.32	4.01
HB6	8.87	10.18	8.87	-1.31	0.00	4.86	4.01	5.32	4.01
HB7	8.87	10.18	8.87	-1.31	0.00	4.86	4.01	5.32	4.01
HB8	8.87	10.18	8.87	-1.31	0.00	4.86	4.01	5.32	4.01
HB9	6.93	7.19	6.77	-0.26	0.16	2.76	4.17	4.43	4.01
HB10	18.04	19.34	17.96	-1.30	0.08	9.80	8.24	9.54	8.16
HB11	6.93	7.19	6.77	-0.26	0.16	2.76	4.17	4.43	4.01
HB12	18.04	19.34	17.96	-1.30	0.08	9.80	8.24	9.54	8.16
HB13	7.75	8.25	7.94	-0.50	-0.19	4.44	3.31	3.81	3.5
HB14	5.59	5.61	5.63	-0.02	-0.04	2.43	3.16	3.18	3.2
HB15	7.75	8.25	7.94	-0.5	-0.19	4.44	3.31	3.81	3.5
HB16	5.59	5.61	5.63	-0.02	-0.04	2.43	3.16	3.18	3.2
HB17	5.59	5.61	5.63	-0.02	-0.04	2.43	3.16	3.18	3.2
HB18	7.75	8.25	7.94	-0.50	-0.19	4.44	3.31	3.81	3.5
HB19	5.59	5.61	5.63	-0.02	-0.04	2.43	3.16	3.18	3.2
HB20	7.75	8.25	7.94	-0.50	-0.19	4.44	3.31	3.81	3.5

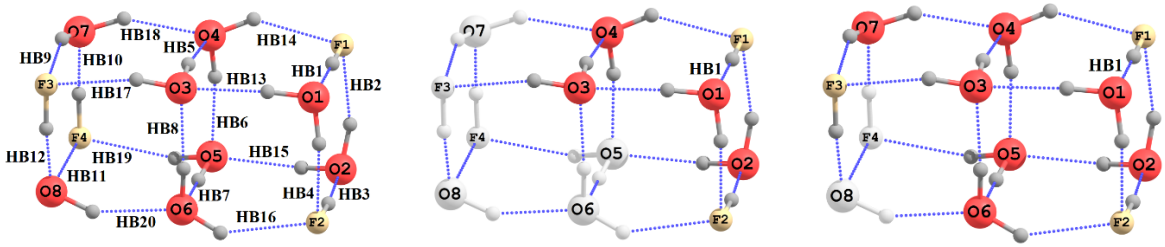

Fig. S11 (a) The MP2/aDZ-optimized geometry of the $(HF)_4(H_2O)_8$ cluster, (b) the shell-1 model and (c) the shell-2 model for estimation of energy of hydrogen bond HB1 in $(HF)_4(H_2O)_8$ cluster.

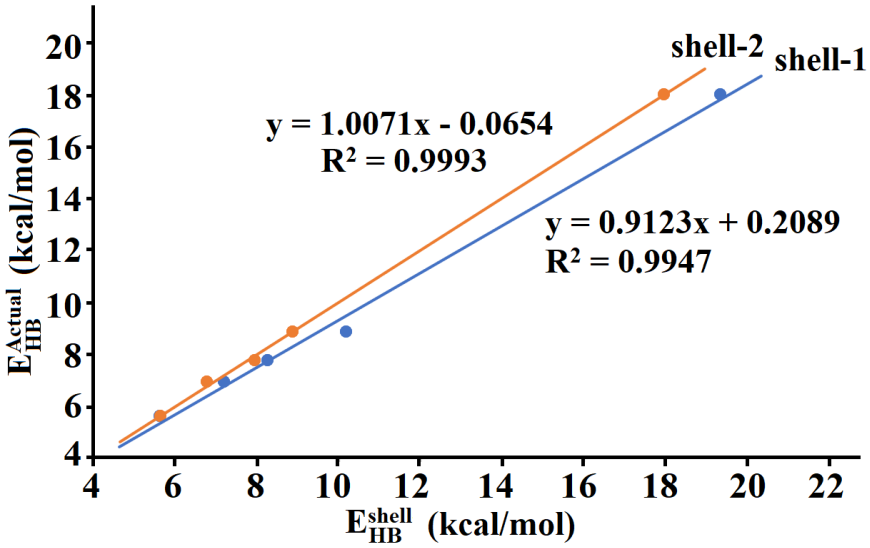

Fig. S12 Correlation plot between the HB energy in $(HF)_4(H_2O)_8$ cluster, estimated by the actual MTA-based method versus shell-1 (blue line) or the shell-2 (orange line) models.

Table S15 Cartesian coordinates of large W_n, (n = 10-16, 18, and 20) clusters.

$W_{10:1}$			
E(MP2/aTZ) = -763.445748 a.u.			
O	0.993720000	2.391230000	1.066350000
H	1.371210000	3.140220000	1.543670000
H	1.625480000	1.645810000	1.197230000
O	-1.683460000	1.482720000	1.388710000
H	-0.779400000	1.852030000	1.366380000
H	-1.981420000	1.520050000	0.458070000
O	-1.700590000	-1.133480000	1.901760000
H	-1.716700000	-0.141290000	1.809160000
H	-2.261250000	-1.338560000	2.659730000
O	0.946410000	-1.944860000	1.432120000
H	0.036740000	-1.714610000	1.710820000
H	0.839470000	-2.288930000	0.523070000
O	2.551960000	0.141080000	1.157710000
H	3.346650000	-0.005300000	1.685630000
H	1.963330000	-0.648410000	1.336800000
O	2.075780000	-0.197810000	-1.700890000
H	2.462670000	-0.041620000	-0.821100000
H	1.504320000	0.594010000	-1.840230000
O	0.610340000	-2.373510000	-1.343540000
H	0.891930000	-3.078650000	-1.938940000
H	1.173660000	-1.579170000	-1.572790000
O	-2.033890000	-1.509250000	-0.917020000
H	-1.158750000	-1.870140000	-1.166410000
H	-2.042620000	-1.559990000	0.057530000
O	-2.225900000	1.114890000	-1.361960000
H	-2.197750000	0.121510000	-1.290900000
H	-2.992620000	1.318530000	-1.911200000
O	0.441100000	2.023160000	-1.771350000
H	-0.499710000	1.761430000	-1.747650000
H	0.611100000	2.359640000	-0.873880000

$W_{10:2}$			
E(MP2/aTZ) = -763.442994 a.u.			
O	2.942410000	-1.246460000	0.066280000
H	2.363640000	-1.445920000	0.827040000
H	2.392570000	-1.468310000	-0.709630000
O	2.999550000	1.443090000	0.024670000
H	3.118500000	0.456670000	0.043160000
H	3.887690000	1.819940000	0.036690000
O	0.946920000	1.287480000	-1.953110000
H	1.699840000	1.534610000	-1.382700000
H	0.158020000	1.492680000	-1.408610000
O	0.999390000	-1.366340000	-2.022280000
H	1.023770000	-1.719130000	-2.920120000
H	0.981710000	-0.370610000	-2.115660000
O	-0.928850000	-1.482640000	-0.011920000
H	-0.329430000	-1.616260000	-0.775840000
H	-0.361240000	-1.598630000	0.778810000
O	0.913530000	-1.304590000	2.072060000
H	0.881480000	-1.626740000	2.981120000
H	0.885570000	-0.306950000	2.129320000
O	0.851640000	1.347940000	1.900320000
H	0.096350000	1.527210000	1.301240000
H	1.636140000	1.577000000	1.366070000
O	-1.124720000	1.324570000	-0.076560000
H	-1.143930000	0.343650000	-0.055950000
H	-2.074760000	1.571620000	-0.083100000
O	-3.900210000	1.449800000	-0.096140000
H	-3.971490000	0.472220000	-0.037050000
H	-4.398510000	1.778860000	0.662220000
O	-3.696260000	-1.320440000	0.078460000
H	-2.740550000	-1.529510000	0.014790000
H	-4.132610000	-1.951750000	-0.506070000

$W_{10:3}$			
E(MP2/aTZ) = -763.4423504 a.u.			
O	-2.531320000	0.273970000	1.499680000
H	-3.103340000	0.458740000	2.254360000
H	-1.601310000	0.244610000	1.868840000
O	-2.374940000	1.544750000	-1.057950000
H	-2.490440000	1.314340000	-0.116640000
H	-2.618890000	0.716960000	-1.499180000
O	0.339330000	2.112600000	-1.352240000
H	0.698170000	1.333400000	-1.819100000
H	-0.628130000	1.948350000	-1.304930000
O	1.533960000	2.067340000	1.000860000
H	1.820610000	2.949800000	1.265550000
H	1.060490000	2.182410000	0.125940000
O	-0.050190000	0.204040000	2.388910000
H	0.495240000	0.920680000	2.003870000
H	0.432120000	-0.613750000	2.156420000
O	1.433160000	-1.973070000	1.331960000
H	2.118280000	-1.376750000	0.918790000
H	1.927490000	-2.650310000	1.809810000
O	2.999450000	-0.192650000	0.119610000
H	2.673140000	-0.201930000	-0.801970000
H	2.684800000	0.666300000	0.465330000
O	1.493180000	-0.312880000	-2.284210000
H	1.730760000	-0.582100000	-3.179790000
H	0.888700000	-1.024220000	-1.937970000
O	-0.030890000	-2.157090000	-1.099360000
H	-0.968630000	-1.938120000	-0.929140000
H	0.375520000	-2.253350000	-0.216520000
O	-2.729470000	-1.437220000	-0.635780000
H	-2.782190000	-0.976280000	0.230580000
H	-3.370640000	-2.156980000	-0.586100000

$W_{10:4}$			
E(MP2/aTZ) = -763.4422554 a.u.			
O	-2.513890000	-0.437780000	1.491460000
H	-1.583580000	-0.670000000	1.777580000
H	-3.077970000	-0.670410000	2.238900000
O	-2.334270000	1.955110000	-0.070550000
H	-2.594690000	1.444320000	-0.852570000
H	-2.456030000	1.301170000	0.643200000
O	0.390310000	2.510990000	-0.264830000
H	0.785280000	2.206740000	0.573770000
H	-0.576560000	2.370800000	-0.161100000
O	1.753220000	1.155320000	1.859050000
H	2.331860000	0.668070000	1.210540000
H	2.351410000	1.518490000	2.523750000
O	-0.032590000	-1.023230000	2.176180000
H	0.561340000	-0.246500000	2.204600000
H	0.397380000	-1.629250000	1.539920000
O	1.222120000	-2.469870000	0.102620000
H	1.376930000	-3.414370000	-0.018900000
H	0.696040000	-2.172070000	-0.691700000
O	3.002240000	-0.254240000	-0.036390000
H	2.650320000	0.131020000	-0.863450000
H	2.570910000	-1.129740000	0.008590000
O	1.454590000	0.928520000	-2.099150000
H	1.710860000	1.432310000	-2.881220000
H	1.037150000	1.588490000	-1.473620000
O	-0.090990000	-1.417770000	-1.948610000
H	-1.019190000	-1.179670000	-1.755770000
H	0.365070000	-0.570950000	-2.129800000
O	-2.759750000	-0.791330000	-1.222960000
H	-3.457490000	-1.375410000	-1.544840000
H	-2.796920000	-0.848720000	-0.242520000

$W_{10:5}$
E(MP2/aTZ) = -763.4415717 a.u.

O	0.000000000	-1.092250000	2.085120000
H	-0.000060000	-0.098970000	2.014520000
H	0.000020000	-1.287120000	3.030190000
O	0.000010000	1.558900000	1.715930000
H	0.769480000	1.796350000	1.162330000
H	-0.769440000	1.796330000	1.162290000
O	2.091830000	1.996880000	-0.161410000
H	2.556080000	2.821660000	-0.349770000
H	2.800460000	1.303370000	-0.101530000
O	3.788100000	-0.067700000	-0.085880000
H	3.152330000	-0.823980000	0.025720000
H	4.481800000	-0.220580000	0.566730000
O	1.921680000	-1.971780000	0.178040000
H	1.316240000	-1.747580000	0.911180000
H	1.341220000	-1.971730000	-0.608050000
O	-0.000090000	-1.605450000	-1.880620000
H	-0.000090000	-0.613350000	-1.956660000
H	-0.000110000	-1.938080000	-2.786370000
O	0.000050000	1.072190000	-1.875750000
H	0.769540000	1.417590000	-1.382410000
H	-0.769310000	1.417750000	-1.382330000
O	-2.091750000	1.996940000	-0.161460000
H	-2.555970000	2.821730000	-0.349840000
H	-2.800370000	1.303430000	-0.101640000
O	-3.788080000	-0.067610000	-0.085880000
H	-4.481860000	-0.220340000	0.566680000
H	-3.152400000	-0.823940000	0.025890000
O	-1.921740000	-1.971780000	0.178130000
H	-1.341330000	-1.971720000	-0.607990000
H	-1.316270000	-1.747590000	0.911240000

$W_{11:1}$
E(MP2/aTZ) = -839.79015 a.u.

O	-2.292770000	-2.059480000	0.533810000
H	-2.819780000	-2.848970000	0.706370000
H	-1.509410000	-2.360580000	0.001420000
O	-0.160490000	-2.540190000	-1.005240000
H	-0.124160000	-1.770240000	-1.598530000
H	0.676690000	-2.495170000	-0.496590000
O	2.191600000	-2.091220000	0.410960000
H	2.794100000	-2.743550000	0.787920000
H	1.964230000	-1.454040000	1.152750000
O	1.542550000	-0.251460000	2.170730000
H	1.846250000	0.590970000	1.787890000
H	0.564600000	-0.157990000	2.264140000
O	-1.195550000	-0.085020000	2.323320000
H	-1.617320000	-0.810810000	1.827390000
H	-1.564530000	0.724340000	1.924230000
O	-2.129130000	2.161790000	0.784930000
H	-2.592930000	2.967560000	1.042680000
H	-1.320020000	2.455400000	0.289080000
O	-2.652570000	0.171210000	-1.117260000
H	-2.729210000	-0.630780000	-0.561640000
H	-2.669030000	0.907740000	-0.473260000
O	-0.306170000	0.144720000	-2.337090000
H	-0.470010000	0.207360000	-3.287790000
H	-1.216400000	0.156420000	-1.912980000
O	2.480440000	0.001010000	-1.431890000
H	2.516740000	-0.823780000	-0.905940000
H	1.578730000	0.011970000	-1.799000000
O	2.474840000	1.902160000	0.463630000
H	3.273290000	2.443360000	0.497810000
H	2.621130000	1.243110000	-0.264770000
O	0.032810000	2.638550000	-0.713990000
H	0.892140000	2.524430000	-0.258900000
H	0.020430000	1.926740000	-1.377480000

$W_{11:2}$
E(MP2/aTZ) = -839.7898948 a.u.

O	-1.986000000	-1.017320000	-1.800960000
H	-1.392050000	-0.231860000	-2.001510000
H	-2.266070000	-1.347570000	-2.663850000
O	-0.414930000	1.043870000	-2.227140000
H	0.540010000	0.797780000	-2.223510000
H	-0.487480000	1.690800000	-1.500400000
O	2.255210000	0.403490000	-1.961890000
H	2.325110000	-0.492720000	-1.579890000
H	2.477260000	0.993240000	-1.219920000
O	2.226370000	-2.079330000	-0.568000000
H	2.685000000	-2.896410000	-0.797940000
H	1.269260000	-2.328050000	-0.446360000
O	-0.355120000	-2.538260000	-0.064480000
H	-0.485230000	-2.122880000	0.809720000
H	-0.956110000	-2.060740000	-0.671600000
O	-0.239230000	-1.104590000	2.408600000
H	-0.262630000	-1.486510000	3.294820000
H	0.713340000	-0.855210000	2.251180000
O	2.266530000	-0.474740000	1.754570000
H	2.445180000	-1.062840000	0.994070000
H	2.322670000	0.426870000	1.381980000
O	2.257870000	2.044000000	0.440080000
H	1.333430000	2.385080000	0.389280000
H	2.796050000	2.791740000	0.727490000
O	-0.389540000	2.665210000	0.150380000
H	-0.951370000	2.103920000	0.765400000
H	-0.767380000	3.552250000	0.201110000
O	-1.829610000	1.111530000	1.706720000
H	-2.567700000	0.704680000	1.203760000
H	-1.308620000	0.351840000	2.036300000
O	-3.771000000	-0.023910000	0.075660000
H	-3.247560000	-0.445680000	-0.640320000
H	-4.379530000	-0.707270000	0.381910000

$W_{11:3}$
E(MP2/aTZ) = -839.7893428 a.u.

O	-1.539920000	2.122240000	1.084660000
H	-1.949670000	2.698370000	1.742090000
H	-1.074930000	1.402000000	1.610080000
O	0.330210000	2.629860000	-0.799120000
H	-0.345900000	2.628590000	-0.078840000
H	0.197740000	3.454080000	-1.283800000
O	2.814000000	1.267550000	-0.329850000
H	2.737360000	0.583490000	-1.023640000
H	2.043270000	1.847190000	-0.474360000
O	2.477150000	-0.146760000	1.925550000
H	2.680770000	0.439100000	1.149050000
H	3.192180000	-0.006210000	2.558140000
O	-0.329330000	0.124250000	2.273600000
H	-0.558360000	-0.622730000	1.676060000
H	0.647210000	0.111420000	2.297680000
O	-0.854960000	-1.724070000	0.280810000
H	-0.759280000	-1.093470000	-0.464960000
H	-1.799960000	-1.987560000	0.255610000
O	1.854570000	-2.390450000	0.242850000
H	2.145660000	-1.788410000	0.954060000
H	0.880520000	-2.407650000	0.335540000
O	2.234760000	-0.981790000	-1.985810000
H	2.765380000	-1.454990000	-2.638290000
H	2.150070000	-1.596590000	-1.203240000
O	-0.356050000	0.081100000	-1.830820000
H	0.473490000	-0.337150000	-2.137100000
H	-0.079990000	0.983180000	-1.573560000
O	-3.084060000	0.674100000	-0.932800000
H	-2.327420000	0.460360000	-1.504530000
H	-2.681850000	1.207030000	-0.220830000
O	-3.609070000	-1.814870000	0.152390000
H	-3.592380000	-0.922170000	-0.262320000
H	-4.242230000	-2.327220000	-0.364270000

$W_{11:4}$
E(MP2/aTZ) = -839.7888741 a.u.

O	-1.491790000	2.211130000	1.100550000
H	-0.741950000	2.527220000	0.547800000
H	-1.801770000	2.986360000	1.585630000
O	-0.218380000	-0.072350000	2.324750000
H	-0.660010000	0.758610000	2.071300000
H	-0.558510000	-0.716080000	1.663530000
O	2.389700000	-0.376690000	1.974460000
H	2.859340000	-0.426440000	2.815950000
H	1.434750000	-0.196610000	2.204230000
O	2.789830000	1.232820000	-0.277660000
H	2.774730000	0.731100000	0.564150000
H	2.749230000	0.540100000	-0.966150000
O	0.585000000	2.625710000	-0.633790000
H	1.461190000	2.174020000	-0.448850000
H	0.802350000	3.429470000	-1.122180000
O	-0.411530000	0.230770000	-1.805500000
H	0.397170000	-0.185900000	-2.164350000
H	-0.096170000	1.102440000	-1.494520000
O	2.163020000	-0.886420000	-2.086470000
H	2.682350000	-1.320180000	-2.774600000
H	2.074970000	-1.554880000	-1.349360000
O	1.793560000	-2.427510000	0.048680000
H	0.820760000	-2.426930000	0.158490000
H	2.108470000	-1.887360000	0.798810000
O	-0.898910000	-1.706470000	0.195380000
H	-1.848780000	-1.952710000	0.168520000
H	-0.805260000	-1.026600000	-0.505700000
O	-3.653270000	-1.762640000	0.105930000
H	-4.293330000	-2.244150000	-0.431520000
H	-3.634090000	-0.850010000	-0.263220000
O	-3.126100000	0.764760000	-0.875340000
H	-2.721310000	1.294620000	-0.163800000
H	-2.373080000	0.579080000	-1.462080000

$W_{11:5}$
E(MP2/aTZ) = -839.7882228 a.u.

O	0.366430000	-0.752050000	-2.405040000
H	-0.513910000	-1.129420000	-2.203890000
H	0.965600000	-1.186390000	-1.764150000
O	-2.077770000	-1.772890000	-1.461560000
H	-2.774850000	-2.210480000	-1.965170000
H	-2.519550000	-1.024480000	-0.975760000
O	-3.047230000	0.222460000	0.027140000
H	-2.610110000	1.076050000	-0.156790000
H	-2.740610000	-0.015340000	0.924710000
O	-1.518220000	2.597930000	-0.368220000
H	-0.794850000	2.426100000	-1.015340000
H	-1.909870000	3.439660000	-0.632060000
O	0.607660000	1.828470000	-1.916970000
H	0.489000000	0.864080000	-2.166670000
H	0.953000000	2.257850000	-2.709670000
O	1.961090000	1.090790000	0.505350000
H	1.673010000	1.511010000	-0.326490000
H	1.262670000	1.349080000	1.157160000
O	-0.167860000	1.756130000	2.066940000
H	-0.665930000	0.943390000	2.285990000
H	-0.719530000	2.193110000	1.393900000
O	-1.680680000	-0.625500000	2.353620000
H	-1.997400000	-0.987670000	3.190130000
H	-1.237380000	-1.383970000	1.880490000
O	-0.585250000	-2.543220000	0.866740000
H	0.330360000	-2.331570000	0.589660000
H	-1.098510000	-2.502410000	0.038090000
O	1.827270000	-1.564680000	-0.146270000
H	2.758310000	-1.808950000	-0.023660000
H	1.822660000	-0.624000000	0.155380000
O	4.376450000	-0.367840000	0.542190000
H	5.108090000	-0.157600000	1.134250000
H	3.724650000	0.345110000	0.678420000

$W_{12:1}$
E(MP2/aTZ) = -916.1436611 a.u.

O	2.772110000	1.869460000	-0.353360000
H	2.900110000	1.480480000	0.533520000
H	1.846350000	2.175820000	-0.349560000
O	2.876610000	-0.246750000	-2.004630000
H	3.560310000	-0.166130000	-2.680920000
H	2.918350000	0.592620000	-1.471820000
O	2.772120000	-1.869460000	0.353320000
H	1.846360000	-2.175810000	0.349530000
H	2.900100000	-1.480480000	-0.533560000
O	2.876650000	0.246760000	2.004610000
H	3.560370000	0.166110000	2.680880000
H	2.918340000	-0.592620000	1.471800000
O	-0.068530000	1.905110000	-0.398500000
H	-0.991140000	2.225770000	-0.413500000
H	-0.064550000	1.142850000	-1.024470000
O	0.068490000	-0.398510000	-1.905080000
H	0.991110000	-0.413520000	-2.225750000
H	0.064520000	-1.024480000	-1.142810000
O	-0.068520000	-1.905090000	0.398520000
H	-0.064540000	-1.142820000	1.024470000
H	-0.991130000	-2.225780000	0.413460000
O	0.068540000	0.398510000	1.905100000
H	0.991160000	0.413500000	2.225750000
H	0.064550000	1.024490000	1.142850000
O	-2.876650000	2.004660000	-0.246720000
H	-3.560320000	2.680990000	-0.166220000
H	-2.918410000	1.471930000	0.592690000
O	-2.772130000	-0.353340000	-1.869420000
H	-2.900120000	0.533530000	-1.480430000
H	-1.846370000	-0.349530000	-2.175770000
O	-2.876620000	-2.004650000	0.246730000
H	-2.918380000	-1.471850000	-0.592650000
H	-3.560330000	-2.680940000	0.166160000
O	-2.772070000	0.353310000	1.869450000
H	-2.900060000	-0.533560000	1.480450000
H	-1.846310000	0.349490000	2.175800000

$W_{12:2}$
E(MP2/aTZ) = -916.1432555 a.u.

O	-2.772320000	1.401520000	-1.285740000
H	-1.846460000	1.581630000	-1.533010000
H	-2.900680000	0.458330000	-1.505520000
O	-2.885150000	1.457330000	1.399800000
H	-2.923020000	1.533000000	0.408550000
H	-3.574590000	2.042480000	1.736860000
O	-2.772300000	-1.401550000	1.285750000
H	-1.846440000	-1.581650000	1.533020000
H	-2.900680000	-0.458370000	1.505540000
O	-2.885120000	-1.457330000	-1.399760000
H	-2.922810000	-1.533140000	-0.408530000
H	-3.574570000	-2.042470000	-1.736800000
O	0.071230000	1.448260000	-1.290920000
H	0.990620000	1.670360000	-1.534450000
H	0.064990000	1.498390000	-0.305400000
O	-0.075700000	1.291980000	1.455870000
H	-0.996550000	1.540450000	1.666040000
H	-0.071430000	0.306650000	1.504770000
O	0.071320000	-1.448270000	1.290910000
H	0.065100000	-1.498340000	0.305400000
H	0.990710000	-1.670330000	1.534500000
O	-0.075650000	-1.292050000	-1.455900000
H	-0.996520000	-1.540470000	-1.666080000
H	-0.071390000	-0.306720000	-1.504770000
O	2.891580000	1.497250000	-1.364290000
H	3.577090000	2.096010000	-1.685250000
H	2.937870000	1.537620000	-0.371110000
O	2.770160000	1.364010000	1.313730000
H	2.896860000	0.417100000	1.518630000
H	1.845320000	1.539330000	1.568090000
O	2.891680000	-1.497180000	1.364280000
H	2.937940000	-1.537540000	0.371100000
H	3.577230000	-2.095920000	1.685200000
O	2.770170000	-1.363970000	-1.313730000
H	1.845340000	-1.539330000	-1.568100000
H	2.896820000	-0.417050000	-1.518630000

$W_{12:3}$
E(MP2/aTZ) = -916.1432537 a.u.

O	-1.356950000	-1.321260000	2.771130000
H	-0.408380000	-1.520510000	2.893900000
H	-1.533940000	-1.574920000	1.846300000
O	-1.506260000	1.355370000	2.890460000
H	-1.541130000	0.361780000	2.936480000
H	-2.102710000	1.672740000	3.579630000
O	1.356950000	1.321260000	2.771130000
H	0.408380000	1.520510000	2.893900000
H	1.533940000	1.574920000	1.846300000
O	1.506260000	-1.355370000	2.890460000
H	2.102710000	-1.672740000	3.579630000
H	1.541130000	-0.361780000	2.936480000
O	-1.286050000	-1.459200000	-0.073490000
H	-1.533910000	-1.672800000	-0.993560000
H	-0.300280000	-1.505150000	-0.069000000
O	-1.451260000	1.287980000	0.069510000
H	-1.676700000	1.529480000	0.988550000
H	-1.497850000	0.302300000	0.062480000
O	1.286050000	1.459200000	-0.073490000
H	1.533910000	1.672800000	-0.993560000
H	0.300280000	1.505150000	-0.069000000
O	1.451260000	-1.287980000	0.069510000
H	1.497850000	-0.302300000	0.062480000
H	1.676700000	-1.529480000	0.988550000
O	-1.451260000	-1.407180000	-2.883810000
H	-2.029700000	-1.747880000	-3.577080000
H	-1.532240000	-0.416220000	-2.922530000
O	-1.408760000	1.277500000	-2.773600000
H	-0.466370000	1.502290000	-2.898800000
H	-1.593010000	1.522670000	-1.847950000
O	1.451260000	1.407180000	-2.883810000
H	1.532240000	0.416220000	-2.922530000
H	2.029700000	1.747880000	-3.577080000
O	1.408760000	-1.277500000	-2.773600000
H	1.593010000	-1.522670000	-1.847950000
H	0.466370000	-1.502290000	-2.898800000

$W_{12:4}$
E(MP2/aTZ) = -916.14288 a.u.

O	2.768120000	-0.480920000	1.831300000
H	2.896720000	0.434240000	1.514090000
H	1.842730000	-0.497910000	2.138020000
O	2.900910000	1.988710000	0.385540000
H	3.589830000	2.663440000	0.346020000
H	2.942750000	1.505740000	-0.483410000
O	2.768080000	0.480920000	-1.831320000
H	1.842670000	0.497860000	-2.137990000
H	2.896740000	-0.434240000	-1.514090000
O	2.900960000	-1.988640000	-0.385530000
H	2.942610000	-1.505700000	0.483450000
H	3.589940000	-2.663310000	-0.345900000
O	-0.079450000	-0.354480000	1.907840000
H	-0.997400000	-0.444810000	2.228340000
H	-0.072810000	0.514970000	1.440740000
O	0.079440000	1.907960000	0.354360000
H	0.997400000	2.228440000	0.444820000
H	0.072820000	1.441170000	-0.515240000
O	-0.079470000	0.354380000	-1.907780000
H	-0.997410000	0.444770000	-2.228310000
H	-0.072870000	-0.514990000	-1.440550000
O	0.079460000	-1.908010000	-0.354400000
H	0.997410000	-2.228450000	-0.444910000
H	0.072840000	-1.441170000	0.515180000
O	-2.900950000	-0.385500000	1.988640000
H	-2.942780000	0.483440000	1.505660000
H	-3.589880000	-0.345950000	2.663370000
O	-2.768090000	1.831390000	0.480890000
H	-1.842690000	2.138100000	0.497870000
H	-2.896720000	1.514150000	-0.434260000
O	-2.900870000	0.385520000	-1.988630000
H	-3.589780000	0.345900000	-2.663370000
H	-2.942580000	-0.483450000	-1.505680000
O	-2.768150000	-1.831330000	-0.480930000
H	-2.896760000	-1.514100000	0.434230000
H	-1.842760000	-2.138090000	-0.497890000

$W_{12:5}$
E(MP2/aTZ) = -916.1428818 a.u.

O	-2.767740000	-1.846480000	-0.418990000
H	-2.897120000	-1.498170000	0.484680000
H	-1.842480000	-2.154000000	-0.424520000
O	-2.901310000	0.317680000	-2.000220000
H	-2.942590000	-0.534840000	-1.488610000
H	-3.589460000	0.255030000	-2.673990000
O	-2.767750000	1.846460000	0.419020000
H	-2.897110000	1.498160000	-0.484660000
H	-1.842490000	2.153990000	0.424560000
O	-2.901290000	-0.317670000	2.000210000
H	-3.589450000	-0.254940000	2.673950000
H	-2.942520000	0.534830000	1.488550000
O	0.079530000	-1.919130000	-0.288460000
H	0.997520000	-2.242420000	-0.367970000
H	0.072880000	-1.422340000	0.564360000
O	-0.079540000	0.288530000	-1.919100000
H	-0.072880000	-0.564240000	-1.422240000
H	-0.997530000	0.367990000	-2.242390000
O	0.079550000	1.919150000	0.288490000
H	0.072900000	1.422270000	-0.564280000
H	0.997540000	2.242420000	0.368010000
O	-0.079550000	-0.288450000	1.919070000
H	-0.997530000	-0.367930000	2.242380000
H	-0.072910000	0.564260000	1.422090000
O	2.901270000	-2.000260000	-0.317700000
H	3.589410000	-2.674030000	-0.255070000
H	2.942560000	-1.488660000	0.534820000
O	2.767750000	0.419020000	-1.846450000
H	2.897100000	-0.484660000	-1.498170000
H	1.842480000	0.424590000	-2.153970000
O	2.901360000	2.000190000	0.317690000
H	2.942570000	1.488530000	-0.534810000
H	3.589550000	2.673900000	0.254960000
O	2.767740000	-0.419020000	1.846460000
H	1.842460000	-0.424530000	2.153960000
H	2.897130000	0.484650000	1.498160000

$W_{13:1}$
E(MP2/aTZ) = -992.4881084 a.u.

O	-2.997564044	0.309669061	1.910014780
H	-3.200403723	-0.524984967	1.442667691
H	-2.078750230	0.206481630	2.210653551
O	-3.428483804	-1.822898353	0.073918992
H	-4.190137985	-2.396995509	-0.072065529
H	-3.373050360	-1.233994067	-0.723581503
O	-3.007674877	-0.053580740	-1.912947382
H	-3.060616593	0.803778250	-1.444918819
H	-2.082941746	-0.112744853	-2.206602483
O	-3.026670068	2.111042580	-0.089227162
H	-3.642800786	2.840630544	0.048863937
H	-3.103222790	1.531651764	0.713426715
O	-0.084810737	-0.026563281	1.880904676
H	-0.236465279	-0.816678457	1.308184441
H	0.825921396	-0.148888388	2.208747182
O	-0.581432488	-2.028853410	0.084526582
H	-1.530747807	-2.246923654	0.096777712
H	-0.464325592	-1.446492772	-0.704875398
O	-0.073001118	-0.206990809	-1.897597713
H	0.003360714	0.604733834	-1.346239826
H	0.840512061	-0.418463912	-2.165998125
O	-0.163029009	1.874020649	-0.073674360
H	-1.087053601	2.183567542	-0.096179100
H	-0.121385914	1.267532310	0.707524574
O	2.711950960	-0.593229037	2.081309339
H	3.082423153	0.002593852	1.372263518
H	3.381355773	-0.616908947	2.776119901
O	2.201673395	-2.650358078	0.186819059
H	2.423100973	-2.081575916	0.951794794
H	1.233724240	-2.739138116	0.235412174
O	2.679246607	-1.046399562	-1.931345171
H	2.553123687	-1.727315705	-1.218988141
H	3.236960166	-1.466925490	-2.597506687
O	3.590616588	0.835036857	0.014339580
H	3.377966546	0.308321385	-0.779798861
H	3.197206180	1.717338420	-0.147382701
O	2.233262566	3.244774332	-0.418463138
H	2.349169385	4.016846203	0.148552533
H	1.319707407	2.935961201	-0.251560366

$W_{13:2}$
E(MP2/aTZ) = -992.4870506 a.u.

O	2.741597252	1.115722032	1.916764792
H	1.793424185	1.336430575	1.920678037
H	3.059500321	1.439386429	1.050377028
O	3.501420450	1.547477189	-0.792537656
H	3.569614488	0.573033661	-0.970809450
H	4.301049668	1.939289664	-1.164454232
O	3.404584652	-1.132668569	-1.073266369
H	3.313653073	-1.455506668	-0.154294997
H	2.559356071	-1.365621168	-1.493667059
O	2.929594273	-1.558858926	1.697565385
H	3.493762727	-1.958829871	2.370629644
H	2.926572511	-0.583881607	1.889919100
O	-0.073550826	1.214397449	1.278715079
H	0.143844785	1.399057220	0.332972735
H	-0.961607101	1.594549900	1.396905440
O	0.674344073	1.462554327	-1.342182748
H	0.709073103	0.495670415	-1.545434986
H	1.606033045	1.745127422	-1.351581069
O	0.558544394	-1.245234348	-1.648272297
H	-0.289727468	-1.408056271	-2.098352120
H	0.367082729	-1.442943336	-0.699129619
O	0.132008475	-1.520864185	1.039099275
H	0.990977513	-1.756504806	1.433853368
H	0.014393174	-0.566249631	1.256596534
O	-2.830711433	2.054469540	0.813140608
H	-3.212433691	2.938658406	0.876483535
H	-2.649925517	1.913302597	-0.155875045
O	-2.185265901	1.579104909	-1.743676864
H	-2.288697558	0.635320413	-1.988347500
H	-1.229575138	1.740793619	-1.824361150
O	-2.276653379	-1.199823784	-2.205448195
H	-2.461329034	-1.581907729	-1.303020440
H	-2.870054806	-1.662922961	-2.809450527
O	-2.574969492	-2.124518695	0.277840423
H	-1.696596235	-2.153236121	0.694836310
H	-3.097598508	-1.525991131	0.854383821
O	-3.932338982	-0.273609512	1.839309621
H	-4.896025556	-0.247644543	1.876792224
H	-3.661249805	0.610058377	1.509862772

$W_{13:3}$
E(MP2/aTZ) = -992.4869148 a.u.

O	-2.914752791	-2.171692983	-0.520650880
H	-3.524014588	-2.919066332	-0.503472064
H	-3.019738140	-1.704510739	0.358399867
O	-3.020442858	-0.713702711	1.695215934
H	-2.088283041	-0.607557655	2.006597208
H	-3.243430393	0.161637795	1.333483078
O	-3.266289981	1.669391636	-0.053652925
H	-4.021049763	2.225179932	-0.282121104
H	-3.055735866	1.154160818	-0.872363772
O	-2.601695323	0.063395208	-2.141353378
H	-2.764914715	-0.806145887	-1.716586204
H	-1.663738278	0.044316453	-2.385587341
O	-0.115830479	-1.713648852	-0.294219801
H	-0.991203548	-2.096546199	-0.483695741
H	0.028428025	-1.014938388	-0.977258320
O	-0.275890078	-0.289771252	2.052591131
H	-0.434819259	0.649663703	1.767793221
H	-0.220572699	-0.791587285	1.204121544
O	-0.825367382	2.220419430	1.215163535
H	-1.687237948	2.202392824	0.755095580
H	-0.186183792	2.507011551	0.533155246
O	0.470385278	0.236397210	-2.110035960
H	1.379308232	-0.061282948	-2.301456180
H	0.604857056	1.127923959	-1.725399767
O	2.594662378	-2.307999496	0.235059288
H	1.633651933	-2.395791229	0.094047534
H	2.647403775	-1.776758317	1.054402155
O	2.376791848	-0.376437960	2.324185426
H	2.681164052	-0.394294203	3.239786143
H	1.378163102	-0.323971088	2.368827290
O	3.214305913	1.370952931	0.243824887
H	2.993440745	0.841061029	1.036869933
H	3.393991521	0.707088230	-0.450553049
O	3.218225889	-0.645992414	-1.772790528
H	3.945432802	-0.968979702	-2.319082245
H	3.065972294	-1.349957644	-1.086065777
O	1.115205179	2.627243371	-0.760074569
H	1.943679940	2.248669839	-0.347778330
H	1.371537077	3.480123281	-1.132338461

$W_{13:4}$
E(MP2/aTZ) = -992.4844824 a.u.

O	3.410011192	0.625428764	1.517896561
H	2.572616066	1.070450747	1.734493074
H	3.594566645	0.894502385	0.595880056
O	3.619985515	0.981653274	-1.295095614
H	4.394587332	1.202088476	-1.826771202
H	3.430684486	0.023627129	-1.476211575
O	2.900679519	-1.609235981	-1.514024594
H	1.953023508	-1.633469091	-1.732353490
H	2.943028149	-1.930520636	-0.591069349
O	2.912084351	-2.018171208	1.296828596
H	3.505130221	-2.557029714	1.834593528
H	3.162237278	-1.074855830	1.480311707
O	0.601258763	1.268380107	1.570757768
H	-0.238279805	1.689335134	1.827356997
H	0.386758334	0.306821610	1.513453665
O	0.830726480	1.669552050	-1.142685375
H	0.810651537	1.625205522	-0.157552599
H	1.778556628	1.705942435	-1.364333399
O	0.097672958	-0.939948346	-1.574203620
H	-0.831628533	-0.958365480	-1.866858272
H	0.324547398	0.019922964	-1.530672229
O	0.103777359	-1.396347388	1.120907952
H	0.933471717	-1.853840952	1.345909266
H	0.108640156	-1.343454885	0.133640007
O	-2.180647741	2.028532635	1.539601518
H	-2.160912142	2.219941436	0.563231639
H	-2.763174192	2.694159651	1.925733981
O	-2.003484070	2.265990592	-1.131157090
H	-1.065835531	2.280205366	-1.388033622
H	-2.334133236	1.407822614	-1.467980594
O	-2.713692578	-0.425600915	-1.571300986
H	-2.689729356	-0.574574390	-0.599574051
H	-3.566177066	-0.816156882	-1.816942851
O	-2.654565941	-0.711270137	1.209929083
H	-1.802750120	-1.124324839	1.438053267
H	-2.567537633	0.223745717	1.492302194
O	-4.942583401	-1.694028629	-0.160141596
H	-5.643840799	-2.219058281	0.243052834
H	-4.317757898	-1.503675225	0.561931197

$W_{13:5}$
E(MP2/aTZ) = -992.4769471 a.u.

O	-2.266157993	1.225642055	2.065896083
H	-2.551357490	1.587054558	1.202708032
H	-1.351479511	1.544850287	2.150514567
O	-2.795015642	2.155523200	-0.559847962
H	-2.872578633	1.319252801	-1.093815189
H	-3.557939647	2.691479334	-0.808986030
O	-2.750020590	-0.109715486	-1.989604935
H	-1.866552365	-0.087415991	-2.403447540
H	-2.733949332	-0.937143787	-1.467122375
O	-2.335122430	-2.444022580	-0.430676646
H	-2.298773423	-2.134463680	0.517339453
H	-2.916650496	-3.214283519	-0.428934617
O	-2.020875640	-1.515570663	2.043407255
H	-1.070177473	-1.584040441	2.226250798
H	-2.190054900	-0.543380315	2.083246786
O	0.583429610	1.690126120	1.696360033
H	0.476782401	1.880628296	0.733636923
H	1.295834311	2.272162946	1.990589035
O	0.074444353	2.221219931	-0.935937230
H	-0.860680663	2.490208663	-0.878400435
H	0.066716513	1.462374233	-1.562893847
O	0.031863120	0.021211074	-2.559425743
H	0.582939690	-0.127508470	-3.337873685
H	0.250176289	-0.711775803	-1.914934465
O	0.451654304	-1.866056200	-0.769843493
H	0.596242910	-1.578763763	0.169059310
H	-0.408300468	-2.326568104	-0.743623947
O	0.895321634	-1.093897470	1.785080304
H	1.824736527	-1.341294999	1.963520791
H	0.879431945	-0.115726002	1.833630055
O	3.622271484	-1.748698964	1.661848546
H	4.442324340	-1.507307698	2.107650823
H	3.689868015	-1.369476110	0.757928259
O	3.318847747	-0.781206576	-0.924028400
H	3.087927589	0.168015607	-0.941389530
H	2.491594875	-1.247153195	-1.118544912
O	2.892882992	2.069793019	-0.890025790
H	1.990800946	2.415508022	-1.006220892
H	3.430740259	2.561799613	-1.523179569

$W_{14:1}$
E(MP2/aTZ) = -1068.835622 a.u.

O	-3.323387000	-2.026150000	0.314178000
H	-3.989767000	-2.721288000	0.252447000
H	-3.331973000	-1.560679000	-0.569431000
O	-3.169185000	-0.580802000	-1.917787000
H	-2.222597000	-0.574128000	-2.150641000
H	-3.347072000	0.335194000	-1.622331000
O	-3.457382000	1.868610000	-0.542980000
H	-4.153860000	2.536071000	-0.546170000
H	-3.484780000	1.452501000	0.351967000
O	-3.326515000	0.410033000	1.756228000
H	-3.417849000	-0.492100000	1.387765000
H	-2.413938000	0.438189000	2.085689000
O	-0.511916000	-1.846544000	0.692475000
H	-0.506381000	-1.243415000	1.469950000
H	-1.434049000	-2.160681000	0.635480000
O	-0.328757000	-0.540038000	-1.734339000
H	-0.334878000	-0.985560000	-0.856179000
H	0.524540000	-0.789483000	-2.135724000
O	-0.572558000	2.171228000	-1.366987000
H	-1.476747000	2.273432000	-1.030641000
H	-0.481831000	1.204105000	-1.526763000
O	-0.532963000	0.013718000	2.723991000
H	-0.502674000	-0.227868000	3.658370000
H	0.292346000	0.544161000	2.570568000
O	2.202831000	-2.575090000	0.109865000
H	1.254232000	-2.529629000	0.328085000
H	2.252351000	-2.287028000	-0.823297000
O	2.358701000	-1.211234000	-2.373967000
H	2.830345000	-0.417430000	-2.002478000
H	2.804094000	-1.419780000	-3.203958000
O	3.549254000	0.818736000	-1.100623000
H	3.756181000	0.402809000	-0.241541000
H	2.961932000	1.564840000	-0.867870000
O	3.610794000	-0.649744000	1.331700000
H	3.112377000	-1.425530000	0.957698000
H	4.340115000	-1.025307000	1.839661000
O	1.771581000	1.316883000	2.241049000
H	2.448494000	0.652665000	2.006851000
H	1.759878000	1.930622000	1.481677000
O	1.736467000	2.815381000	-0.173086000
H	1.926332000	3.754979000	-0.284645000
H	0.844229000	2.674456000	-0.582307000

$W_{14:2}$
E(MP2/aTZ) = -1068.835392 a.u.

O	3.664271000	1.535343000	1.156020000
H	3.677798000	1.455518000	0.170649000
H	4.427072000	2.081204000	1.382784000
O	3.420228000	1.052946000	-1.517891000
H	3.391841000	0.078849000	-1.576297000
H	2.513247000	1.324877000	-1.739324000
O	3.063634000	-1.798210000	-1.176911000
H	3.177176000	-1.672364000	-0.182589000
H	3.677898000	-2.499918000	-1.426009000
O	3.184111000	-1.283293000	1.396717000
H	3.470430000	-0.354362000	1.492204000
H	2.234429000	-1.259831000	1.667711000
O	0.703305000	1.714172000	1.210273000
H	1.629234000	1.922901000	1.420199000
H	0.695072000	1.635236000	0.224523000
O	0.532065000	1.289148000	-1.486828000
H	0.389006000	0.315753000	-1.489353000
H	-0.315036000	1.674287000	-1.779399000
O	0.421286000	-1.415382000	-1.103630000
H	-0.325732000	-2.011106000	-1.336874000
H	1.287660000	-1.821052000	-1.333214000
O	0.440171000	-1.019016000	1.634230000
H	0.448616000	-0.034503000	1.654388000
H	0.425455000	-1.196924000	0.664603000
O	-2.073727000	2.427428000	0.996111000
H	-2.571505000	1.650970000	1.323624000
H	-1.161859000	2.305449000	1.314828000
O	-2.141396000	2.228180000	-1.672117000
H	-2.542702000	3.002537000	-2.085388000
H	-2.140602000	2.412970000	-0.693429000
O	-3.439759000	-0.274308000	-1.302636000
H	-3.029597000	0.564118000	-1.593789000
H	-3.691304000	-0.095985000	-0.374520000
O	-3.625286000	0.124435000	1.491207000
H	-3.094726000	-0.703771000	1.671318000
H	-4.365068000	0.101785000	2.110531000
O	-2.117158000	-2.042306000	1.730303000
H	-1.194602000	-1.710897000	1.848877000
H	-2.105150000	-2.435685000	0.840355000
O	-2.016592000	-2.518865000	-1.223269000
H	-2.451106000	-3.183817000	-1.771464000
H	-2.558497000	-1.687131000	-1.334252000

$W_{14:3}$
E(MP2/aTZ) = -1068.833227 a.u.

O	-3.508232000	1.016237000	-1.194527000
H	-3.472422000	0.031464000	-1.260258000
H	-4.375617000	1.269807000	-1.533067000
O	-2.492468000	2.007468000	1.266628000
H	-1.634609000	2.398936000	1.031550000
H	-2.877592000	1.719275000	0.415028000
O	-2.053560000	-0.109555000	2.858588000
H	-2.297556000	0.693095000	2.327126000
H	-2.540733000	-0.032728000	3.688037000
O	-2.074077000	-2.311890000	1.087445000
H	-2.126405000	-1.601579000	1.759599000
H	-1.118894000	-2.459679000	0.967848000
O	-3.054789000	-1.675699000	-1.307182000
H	-3.710892000	-2.343812000	-1.542558000
H	-2.737686000	-1.935072000	-0.397162000
O	-0.804425000	1.513277000	-2.065866000
H	-0.554988000	0.563932000	-2.114597000
H	-1.771793000	1.488513000	-1.960687000
O	0.260797000	2.306533000	0.261628000
H	-0.106980000	2.035696000	-0.621427000
H	1.177430000	2.558214000	0.053152000
O	0.666815000	0.239156000	1.953391000
H	0.460319000	0.999958000	1.350794000
H	-0.116638000	0.149847000	2.523904000
O	0.680053000	-1.984249000	0.414174000
H	1.606254000	-2.268320000	0.318815000
H	0.730707000	-1.172810000	0.979536000
O	-0.163655000	-1.192324000	-2.060259000
H	-1.055672000	-1.561483000	-2.160581000
H	0.113119000	-1.489082000	-1.159606000
O	2.656215000	-0.164101000	-2.125074000
H	1.787227000	-0.475376000	-2.422327000
H	2.986784000	-0.877817000	-1.543088000
O	3.020493000	2.062202000	-0.602783000
H	3.636599000	2.655836000	-1.049738000
H	2.858992000	1.324800000	-1.243482000
O	3.513104000	0.272492000	1.546426000
H	3.463649000	1.009560000	0.905017000
H	2.636923000	0.282765000	1.971426000
O	3.514132000	-1.889960000	-0.050642000
H	4.309945000	-2.429052000	0.032756000
H	3.621998000	-1.142845000	0.596236000

$W_{14:4}$
E(MP2/aTZ) = -1068.832449 a.u.

O	-4.063929000	1.008054000	-1.162668000
H	-4.103089000	0.839174000	-0.184487000
H	-4.901792000	1.428641000	-1.391431000
O	-3.898727000	0.346595000	1.445744000
H	-3.739980000	-0.618265000	1.420509000
H	-3.068775000	0.717150000	1.792667000
O	-3.209637000	-2.351318000	0.880066000
H	-3.228606000	-2.201023000	-0.101010000
H	-3.719118000	-3.156568000	1.032551000
O	-3.153551000	-1.624330000	-1.720611000
H	-2.225326000	-1.485808000	-1.975138000
H	-3.535821000	-0.724122000	-1.705138000
O	-1.269856000	1.671166000	-1.080013000
H	-0.975454000	0.773333000	-1.367114000
H	-2.219119000	1.695732000	-1.297774000
O	-1.152334000	1.200888000	1.607600000
H	-1.184782000	1.480126000	0.659566000
H	-0.352219000	1.626454000	1.962408000
O	-0.492887000	-1.416210000	1.153618000
H	-0.773357000	-0.506041000	1.416136000
H	-1.294939000	-1.958525000	1.256586000
O	-0.368009000	-0.876030000	-1.565234000
H	-0.348022000	-1.162971000	-0.623458000
H	0.572023000	-0.763532000	-1.800255000
O	1.481950000	2.577621000	-0.873672000
H	1.538667000	2.561343000	0.100232000
H	0.526718000	2.578194000	-1.055430000
O	1.618310000	1.944864000	1.947402000
H	1.927308000	1.019833000	1.795093000
H	2.214273000	2.313227000	2.611347000
O	2.232333000	-0.622570000	1.173226000
H	1.435820000	-1.163640000	1.322111000
H	2.230914000	-0.446428000	0.193140000
O	2.316263000	0.019495000	-1.440168000
H	2.130992000	0.985255000	-1.369791000
H	3.263424000	-0.076714000	-1.680294000
O	5.015207000	-0.542836000	-1.612541000
H	5.722421000	0.092783000	-1.777002000
H	5.121564000	-0.807497000	-0.672585000
O	4.932900000	-1.276128000	1.076379000
H	5.151428000	-2.182862000	1.324641000
H	3.974159000	-1.184860000	1.263816000

$W_{14:5}$
E(MP2/aTZ) = -1068.832599 a.u.

O	-2.977240000	1.846339000	-1.294001000
H	-2.991583000	1.793784000	-0.302731000
H	-3.720765000	2.412484000	-1.534825000
O	-2.789629000	1.595325000	1.387712000
H	-2.872859000	0.665558000	1.682293000
H	-1.878877000	1.839132000	1.625224000
O	-2.832365000	-1.158986000	2.091773000
H	-3.294506000	-1.645855000	1.360981000
H	-3.273310000	-1.436913000	2.904052000
O	-4.003877000	-2.256057000	-0.056497000
H	-4.004620000	-3.192621000	-0.287534000
H	-3.568147000	-1.799660000	-0.822342000
O	-2.766551000	-0.889203000	-2.021283000
H	-1.801064000	-1.003477000	-1.976663000
H	-2.903570000	0.066826000	-1.864982000
O	0.041614000	-0.927223000	-1.383376000
H	0.043328000	-1.064905000	-0.406848000
H	0.943116000	-1.142012000	-1.686643000
O	-0.102752000	1.807782000	-1.408408000
H	-1.023487000	2.059798000	-1.601393000
H	-0.098394000	0.823907000	-1.491181000
O	0.085975000	1.822228000	1.322061000
H	1.002555000	2.036047000	1.572609000
H	0.065561000	1.933350000	0.340805000
O	-0.064271000	-0.906619000	1.362961000
H	-0.928606000	-1.165456000	1.732314000
H	-0.058280000	0.079468000	1.429093000
O	2.754825000	-0.997760000	1.974958000
H	1.789893000	-1.115567000	1.917504000
H	2.883217000	-0.032159000	1.883482000
O	2.960275000	1.779937000	1.414377000
H	3.688716000	2.344851000	1.700103000
H	2.993618000	1.782006000	0.422071000
O	2.793480000	1.685741000	-1.274120000
H	2.861594000	0.770725000	-1.615734000
H	1.894573000	1.963605000	-1.517953000
O	2.824859000	-1.036369000	-2.088735000
H	3.323962000	-1.552679000	-1.403689000
H	3.221531000	-1.281276000	-2.933884000
O	4.070042000	-2.215049000	-0.030828000
H	3.605490000	-1.820314000	0.752504000
H	4.115759000	-3.161276000	0.150897000

$W_{15:1}$
E(MP2/aTZ) = -1145.184657 a.u.

O	-2.987031127	2.217087135	0.962544955
H	-3.690642416	2.861357606	1.108041283
H	-3.079825870	1.929772560	0.015283019
O	-2.686949002	-0.169654707	2.463812015
H	-2.853181610	0.680461425	2.008549459
H	-1.768485010	-0.098458687	2.768654863
O	-2.812107511	-2.301698529	0.719704387
H	-2.837050862	-1.560583943	1.370514065
H	-1.905315243	-2.638144957	0.797833969
O	-3.113157408	-1.420561522	-1.777112478
H	-3.088373260	-1.776878150	-0.845989152
H	-3.825564622	-1.898544347	-2.219233235
O	-2.990464424	1.387314858	-1.589891912
H	-3.114274388	0.421126764	-1.698678283
H	-2.093902416	1.550984585	-1.928364259
O	-0.128347122	2.164952861	0.734836367
H	-0.160467588	1.877566739	-0.211319709
H	-1.037585258	2.457956377	0.927573068
O	0.263221545	0.016785303	2.346024794
H	0.151873873	0.805631252	1.758949741
H	1.193773763	0.050784552	2.622704908
O	0.143749544	-2.211210132	0.761701582
H	1.068508855	-2.511115237	0.762201874
H	0.157068055	-1.419951769	1.354089638
O	-0.243576521	-1.362354401	-1.791328487
H	-0.158080625	-1.680592558	-0.858109089
H	-1.170187317	-1.547022650	-2.030460273
O	-0.102729927	1.343746744	-1.855508437
H	-0.113465121	0.354368405	-1.845649250
H	0.782088491	1.577311430	-2.187203709
O	2.740171947	2.242613357	0.552961063
H	2.955440589	1.482923489	1.130557877
H	1.820785862	2.466224893	0.780535802
O	3.196249133	-0.054736777	2.153729329
H	3.961365285	-0.104357692	2.740014145
H	3.251809956	-0.855075502	1.580978036
O	3.073163313	-2.196336843	0.423696552
H	3.734681662	-2.895211045	0.346630180
H	2.958062302	-1.843783339	-0.502106047
O	2.619502430	-1.228430227	-2.022629857
H	2.741401046	-0.259143612	-2.097655173
H	1.678693515	-1.372213080	-2.225649640
O	2.763175921	1.579042408	-2.049414338
H	3.417910407	2.104618686	-2.525079845
H	2.827007358	1.864597002	-1.099287466

$W_{15:2}$
E(MP2/aTZ) = -1145.18208 a.u.

O	4.731408026	1.516454339	-0.350840084
H	4.206173974	1.041702977	-1.046004534
H	4.960121435	2.367670909	-0.742742497
O	3.213275985	0.135344731	-2.095215518
H	2.292636600	0.450183408	-2.096805858
H	3.144546416	-0.790741494	-1.786111226
O	2.830536962	-2.420176562	-0.929946862
H	3.431137150	-3.167730025	-1.039065361
H	2.860245004	-2.192920503	0.036583611
O	2.682779572	-1.662505227	1.649775062
H	1.741485244	-1.679119206	1.893821854
H	2.944764049	-0.728625850	1.783696911
O	3.266676857	1.107152275	1.858994976
H	3.710413041	1.445842124	2.646362772
H	3.858017519	1.348103680	1.099913252
O	0.503264378	1.386487257	1.041953318
H	1.419217601	1.478265688	1.362681457
H	0.579702875	1.190608627	0.068522622
O	0.430864863	0.715970214	-1.554611979
H	-0.371628933	1.190904893	-1.866795309
H	0.166558427	-0.229604115	-1.476596314
O	-0.019408058	-1.936376782	-0.957614935
H	-0.022627603	-1.770322632	0.015670167
H	0.844625072	-2.352985793	-1.126351680
O	-0.168694075	-1.212125030	1.680527637
H	-1.098505000	-1.344865309	1.946698642
H	-0.052307316	-0.240646476	1.573597296
O	-2.977516009	-1.542428159	1.882602657
H	-3.524002068	-1.906552806	2.589682576
H	-3.342688401	-0.634840405	1.699840942
O	-2.872589959	-2.197277880	-0.900093203
H	-2.919722671	-2.169649829	0.075560676
H	-1.921174815	-2.283477588	-1.091172018
O	-3.979034567	0.140267801	-1.604514208
H	-3.580928810	-0.756624944	-1.443040583
H	-4.728637921	-0.009162615	-2.193561167
O	-3.869248999	0.863647886	1.127410064
H	-3.207532030	1.581031237	1.139258171
H	-4.062626894	0.727289275	0.178707027
O	-1.823734343	2.845465767	0.889945399
H	-0.934106891	2.476866571	1.082900617
H	-1.838135910	3.719597581	1.298751245
O	-1.941445490	2.111202450	-1.968337135
H	-2.676958468	1.468965270	-1.965037734
H	-1.995609089	2.529716591	-1.091860927

$W_{15:3}$
E(MP2/aTZ) = -1145.181424 a.u.

O	3.400805764	1.312968818	1.341342208
H	4.211386759	1.695486130	1.699303529
H	3.537903154	1.272947744	0.366564798
O	3.494357006	1.097186860	-1.413217703
H	3.195568564	0.186611946	-1.686972299
H	4.254805215	1.294669063	-1.974061778
O	2.542542590	-1.301176446	-2.095832958
H	2.536685873	-1.918083500	-1.335043090
H	1.609970598	-1.217609264	-2.357935471
O	2.382900000	-2.878235012	0.222352335
H	2.453291152	-2.286572385	1.018312798
H	2.893417461	-3.669296743	0.432934705
O	2.395383428	-1.154383634	2.277923785
H	2.788794861	-0.299428586	2.009529877
H	1.476914556	-0.937960626	2.513795888
O	0.523332715	1.950121232	1.279677450
H	0.160724449	1.082694280	1.591653572
H	1.451105345	1.953630460	1.565711049
O	0.692165603	1.960568925	-1.467138505
H	1.645421982	1.903214066	-1.651715345
H	0.652000338	1.933740893	-0.482962417
O	-0.270245872	-0.485613469	-2.179722235
H	-1.222116456	-0.431842074	-2.386260358
H	0.001098063	0.437378137	-1.950978423
O	-0.363483772	-2.163461449	-0.053197934
H	-0.281689527	-1.567233222	-0.839427402
H	0.475192676	-2.656553918	-0.012263968
O	-0.423234489	-0.460827153	2.070145179
H	-1.364566193	-0.381642922	2.315297804
H	-0.430866111	-1.083439147	1.302669584
O	-1.541224341	3.530199656	0.009697955
H	-1.072629810	3.547251008	-0.837710168
H	-0.861803422	3.206634582	0.626956241
O	-3.492487226	1.505051393	0.053538234
H	-2.848728105	2.241674831	-0.003854200
H	-3.384223421	0.994081295	-0.770891473
O	-3.139167272	-0.431547641	-2.041110140
H	-3.822599995	-0.606858915	-2.700037368
H	-3.240480001	-1.147649550	-1.358431988
O	-3.202414774	-2.212418133	-0.020744508
H	-2.270010388	-2.488685450	0.036313339
H	-3.331758814	-1.670674759	0.783641909
O	-3.273043283	-0.255123304	2.039657375
H	-3.384557414	0.472593671	1.367194930
H	-3.968358435	-0.113567620	2.693745654

$W_{15:4}$
E(MP2/aTZ) = -1145.181114 a.u.

O	-3.870277015	0.218524919	-1.469626879
H	-3.905662087	0.457541121	-0.502121485
H	-4.694085998	0.541497329	-1.854726932
O	-3.657099424	0.708114692	1.146045060
H	-2.894411337	1.299944042	1.292667203
H	-3.389479037	-0.148535511	1.532861475
O	-2.785277841	-1.946557124	1.733317509
H	-2.895881531	-2.220278302	0.785054723
H	-3.268729356	-2.602782506	2.250647947
O	-2.926763957	-2.396538328	-0.923688377
H	-3.341899492	-1.582052882	-1.271152596
H	-2.017321049	-2.359792159	-1.266881325
O	-1.167654677	1.008372644	-1.444765459
H	-1.262571948	1.402703589	-0.547993132
H	-2.091180602	0.855079653	-1.724668530
O	-1.245134787	2.207917800	1.094527394
H	-0.963829638	3.114828878	0.850360545
H	-0.443187414	1.829569039	1.504112877
O	0.064888224	4.375841214	-0.035714636
H	0.581305181	5.115606175	0.305800303
H	0.717168626	3.751757850	-0.418497814
O	1.417931559	2.098915363	-0.988109640
H	0.664256374	1.824352053	-1.541214261
H	1.279576866	1.590072621	-0.153997256
O	1.140668629	0.799738229	1.451695163
H	0.749560509	-0.108043427	1.467688466
H	2.073454396	0.672359113	1.712060294
O	0.059324144	-1.690811092	1.311972385
H	-0.825660211	-1.848929026	1.689010221
H	-0.085740975	-1.714064489	0.333832134
O	-0.192878248	-1.553478736	-1.386441718
H	0.714517009	-1.660426804	-1.728444297
H	-0.431384094	-0.602245436	-1.483519094
O	3.808829279	0.570620638	-1.174198403
H	3.056764679	1.182680735	-1.302661159
H	3.487088761	-0.274896086	-1.544164404
O	3.860532170	0.085155565	1.454276303
H	4.687720122	0.347274051	1.876361807
H	3.956283617	0.317599727	0.488883088
O	2.796336860	-2.487979505	0.904206622
H	3.245137184	-1.692869653	1.254043912
H	1.894787521	-2.434181329	1.267232345
O	2.627322172	-1.967248844	-1.738106461
H	3.009791833	-2.672193362	-2.275758185
H	2.723636518	-2.268662519	-0.796274995

$W_{15:5}$
E(MP2/aTZ) = -1145.17937 a.u.

O	-2.869460038	2.181531829	0.257075755
H	-1.967428902	2.530666837	0.145782447
H	-3.031168755	1.666075174	-0.558714610
O	-2.728052895	0.656666044	2.462025811
H	-3.378004242	0.949018015	3.112755424
H	-2.858109650	1.244898784	1.670942241
O	-2.559810714	-1.954833637	1.430353420
H	-1.615786895	-2.146803010	1.573492573
H	-2.694118834	-1.078059294	1.846414734
O	-2.959673740	-2.009442056	-1.208477050
H	-2.864904532	-1.997899809	-0.215370247
H	-3.605176328	-2.703857971	-1.390466334
O	-3.155225001	0.598097371	-2.084693367
H	-3.177403148	-0.353536720	-1.828524481
H	-3.915386350	0.724148811	-2.666031030
O	-0.022747026	2.412311304	0.127921174
H	0.117032215	1.789972672	0.880564606
H	0.818047014	2.899956827	0.017596094
O	0.154560533	0.590518782	2.155167802
H	-0.727960689	0.682192537	2.555848981
H	0.175775047	-0.339029596	1.821528180
O	0.285643529	-1.972721665	1.214423520
H	1.185691697	-2.292261045	1.404128860
H	0.229055939	-1.950306731	0.226799615
O	-0.021750329	-1.842492298	-1.477938818
H	-0.934987962	-2.149017594	-1.609445491
H	-0.072127753	-0.877247242	-1.684985114
O	-0.214436044	0.824583001	-2.038282763
H	-1.109284431	0.929434171	-2.399587368
H	-0.196558998	1.417496610	-1.243792857
O	2.564483044	3.409988944	-0.514270623
H	2.902610479	2.574335969	-0.885561988
H	3.219459800	3.659846841	0.150060486
O	2.645487741	0.739592126	-1.471289769
H	1.806644783	0.840817372	-1.950346396
H	2.874234012	-0.211958491	-1.601831127
O	2.949284783	0.517446168	1.333307034
H	2.146690506	0.756169224	1.825586414
H	2.722480493	0.687059009	0.394465963
O	3.153389562	-2.177013261	1.282995136
H	3.185163176	-1.193666034	1.407355532
H	3.875409621	-2.535811034	1.813207266
O	2.933783742	-1.997464976	-1.553568303
H	2.012058429	-2.268481212	-1.696607599
H	3.100492501	-2.222342864	-0.616920143

$W_{16:1}$ **E(MP2/aTZ) = -1221.5337 a.u.**			
O	2.745302659	-2.191068115	-1.321176480
H	1.796161788	-2.035604901	-1.473654937
H	2.809075718	-2.376922995	-0.362195752
O	4.181957391	0.047846306	-1.590139619
H	3.667282037	-0.804403737	-1.584540903
H	4.870246723	-0.067324107	-2.256731863
O	2.544168363	2.326316462	-1.326567595
H	1.634315386	2.077415097	-1.567082293
H	3.091290413	1.549568059	-1.561422437
O	-0.190290086	1.371167119	-1.348398845
H	-1.059494554	1.745877087	-1.582578881
H	-0.125706376	-0.404052358	-1.527491920
O	-0.007070865	-1.371832931	-1.382215669
H	0.158297282	-1.434880007	0.362566966
H	-0.868189394	-1.780354777	-1.586325178
O	-2.666739946	-2.470647780	-1.357540130
H	-2.641741278	-2.539258154	-0.366705924
H	-2.972667643	-3.330125593	-1.672583774
O	-4.262915224	-0.120086026	-1.275632332
H	-3.761436850	-0.938585315	-1.461653132
H	-4.435612596	-0.169954503	-0.316344756
O	-2.939944978	2.196762633	-1.497659875
H	-3.449456143	1.342788443	-1.524769198
H	-3.404325445	2.797513692	-2.093016775
O	-2.745276255	2.191077542	1.321180402
H	-1.796134910	2.035587354	1.473650735
H	-2.809053078	2.376935495	0.362199934
O	-4.181945327	-0.047818200	1.590159514
H	-4.870226987	0.067360436	2.256761740
H	-3.667271929	0.804428388	1.584557120
O	-2.544189848	-2.326307540	1.326564383
H	-1.634326221	-2.077426595	1.567079134
H	-3.091300071	-1.549549734	1.561426403
O	0.190292087	-1.371223570	1.348385552
H	0.125710274	0.404000359	1.527471748
H	1.059498393	-1.745918069	1.582565646
O	0.007067950	1.371782744	1.382203276
H	-0.158296117	1.434822928	-0.362585053
H	0.868186224	1.780306574	1.586310550
O	2.666705788	2.470662579	1.357534668
H	2.972598173	3.330154706	1.672581764
H	2.641710072	2.539275974	0.366700169
O	4.262898441	0.120119374	1.275655968
H	3.761414630	0.938610389	1.461667677
H	4.435601767	0.169988770	0.316367112
O	2.939955899	-2.196756481	1.497663210
H	3.449459680	-1.342768041	1.524780725
H	3.404356238	-2.797502128	2.093020060

$W_{16:2}$ **E(MP2/aTZ) = -1221.534288 a.u.**			
O	2.921921226	2.348546946	1.390834034
H	3.306742467	3.177886575	1.699979248
H	2.896655728	2.416006116	0.400172847
O	4.263255201	-0.154906089	1.269187969
H	3.850576278	0.709185620	1.467499104
H	4.439882311	-0.113195021	0.310219140
O	2.715975980	-2.326674426	1.458453847
H	3.108547438	-2.965763800	2.065582525
H	3.306945000	-1.526379499	1.492685288
O	0.030811160	-1.341327153	1.389240176
H	0.906951137	-1.722695260	1.586178689
H	0.130708506	-0.369869845	1.523219590
O	0.179516965	1.404161508	1.325050435
H	0.164560722	1.448592830	0.337286633
H	1.029736628	1.813416370	1.567673703
O	-2.557819927	2.338800138	1.275097181
H	-1.645801360	2.097536198	1.516118510
H	-3.100529312	1.565463777	1.530395707
O	-4.174447179	0.053807010	1.602708117
H	-4.858934036	-0.052311357	2.274701603
H	-3.651780867	-0.793308797	1.614983267
O	-2.721870071	-2.181313217	1.380168354
H	-1.771468482	-2.022985570	1.520032466
H	-2.795478600	-2.391864251	0.426959432
O	-2.955336303	-2.259346581	-1.433622689
H	-3.423964691	-2.875499715	-2.009571505
H	-3.464061594	-1.405820973	-1.480131949
O	-4.270363074	0.066519964	-1.263842273
H	-3.766966131	0.878458325	-1.471963027
H	-4.436760674	0.138392439	-0.304860182
O	-2.674169979	2.418188850	-1.411712367
H	-2.653802031	2.510093818	-0.422577323
H	-2.991331486	3.265796003	-1.747294115
O	-0.003425075	1.340037015	-1.405326435
H	-0.129286679	0.371366975	-1.535979008
H	-0.862675027	1.747180166	-1.620115922
O	-0.214215361	-1.402738077	-1.326082668
H	-1.080731081	-1.791284677	-1.546645540
H	-0.177254797	-1.437736801	-0.338388194
O	2.530867370	-2.302275121	-1.362469291
H	1.589372077	-2.116913852	-1.529181146
H	2.570331167	-2.497517083	-0.404135194
O	4.182513676	-0.210521948	-1.595589524
H	3.577217537	-1.000470592	-1.605235918
H	4.858127954	-0.392202496	-2.260287885
O	2.752179074	2.197320510	-1.290285362
H	1.828154680	1.988756961	-1.514359924
H	3.251169938	1.391633210	-1.534626574

$W_{16:3}$
E(MP2/aTZ) = -1221.533337 a.u.

O	-2.687493771	2.164337437	1.614649119
H	-2.767293690	1.351803737	2.143059082
H	-3.254708609	1.992961285	0.838956463
O	-4.240898215	1.331835896	-0.648856936
H	-4.977317375	1.835433414	-1.016662133
H	-3.671231938	1.082410992	-1.424627850
O	-2.659066323	0.404785008	-2.608010033
H	-1.722261446	0.647416188	-2.490839444
H	-2.677959976	-0.559026167	-2.448189899
O	0.034666412	0.811092191	-1.747347676
H	-0.035780876	1.259012702	-0.873116937
H	0.912338226	1.098798917	-2.083874501
O	-0.024223161	1.770841181	0.842025250
H	-0.920255344	2.072321655	1.109028632
H	0.059487225	0.884315008	1.262966376
O	0.058984595	-0.833862537	1.747280878
H	0.933973527	-1.115036757	2.075910729
H	-0.023046017	-1.253811202	0.852746685
O	2.780768509	-1.550560624	2.199601527
H	3.303412860	-0.752031769	1.920084150
H	3.230651901	-1.899559109	2.978592870
O	4.128348405	0.525245629	1.170592491
H	4.334773742	0.206824324	0.269326819
H	3.617893452	1.343928257	1.024133495
O	2.518528108	2.794215021	0.487646336
H	1.581821932	2.600872965	0.705141044
H	2.685704736	3.681527443	0.828752996
O	2.652704248	1.646544470	-2.235018162
H	3.227753176	0.875076571	-2.068318527
H	2.749198665	2.184218606	-1.430504943
O	4.212625225	-0.609403432	-1.416708539
H	4.940668714	-0.986059437	-1.925930712
H	3.638957341	-1.379697750	-1.156916237
O	2.635381860	-2.555497241	-0.466205794
H	1.691962005	-2.435929641	-0.683625649
H	2.678804772	-2.403218369	0.498003631
O	-0.067174301	-1.722139911	-0.802289363
H	0.000070254	-0.839622379	-1.249048582
H	-0.920724560	-2.088348530	-1.103347169
O	-2.741002916	-2.259503849	-1.586734367
H	-3.273622604	-1.986857981	-0.791481314
H	-3.172353699	-3.049416498	-1.934438042
O	-4.107528244	-1.255427156	0.482864356
H	-3.592982845	-1.103005113	1.298331193
H	-4.331815107	-0.357010186	0.168720550
O	-2.498603745	-0.557441947	2.741045008
H	-1.553836870	-0.744120292	2.549703930
H	-2.656193603	-0.900759148	3.629240755

$W_{16:4}$
E(MP2/aTZ) = -1221.534052 a.u.

O	-4.392588685	-1.479562176	1.352418463
H	-5.080868111	-2.074007943	1.674963443
H	-4.425288730	-1.536760503	0.360921646
O	-4.265413164	-1.360445996	-1.335081202
H	-4.390650311	-0.408170155	-1.518329314
H	-3.339662360	-1.532376037	-1.582452478
O	-4.392542175	1.479628541	-1.352473045
H	-4.425267093	1.536820798	-0.360970745
H	-5.080790213	2.074103101	-1.675028816
O	-4.265401263	1.360498873	1.335021848
H	-4.390666513	0.408225790	1.518269963
H	-3.339672196	1.532414919	1.582435390
O	-1.529032082	-1.354966817	1.404130062
H	-2.457892905	-1.572460991	1.605592088
H	-1.482867464	-0.375894844	1.499936539
O	-1.390092594	-1.411155103	-1.326135046
H	-0.519467760	-1.730405567	-1.612248306
H	-1.380590658	-1.494490897	-0.340829715
O	-1.529011758	1.354925495	-1.404055784
H	-1.482857408	0.375852966	-1.499852114
H	-2.457856411	1.572445468	-1.605547960
O	-1.390082190	1.411112700	1.326212428
H	-0.519460659	1.730389802	1.612342360
H	-1.380572110	1.494459434	0.340906992
O	1.390094766	-1.411131417	1.326217546
H	1.380589256	-1.494487819	0.340912631
H	0.519481989	-1.730425563	1.612351389
O	1.529006911	-1.354953887	-1.404060234
H	2.457846587	-1.572464173	-1.605552664
H	1.482837817	-0.375884801	-1.499848030
O	1.390073371	1.411126590	-1.326129553
H	0.519439712	1.730368375	-1.612244334
H	1.380577681	1.494455641	-0.340832327
O	1.529043093	1.354936639	1.404128674
H	2.457899763	1.572449459	1.605584238
H	1.482878942	0.375867511	1.499929604
O	4.265432403	-1.360465065	1.335004770
H	3.339700619	-1.532395306	1.582418312
H	4.390680084	-0.408189161	1.518242336
O	4.392544093	-1.479596451	-1.352502532
H	4.425279656	-1.536783635	-0.361000308
H	5.080802504	-2.074057046	-1.675060630
O	4.265381667	1.360478636	-1.335102953
H	3.339637189	1.532389203	-1.582471591
H	4.390631090	0.408201899	-1.518361740
O	4.392586675	1.479595179	1.352387922
H	5.080855862	2.074064080	1.674924349
H	4.425278961	1.536798729	0.360883849

$W_{16:5}$
E(MP2/aTZ) = -1221.533868 a.u.

O	-4.264845026	1.073209335	-1.568198096
H	-3.339181329	1.288298398	-1.779597845
H	-4.390648756	1.426131527	-0.664913313
O	-4.404899828	1.592060628	1.225807732
H	-5.090450460	2.011045927	1.760308937
H	-4.441084371	0.623905175	1.447463373
O	-4.264774516	-1.071995923	1.569392568
H	-4.390912888	-1.424879204	0.666144069
H	-3.339095851	-1.287335037	1.780515863
O	-4.405665927	-1.590803360	-1.224572715
H	-4.441623377	-0.622633538	-1.446211353
H	-5.091486445	-2.009588974	-1.758884583
O	-1.385268880	1.194347254	-1.523170896
H	-1.372617443	1.424812737	-0.561295928
H	-0.519137983	1.475361903	-1.858376577
O	-1.532464915	1.552101932	1.176575115
H	-1.485646127	0.599377215	1.422478737
H	-2.459427190	1.796793432	1.353936341
O	-1.385257624	-1.193948399	1.523415178
H	-0.519111915	-1.475164584	1.858404367
H	-1.372896465	-1.424423552	0.561536248
O	-1.533182467	-1.551695250	-1.176283246
H	-1.486142064	-0.598976168	-1.422192184
H	-2.460282882	-1.796093181	-1.353382984
O	1.534685639	1.135608032	-1.589009155
H	1.485256790	0.153340021	-1.540080294
H	2.464709662	1.318409991	-1.817886175
O	1.390985637	1.589639804	1.103135417
H	1.382991720	1.527931877	0.116150759
H	0.520801115	1.949224180	1.337987885
O	1.534629014	-1.135994453	1.588464513
H	1.485491089	-0.153719633	1.539534191
H	2.464642647	-1.319074439	1.817214096
O	1.390348468	-1.590016837	-1.103664089
H	1.382554099	-1.528301747	-0.116684702
H	0.520034156	-1.949388823	-1.338343163
O	4.397146243	1.264352066	-1.553983584
H	4.428967767	1.466551067	-0.581602018
H	5.084854799	1.805942793	-1.960010639
O	4.266808641	1.541296552	1.121504449
H	3.340693538	1.746885025	1.340185310
H	4.392744587	0.626294152	1.442382116
O	4.397029909	-1.265604629	1.553157639
H	4.428659581	-1.467819484	0.580770169
H	5.084604757	-1.807425815	1.959099471
O	4.266221805	-1.542508640	-1.122312498
H	4.392360706	-0.627535971	-1.443201300
H	3.340023080	-1.747845975	-1.340891636

$W_{18:1}$
E(MP2/aTZ) = -1374.2301304 a.u.

O	4.853990097	0.506247249	1.396954140
H	4.003091501	0.900667142	1.657342790
H	4.729682134	-0.452027922	1.547782239
O	4.990785715	0.671077389	-1.290580160
H	5.042800468	0.689637712	-0.298948241
H	5.801530937	1.088603159	-1.605974573
O	4.137475890	-2.033607745	-1.356611602
H	4.513061964	-1.144269033	-1.512476038
H	3.199748676	-1.941045802	-1.602424983
O	4.226544917	-2.260162001	1.324791228
H	4.242211453	-2.294537008	0.331579504
H	4.726275609	-3.029287882	1.624463285
O	2.073587067	1.274959952	1.413909372
H	2.107451711	1.372702247	0.436995392
H	1.385195878	1.921868736	1.681110800
O	2.177730303	1.304151386	-1.379748140
H	1.845058756	0.381392732	-1.501165409
H	3.134607803	1.250534763	-1.555638493
O	1.359143249	-1.294780032	-1.353670063
H	0.445541237	-1.471647619	-1.636677701
H	1.343500986	-1.404837523	-0.370159042
O	1.492974491	-1.390236978	1.373195810
H	1.669001027	-0.430697130	1.531597743
H	2.336319707	-1.833045772	1.579714787
O	-0.061991318	3.080666574	1.636779866
H	-0.061589848	3.320977145	0.693760352
H	-0.867071318	2.543337108	1.740136321
O	0.191914883	3.242464926	-1.314738970
H	0.966255374	2.661674151	-1.470689706
H	0.331796949	4.013814851	-1.877860866
O	-2.225733163	1.156233693	1.492899096
H	-3.178363697	1.087764114	1.688464821
H	-1.891177089	0.231368710	1.553551454
O	-2.057054370	1.440416889	-1.220414072
H	-2.100381026	1.428965573	-0.233172522
H	-1.383688105	2.113120846	-1.427372337
O	-1.509038271	-1.237236194	-1.492884998
H	-1.676358053	-0.266704811	-1.535651175
H	-2.359244344	-1.646623677	-1.736730554
O	-1.385577269	-1.453753661	1.247858009
H	-1.359556043	-1.455271434	0.261057989
H	-0.471113603	-1.645462745	1.517767570
O	-5.021710574	0.545009410	1.383156466
H	-5.836474286	0.928446408	1.729841003
H	-5.055641024	0.675000086	0.398384526
O	-4.834670280	0.688094226	-1.298348453
H	-3.973810508	1.097129870	-1.499114019
H	-4.722500660	-0.247739584	-1.558587201
O	-4.251346726	-2.081166131	-1.534337051
H	-4.755844096	-2.806589526	-1.922040513
H	-4.274004172	-2.227251022	-0.551834381
O	-4.176275321	-2.156827938	1.157658866
H	-4.547074798	-1.287387571	1.407916923
H	-3.239622345	-2.100251838	1.417455526

$W_{18:2}$
E(MP2/aTZ) = -1374.2278407 a.u.

O	2.985837276	2.762207709	-0.219738379
H	2.984688995	2.183410371	-1.027760176
H	3.666656919	3.426695831	-0.382144460
O	2.775488586	1.479163810	2.277659618
H	1.850293685	1.689940890	2.489497251
H	2.929970122	1.908215410	1.410824775
O	2.992995794	-1.186494321	2.494395078
H	2.990333401	-0.197260720	2.397445380
H	3.675330730	-1.377329216	3.149718919
O	2.779433655	-2.709239162	0.135751577
H	2.934866690	-2.172533794	0.940159120
H	1.854923042	-2.999696149	0.214600311
O	2.989612441	-1.563685417	-2.281434486
H	3.671263761	-2.034816163	-2.776217463
H	2.989664294	-1.974648849	-1.376364284
O	2.772144975	1.240167743	-2.419167288
H	2.929132987	0.275374379	-2.357129471
H	1.846807325	1.315818178	-2.707815645
O	0.114570841	2.698067487	-0.053838149
H	0.061647989	2.180483168	0.787201736
H	1.034652419	3.015777190	-0.087756666
O	-0.118159735	1.394708079	2.308038110
H	-1.038736615	1.580492468	2.566293732
H	-0.062581368	0.407718561	2.280432218
O	0.121669889	-1.301783398	2.361611934
H	0.067277090	-1.772257740	1.493445078
H	1.042550920	-1.429990906	2.651748488
O	-0.114553889	-2.698083124	0.053845222
H	-1.034651552	-3.015777337	0.087774657
H	-0.061639590	-2.180477427	-0.787179416
O	0.118163389	-1.394705082	-2.308028217
H	0.062595979	-0.407734700	-2.280416529
H	1.038744884	-1.580504040	-2.566281949
O	-0.121657464	1.301771602	-2.361596945
H	-0.067274776	1.772256274	-1.493426810
H	-1.042534564	1.429997639	-2.651734869
O	-2.779421244	2.709267528	-0.135736418
H	-2.934867458	2.172517749	-0.940157305
H	-1.854911548	2.999699557	-0.214576902
O	-2.989597221	1.563669435	2.281442422
H	-3.671268384	2.034809837	2.776237072
H	-2.989653510	1.974626749	1.376389097
O	-2.772142610	-1.240177031	2.419170943
H	-2.929136092	-0.275384304	2.357121574
H	-1.846787155	-1.315835975	2.707824298
O	-2.985838084	-2.762207287	0.219710613
H	-3.666672061	-3.426685514	0.382117148
H	-2.984681481	-2.183396185	1.027755708
O	-2.775474893	-1.479139074	-2.277651268
H	-1.850285337	-1.689934544	-2.489509043
H	-2.929966758	-1.908203871	-1.410850609
O	-2.992977751	1.186513313	-2.494382784
H	-3.675308624	1.377351860	-3.149711554
H	-2.990326368	0.197285044	-2.397451547

$W_{20:1}$
E(MP2/aTZ) = -1526.928884 a.u.

O	-4.145836579	-0.958124891	-1.352371619
H	-3.693473488	-0.114374057	-1.523016805
H	-4.362230551	-0.931315491	-0.398091202
O	-4.327106086	-1.119553115	1.461446503
H	-5.093087338	-1.342362585	2.004460722
H	-3.725310273	-1.907241066	1.515295326
O	-2.687056045	-3.248871149	1.300090757
H	-2.671475677	-3.430200829	0.340020032
H	-1.748044661	-3.170875533	1.544449318
O	-2.731428880	-3.238825785	-1.560078521
H	-3.257972296	-2.396924455	-1.584913875
H	-3.195245857	-3.847656794	-2.148166259
O	0.054327689	-2.614519478	-1.393153179
H	0.047516691	-1.637530272	-1.532259090
H	-0.840362812	-2.911321474	-1.644383831
O	0.140116960	-2.680414240	1.352771375
H	1.044255071	-2.932951935	1.618245855
H	0.153602595	-2.732406520	0.366462764
O	-0.023262462	0.028666552	1.401987166
H	-0.936748624	0.362180022	1.559953194
H	-0.027730102	-0.947928508	1.546540119
O	0.067360465	0.107862192	-1.335652001
H	0.062806359	0.102860575	-0.346571710
H	0.914909538	0.567463485	-1.543785882
O	-2.377641664	1.338172760	-1.380114501
H	-2.246016947	2.284376913	-1.571573755
H	-1.489443907	0.937926610	-1.529660448
O	-2.524279017	1.131687031	1.351011566
H	-3.238005780	0.508076538	1.574960000
H	-2.555859726	1.196514954	0.365394997
O	-1.461436523	3.855779636	1.392905747
H	-1.915563367	3.021713772	1.599802953
H	-1.637623073	4.000537113	0.440763686
O	-1.505171238	4.085560408	-1.419845825
H	-0.516634130	4.043046486	-1.503149202
H	-1.773724726	4.840398588	-1.957910305
O	1.186217013	3.999986194	-1.349776813
H	1.684001170	3.200667639	-1.595378923
H	1.368832360	4.116922574	-0.397196841
O	1.217347343	4.116121598	1.509930537
H	0.231641174	4.016834094	1.571070846
H	1.434077870	4.868029416	2.074837130
O	2.281656412	1.480172247	1.337415347
H	2.059108672	2.398516805	1.579965417
H	1.451755302	0.978262372	1.506406266
O	2.473776028	1.402315797	-1.388679237
H	3.188996835	0.787628702	-1.629694299
H	2.500196632	1.433285311	-0.400711777
O	4.328874706	-0.834785368	-1.505056761
H	3.790071288	-1.667717394	-1.540062054
H	5.106040046	-1.010428314	-2.049720557
O	4.198053034	-0.687798320	1.310345179
H	4.388842601	-0.651006267	0.350619082
H	3.698393931	0.127243042	1.488029658
O	2.966272966	-3.067936425	1.570700414
H	3.496062453	-3.636282769	2.143308609
H	3.422301112	-2.185687750	1.579807284
O	2.879738298	-3.100711633	-1.290742851
H	1.929625093	-3.076463930	-1.503127727
H	2.906892077	-3.273090424	-0.329572141

$W_{20:2}$
E(MP2/aTZ) = -1526.924889 a.u.

O	-4.273911407	1.294195857	1.987155807
H	-4.416575684	1.700130236	1.108870884
H	-3.354027193	1.520802905	2.201693258
O	-4.455400452	2.307713660	-0.661793941
H	-4.509606640	1.510585390	-1.254501046
H	-5.137021203	2.913374564	-0.977688961
O	-4.345731361	0.122974371	-2.208345790
H	-4.488214290	-0.717139243	-1.724538480
H	-3.421910457	0.068214543	-2.508846108
O	-4.503815847	-2.242122958	-0.684581873
H	-4.525138366	-1.973523737	0.276539561
H	-5.191019234	-2.912492656	-0.783120459
O	-4.320592071	-1.459532677	1.850253977
H	-3.409685273	-1.644839415	2.131438629
H	-4.386302870	-0.478213641	1.929359954
O	-1.336459101	1.398350747	1.915046343
H	-0.495181988	1.742839844	2.250073225
H	-1.382882849	1.710393441	0.974011686
O	-1.597179836	2.211372341	-0.643459102
H	-2.524966433	2.505472859	-0.713202476
H	-1.553027267	1.421939474	-1.234557987
O	-1.461124972	-0.010737200	-2.245055075
H	-1.467821766	-0.819290852	-1.672203763
H	-0.603324128	-0.032163316	-2.698058756
O	-1.641545995	-2.188275120	-0.647889180
H	-1.570510404	-1.899584282	0.292708531
H	-2.573526148	-2.459528599	-0.747039106
O	-1.382997170	-1.341131239	1.954564191
H	-0.518612393	-1.617174822	2.295770339
H	-1.345997796	-0.354167618	1.968792787
O	1.637749545	1.332098618	1.940863716
H	2.580665796	1.490476998	2.121245056
H	1.565294183	0.347357753	1.936894535
O	1.326059268	2.202277671	-0.601648690
H	1.374743191	1.891681847	0.338862844
H	0.449868624	2.611633868	-0.685761806
O	1.443618426	0.084547338	-2.342711592
H	1.402384491	0.858068964	-1.731495055
H	2.361159097	0.079259381	-2.670610637
O	1.273861219	-2.136623179	-0.795847482
H	0.391392236	-2.524606439	-0.910763975
H	1.275922156	-1.333171364	-1.374834044
O	1.590869716	-1.421853575	1.845941893
H	2.520924327	-1.635418735	2.031820920
H	1.467660233	-1.683612550	0.903352853
O	4.561929527	1.376012976	1.731530773
H	4.481994716	1.673549126	0.782035922
H	5.230902394	1.951646122	2.122650038
O	4.186824627	2.132650565	-0.794036964
H	3.251375246	2.389049421	-0.882427957
H	4.305448851	1.406897395	-1.441114161
O	4.304702297	-0.086191372	-2.514597061
H	4.319273991	-0.898444713	-1.940302948
H	4.958241971	-0.241667824	-3.207248815
O	4.133027300	-2.203143259	-0.879946422
H	4.331776262	-1.967117034	0.047986393
H	3.193167447	-2.459264561	-0.867606747
O	4.526379795	-1.375087859	1.806762926
H	4.643406342	-0.397043391	1.841163115
H	5.236898750	-1.739310584	2.349017994

$W_{20:3}$
E(MP2/aTZ) = -1526.925493 a.u.

O	5.397233678	0.434315834	1.409767433
H	5.616103947	0.553305687	0.465648376
H	4.573511301	0.945323750	1.526950891
O	5.604936694	0.326253780	-1.453007970
H	5.334320246	-0.630844943	-1.471286048
H	6.348126290	0.404289843	-2.063594452
O	4.623811986	-2.162924081	-1.258395165
H	3.671215759	-2.103439943	-1.451531027
H	4.661763624	-2.351520465	-0.299060126
O	4.693155820	-2.151531599	1.577815304
H	5.036597859	-1.218624481	1.611785196
H	5.235004277	-2.655190406	2.197343984
O	2.740869316	1.429610158	1.263235045
H	2.093129838	2.120836575	1.499366117
H	2.785380307	1.453447857	0.276509423
O	2.926757147	1.215088363	-1.454978001
H	3.875063329	1.078255706	-1.646236970
H	2.524129255	0.321113302	-1.552957036
O	1.861918232	-1.320613841	-1.320525750
H	0.949719358	-1.468181147	-1.624155647
H	1.806081963	-1.351235305	-0.335325481
O	1.977337272	-1.200632959	1.421382846
H	2.779030965	-1.689756630	1.680687008
H	2.234139401	-0.251378252	1.497737564
O	0.598818618	3.261187225	1.466793283
H	0.479072149	4.051827597	2.007265323
H	-0.228055279	2.741412283	1.568628539
O	0.736653616	3.039548427	-1.505043873
H	0.775394025	3.303596286	-0.570276955
H	1.562541481	2.540131785	-1.644363440
O	-1.546882119	1.505480979	1.296221792
H	-2.489244082	1.626046494	1.548816293
H	-1.581622129	1.513593325	0.306577650
O	-1.560699416	1.438541097	-1.432590002
H	-0.757433935	1.967029264	-1.629680371
H	-1.332059416	0.491536324	-1.593159319
O	-1.039390734	-1.242303233	-1.432503603
H	-0.998271088	-1.290132545	-0.448820628
H	-1.814926858	-1.789714663	-1.662610796
O	-0.893734195	-1.153692151	1.327434888
H	-1.086292492	-0.196270315	1.472842927
H	0.029886931	-1.284148321	1.603923471
O	-4.332954159	1.721748866	1.531477524
H	-4.723229925	0.834555197	1.648268590
H	-4.500523449	1.926257123	0.595902202
O	-4.292689639	1.891089345	-1.424486882
H	-3.322841533	1.847133088	-1.562911610
H	-4.613929716	2.549135631	-2.053355133
O	-5.351057331	-0.954934556	1.548524183
H	-4.603703549	-1.611447567	1.556586166
H	-6.003802520	-1.292743271	2.173798536
O	-5.351768910	-0.760229614	-1.270647053
H	-5.543417874	-0.799386561	-0.312524636
H	-5.034974278	0.151767597	-1.414460253
O	-3.494305042	-2.663417499	-1.568406126
H	-4.209904040	-1.971922620	-1.558302401
H	-3.805540213	-3.354485322	-2.165630204
O	-3.306459595	-2.665273360	1.286777273
H	-2.440196245	-2.246114746	1.446450377
H	-3.310513743	-2.850675881	0.327597746

$(NH3)_{8:1}$
E(MP2/aTZ) = -451.7526727 a.u.

N	-2.109504000	1.726363000	1.261954000
H	-3.067935000	1.462392000	1.466698000
H	-2.040322000	2.717953000	1.467270000
H	-1.966549000	1.609821000	0.253791000
N	1.125441000	1.375173000	1.703012000
H	1.494154000	1.825752000	2.533881000
H	1.376005000	0.390004000	1.761470000
H	0.110179000	1.426298000	1.761222000
N	2.108586000	-1.726831000	1.262704000
H	2.039121000	-2.718481000	1.467634000
H	3.066912000	-1.463068000	1.468204000
H	1.966354000	-1.609927000	0.254480000
N	-1.126643000	-1.375777000	1.701985000
H	-1.377238000	-0.390629000	1.760664000
H	-1.495891000	-1.826680000	2.532440000
H	-0.111418000	-1.426924000	1.760821000
N	-1.726176000	-2.108774000	-1.263200000
H	-2.717715000	-2.039302000	-1.468666000
H	-1.462345000	-3.067145000	-1.468405000
H	-1.609804000	-1.966380000	-0.254937000
N	1.376054000	-1.125773000	-1.702266000
H	1.427226000	-0.110523000	-1.760647000
H	1.827031000	-1.494655000	-2.532845000
H	0.390907000	-1.376324000	-1.761153000
N	1.727100000	2.109242000	-1.261454000
H	2.718791000	2.039848000	-1.466211000
H	1.609979000	1.966501000	-0.253327000
H	1.463409000	3.067680000	-1.466528000
N	-1.374845000	1.126394000	-1.702733000
H	-0.389667000	1.376983000	-1.760941000
H	-1.825319000	1.495521000	-2.533475000
H	-1.425962000	0.111162000	-1.761451000

$(NH3)_{8:2}$
E(MP2/aTZ) = -451.7523221 a.u.

N	1.148330000	-2.084689000	0.010668000
H	1.283427000	-1.568777000	-0.856539000
H	1.520234000	-3.017432000	-0.134688000
H	0.144280000	-2.184349000	0.144848000
N	2.140591000	-0.095341000	2.187823000
H	2.211711000	-0.521316000	3.105980000
H	3.059210000	0.278552000	1.973037000
H	1.940404000	-0.839790000	1.512882000
N	1.148337000	2.084685000	-0.010671000
H	1.520246000	3.017426000	0.134685000
H	0.144288000	2.184350000	-0.144849000
H	1.283434000	1.568773000	0.856537000
N	2.140588000	0.095336000	-2.187825000
H	1.940403000	0.839786000	-1.512884000
H	3.059207000	-0.278559000	-1.973040000
H	2.211708000	0.521311000	-3.105982000
N	-1.148335000	-0.010668000	-2.084684000
H	-0.144287000	-0.144849000	-2.184350000
H	-1.283428000	0.856536000	-1.568764000
H	-1.520244000	0.134698000	-3.017424000
N	-2.140586000	2.187831000	0.095339000
H	-3.059207000	1.973050000	-0.278554000
H	-1.940402000	1.512889000	0.839789000
H	-2.211700000	3.105988000	0.521314000
N	-1.148332000	0.010671000	2.084686000
H	-1.520238000	-0.134685000	3.017429000
H	-0.144283000	0.144847000	2.184347000
H	-1.283432000	-0.856536000	1.568774000
N	-2.140593000	-2.187825000	-0.095338000
H	-1.940408000	-1.512885000	-0.839788000
H	-3.059212000	-1.973041000	0.278557000
H	-2.211711000	-3.105983000	-0.521312000

$(HF)_3(H_2O)_5$
E(MP2/aTZ) = -682.7973725 a.u.

O	1.841245000	-0.002124000	1.510673000
H	1.267501000	0.763727000	1.686548000
H	1.266548000	-0.767562000	1.685252000
O	2.147804000	-0.000242000	-1.140203000
H	2.196807000	-0.001008000	-0.145793000
H	3.058590000	-0.000494000	-1.460611000
O	0.122117000	-1.919951000	-1.185095000
H	0.905412000	-1.352310000	-1.344874000
H	-0.628813000	-1.398292000	-1.523877000
O	-2.074656000	0.000366000	0.985786000
H	-1.557520000	-0.770521000	1.288251000
H	-1.556688000	0.770241000	1.289410000
O	0.124146000	1.921672000	-1.182168000
H	0.906823000	1.353430000	-1.342830000
H	-0.627349000	1.401362000	-1.521766000
F	-0.175475000	-2.032110000	1.258180000
H	-0.048615000	-2.053194000	0.271601000
F	-1.919318000	0.002124000	-1.468891000
H	-2.052359000	0.001464000	-0.480562000
F	-0.173399000	2.030432000	1.261281000
H	-0.046458000	2.052874000	0.274749000

$(HF)_4(H_2O)_4$
E(MP2/aTZ) = -706.8099142 a.u.

O	-0.218971000	-1.948088000	1.195587000
H	0.606289000	-1.497623000	1.455741000
H	-0.923668000	-1.325873000	1.456155000
O	1.948088000	-0.218972000	-1.195591000
H	1.325874000	-0.923670000	-1.456158000
H	1.497623000	0.606287000	-1.455744000
O	-1.948091000	0.218973000	-1.195584000
H	-1.497622000	-0.606286000	-1.455736000
H	-1.325879000	0.923673000	-1.456154000
O	0.218975000	1.948090000	1.195587000
H	-0.606283000	1.497622000	1.455740000
H	0.923675000	1.325878000	1.456156000
F	-0.224940000	-2.001337000	-1.265766000
H	-0.230871000	-2.050738000	-0.271184000
F	2.001342000	-0.224937000	1.265763000
H	2.050740000	-0.230872000	0.271182000
F	-2.001335000	0.224938000	1.265769000
H	-2.050738000	0.230875000	0.271187000
F	0.224936000	2.001339000	-1.265767000
H	0.230875000	2.050739000	0.271186000

$(HF)_4(H_2O)_8$
E(MP2/aTZ) = -1012.201323 a.u.

O	2.794865000	1.773670000	-0.429186000
H	2.949750000	1.437444000	0.473393000
H	1.880975000	2.119535000	-0.405634000
F	2.848815000	-0.200709000	-1.913872000
H	2.859279000	0.623045000	-1.361616000
O	2.794903000	-1.773668000	0.429160000
H	1.881015000	-2.119534000	0.405624000
H	2.949780000	-1.437433000	-0.473418000
F	2.848835000	0.200712000	1.913844000
H	2.859310000	-0.623043000	1.361586000
O	0.004651000	1.907473000	-0.364706000
H	-0.868773000	2.332746000	-0.394329000
H	-0.062910000	1.161949000	-1.007199000
O	-0.004682000	-0.364683000	-1.907465000
H	0.868744000	-0.394324000	-2.332731000
H	0.062872000	-1.007143000	-1.161909000
O	0.004665000	-1.907467000	0.364697000
H	-0.062893000	-1.161938000	1.007186000
H	-0.868758000	-2.332741000	0.394328000
O	-0.004647000	0.364687000	1.907432000
H	0.868775000	0.394262000	2.332709000
H	0.062890000	1.007196000	1.161924000
F	-2.848851000	1.913862000	-0.200712000
H	-2.859281000	1.361615000	0.623056000
O	-2.794900000	-0.429190000	-1.773623000
H	-2.949786000	0.473389000	-1.437398000
H	-1.881021000	-0.405649000	-2.119511000
F	-2.848835000	-1.913849000	0.200755000
H	-2.859308000	-1.361642000	-0.623036000
O	-2.794848000	0.429199000	1.773681000
H	-2.949737000	-0.473383000	1.437459000
H	-1.880954000	0.405651000	2.119531000