

Microsolvation of F⁻

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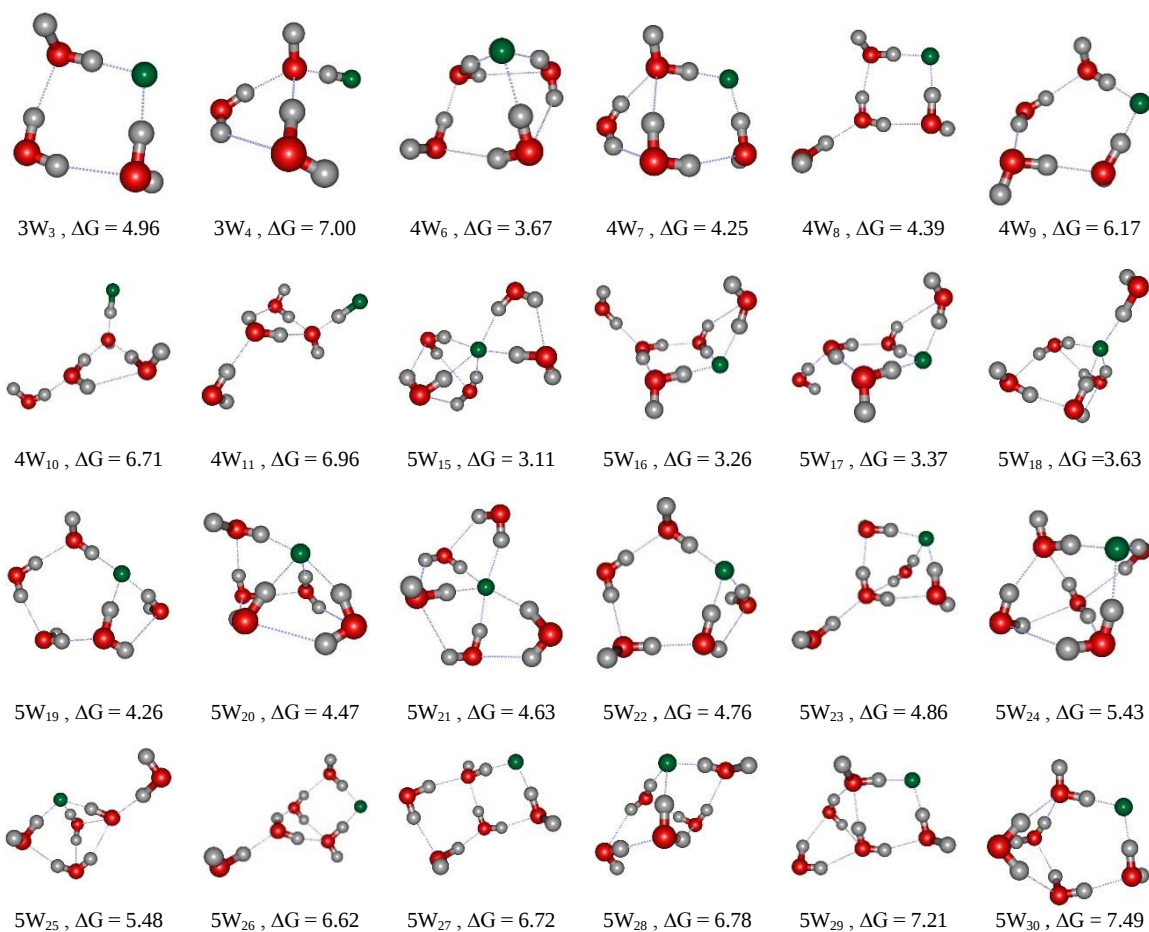
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Supporting Information

Figure S1: MP2/6–311++G(d, p) optimized structures responsible for the microsolvation of F⁻ with up to 6 water molecules. Relative energies in kcal/mol



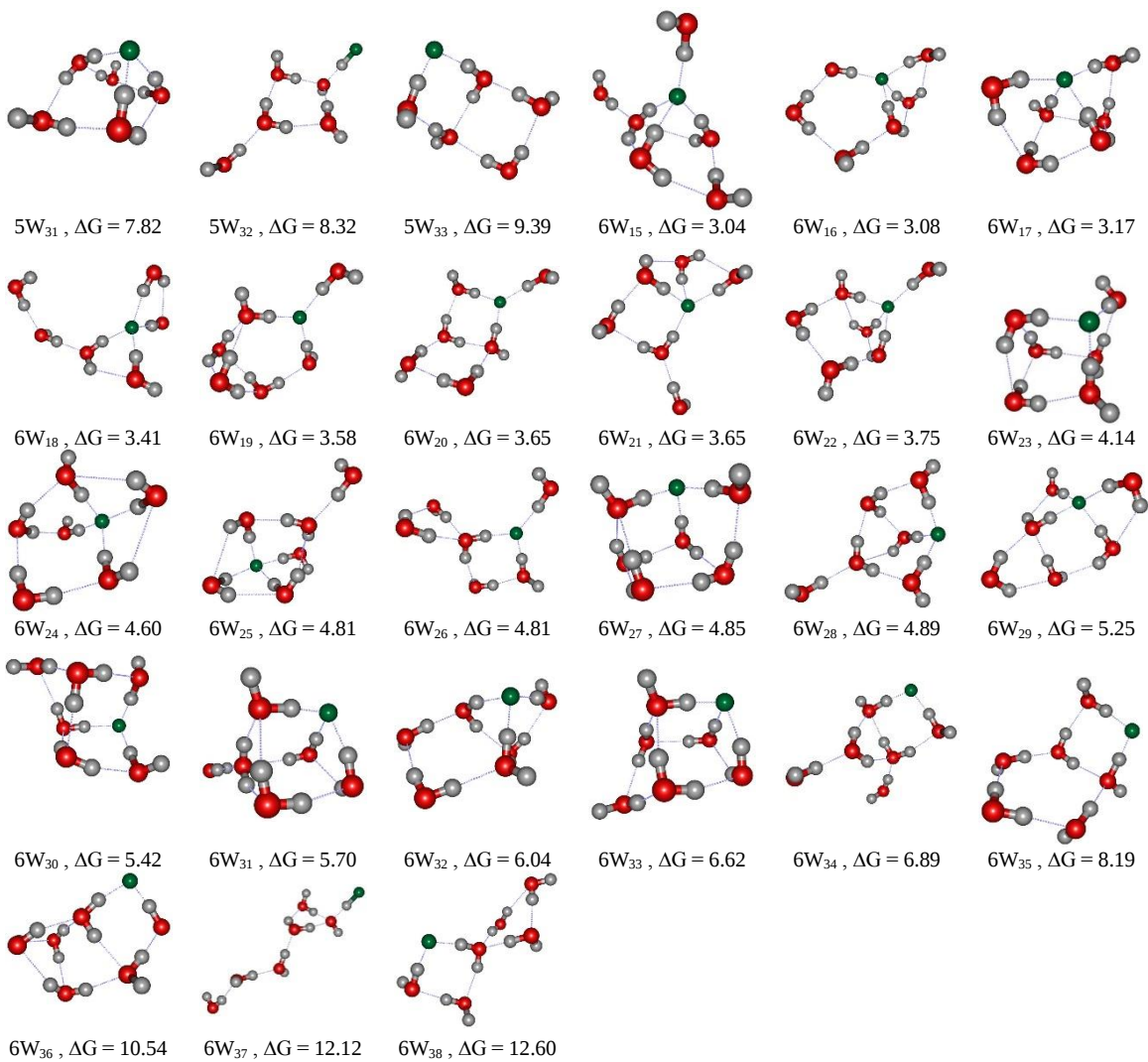


Table S1. Structural motifs within 3 kcal mol⁻¹ of the global minimum on the potential energy surfaces for $[F(H_2O)_n]^{-1}$. Isomer populations (% x_i) estimated using standard Boltzmann distributions at 298 K, 1 atm. ΔE and ΔE_G , refer to “binding energies” calculated as the difference between the energy of a particular cluster and the energy of its isolated moieties using the electronic energies, enthalpies of formation, and Gibbs energies, respectively. All energies in kcal mol⁻¹ and corrected for ZPEs. Data taken from the MP2/6-311++g(d,p) optimized geometries. *CCSD(T)/6-311++g(d,p)

<i>Structure</i>	<i>BE*</i>	<i>ΔE*</i>	<i>BE</i>	<i>ΔE</i>	<i>BE_H</i>	<i>ΔE_H</i>	<i>BE_G</i>	<i>ΔE_G</i>	<i>%x_iE*</i>	<i>%x_iE</i>	<i>%x_iH</i>	<i>%x_iG</i>
$[F(H_2O)_2]^{-1}$ 2W ₁	-46.23		-46.10		-47.57		-34.00					
$[F(H_2O)_3]^{-1}$ 3W ₁	-62.22	0.00	-61.85	0.00	-63.79	0.00	-42.78	0.00	73.13	71.72	48.91	98.25
3W ₂	-61.45	0.76	-61.02	0.83	-63.35	0.44	-40.36	2.42	20.25	18.04	23.38	1.72
3W ₃	-60.77	1.44	-60.67	1.18	-63.44	0.35	-37.82	4.96	6.59	10.12	27.44	0.02
3W ₄	-57.61	4.60	-58.02	3.83	-60.70	3.09	-35.77	7.00	0.03	0.12	0.28	0.00
$[F(H_2O)_4]^{-1}$ 4W ₁	-75.79	0.13	-75.45	0.00	-78.38	0.00	-45.61	0.00	27.27	39.22	36.97	39.36
4W ₂	-75.92	0.00	-75.18	0.27	-77.92	0.46	-45.54	0.07	34.14	25.02	17.11	34.62
4W ₃	-75.73	0.19	-75.09	0.36	-77.80	0.58	-45.34	0.27	24.77	21.31	14.11	25.11
4W ₄	-74.78	1.14	-74.01	1.44	-77.11	1.27	-42.91	2.71	4.98	3.53	4.44	0.41
4W ₅	-75.08	0.83	-74.62	0.83	-78.14	0.24	-42.80	2.81	8.32	9.86	25.15	0.35
4W ₆	-72.73	3.18	-72.37	3.08	-75.62	2.76	-41.94	3.67	0.17	0.22	0.36	0.08
4W ₇	-73.14	2.78	-73.06	2.39	-76.52	1.82	-41.36	4.25	0.32	0.71	1.64	0.03
4W ₈	-71.83	4.09	-71.93	3.52	-75.23	3.15	-41.23	4.39	0.03	0.11	0.19	0.02
4W ₉	-70.22	5.70	-70.29	5.16	-73.66	4.72	-39.44	6.17	0.00	0.01	0.01	0.00
4W ₁₀	-68.20	7.72	-68.76	6.69	-71.84	6.54	-38.90	6.71	0.00	0.00	0.00	0.00
4W ₁₁	-68.00	7.91	-68.54	6.91	-71.66	6.73	-38.65	6.96	0.00	0.00	0.00	0.00
$[F(H_2O)_5]^{-1}$ 5W ₁	-88.28	0.29	-87.65	0.22	-90.93	0.60	-50.16	0.00	16.37	16.16	9.03	54.89
5W ₂	-88.24	0.33	-87.58	0.29	-91.02	0.52	-49.02	1.14	15.35	14.21	10.26	8.00
5W ₃	-88.26	0.31	-87.66	0.21	-91.14	0.40	-49.01	1.16	15.86	16.69	12.85	8.00
5W ₄	-86.15	2.42	-85.50	2.37	-88.54	3.00	-48.99	1.18	0.46	0.44	0.17	7.74
5W ₅	-86.26	2.31	-86.02	1.85	-89.45	2.08	-48.92	1.24	0.56	1.06	0.76	6.81
5W ₆	-88.57	0.00	-87.87	0.00	-91.54	0.00	-48.70	1.47	26.50	23.75	25.21	4.63
5W ₇	-86.10	2.48	-85.96	1.91	-89.38	2.16	-48.26	1.90	0.42	0.96	0.67	2.29
5W ₈	-85.67	2.91	-85.13	2.76	-88.19	3.34	-48.00	2.16	0.20	0.24	0.09	1.46
5W ₉	-87.01	1.56	-86.05	1.82	-89.19	2.35	-47.98	2.18	1.60	1.13	0.49	1.41
5W ₁₀	-86.91	1.66	-86.56	1.31	-90.20	1.33	-47.69	2.48	1.62	2.59	2.71	0.87
5W ₁₁	-85.51	3.06	-85.35	2.25	-88.78	2.76	-47.63	2.53	0.16	0.34	0.24	0.79
5W ₁₂	-87.72	0.86	-87.29	0.58	-91.14	0.40	-47.62	2.54	6.25	8.78	12.85	0.79
5W ₁₃	-86.84	1.73	-86.50	1.37	-90.12	1.41	-47.52	2.65	1.47	2.36	2.39	0.65
5W ₁₄	-86.74	1.83	-86.32	1.55	-90.02	1.52	-47.50	2.67	1.25	1.71	1.97	0.63
5W ₁₅	-86.72	1.56	-85.71	2.16	-89.07	2.47	-47.06	3.11	1.78	0.63	0.40	0.30
5W ₁₆	-85.53	3.04	-85.32	2.55	-88.93	2.61	-46.91	3.26	0.16	0.33	0.31	0.23
5W ₁₇	-85.53	3.04	-85.33	2.54	-88.97	2.57	-46.79	3.37	0.16	0.33	0.33	0.19

$5W_{18}$	-86.47	2.10	-85.82	2.05	-89.53	2.00	-46.53	3.63	0.78	0.77	0.87	0.12
$5W_{19}$	-84.77	3.51	-88.13	3.41	-84.51	3.37	-45.90	4.26	0.04	0.08	0.08	0.04
$5W_{20}$	-87.83	0.74	-87.04	0.83	-91.24	0.29	-45.70	4.47	7.58	5.79	15.09	0.03
$5W_{21}$	-86.53	2.04	-85.58	2.29	-89.44	2.10	-45.53	4.63	0.85	0.50	0.74	1.41
$5W_{22}$	-84.88	3.70	-84.67	3.20	-88.42	3.11	-45.40	4.76	0.05	0.11	0.13	0.019
$5W_{23}$	-85.24	3.33	-84.94	2.94	-88.85	2.69	-45.31	4.86	0.10	0.17	0.27	0.016
$5W_{24}$	-85.99	2.58	-85.51	2.36	-89.56	1.98	-44.73	5.43	0.36	0.44	0.90	0.00
$5W_{25}$	-85.18	3.40	-84.75	3.12	-88.71	2.82	-44.68	5.48	0.09	0.13	0.22	0.01
$5W_{26}$	-82.87	5.71	-82.96	4.91	-86.88	4.66	-43.54	6.62	0.00	0.01	0.01	0.00
$5W_{27}$	-83.73	4.85	-83.82	4.05	-88.04	3.50	-43.44	6.72	0.01	0.03	0.07	0.00
$5W_{28}$	-85.48	3.09	-85.03	2.84	-89.51	2.03	-43.38	6.78	0.15	0.20	0.81	0.00
$5W_{29}$	-83.48	5.09	-83.41	4.46	-87.51	4.03	-42.95	7.21	0.01	0.01	0.03	0.00
$5W_{30}$	-84.01	4.56	-83.97	3.90	-88.33	3.21	-42.67	7.49	0.01	0.03	0.11	0.00
$5W_{31}$	-83.79	4.78	-83.56	4.31	-87.93	3.61	-42.35	7.82	0.01	0.02	0.06	0.00
$5W_{32}$	-79.94	8.63	-80.65	7.23	-84.51	7.02	-41.85	8.32	0.00	0.00	0.01	0.00
$5W_{33}$	-81.29	7.28	-81.56	5.66	-85.88	5.66	-40.77	9.39	0.00	0.00	0.00	0.00
$[F(H_2O)_6]^{-1}$												
$6W_1$	-100.18	0.28	-99.61	0.09	-103.77	0.85	-52.27	0.00	17.44	19.67	5.62	52.22
$6W_2$	-98.01	2.44	-97.43	2.26	-101.34	3.28	-51.55	0.71	0.45	0.51	0.10	16.44
$6W_3$	-97.63	2.82	-97.07	2.63	-100.89	3.72	-51.10	1.17	0.24	0.28	0.05	7.61
$6W_4$	-97.90	2.56	-97.39	2.31	-101.36	3.25	-50.89	1.37	0.37	0.48	0.10	5.18
$6W_5$	-99.55	0.90	-98.88	0.82	-103.15	1.46	-50.79	1.48	6.24	5.81	2.01	4.55
$6W_6$	-97.72	2.74	-97.19	2.51	-101.09	3.53	-50.76	1.51	0.29	0.34	0.06	4.27
$6W_7$	-98.10	2.35	-97.55	2.15	-101.56	3.05	-50.49	1.77	0.54	0.61	0.14	2.72
$6W_8$	-100.10	0.35	-99.37	0.33	-104.04	0.57	-50.30	1.96	15.33	13.38	8.80	1.98
$6W_9$	-98.52	1.94	-98.10	1.60	-102.53	2.09	-49.74	2.53	1.03	1.61	0.72	0.75
$6W_{10}$	-94.48	5.98	-94.54	5.16	-98.44	6.18	-49.60	2.66	0.00	0.00	0.00	0.62
$6W_{11}$	-94.57	5.89	-94.19	5.51	-97.7	6.8	-49.57	2.70	0.00	0.00	0.00	0.58
$6W_{12}$	-98.09	2.37	-97.33	2.37	-101.49	3.12	-49.57	2.70	0.51	0.42	0.13	0.58
$6W_{13}$	-99.82	0.64	-99.05	0.65	-103.76	0.85	-49.38	2.89	9.18	7.51	5.62	0.42
$6W_{14}$	-99.51	0.94	-98.70	1.00	-103.53	1.08	-49.31	2.95	5.49	4.21	3.82	0.37
$6W_{15}$	-96.24	4.22	-95.71	3.99	-99.69	4.93	-49.22	3.04	0.05	0.03	0.01	0.33
$6W_{16}$	-97.22	3.24	-96.68	3.02	-100.81	3.81	-49.18	3.08	0.07	0.14	0.04	0.31
$6W_{17}$	-100.46	0.00	-99.70	0.00	-104.62	0.00	-49.09	3.17	27.33	22.36	23.06	0.25
$6W_{18}$	-93.99	6.47	-93.61	6.09	-97.23	7.38	-48.86	3.41	0.00	0.00	0.00	0.17
$6W_{19}$	-96.85	3.61	-96.72	2.98	-101.21	3.40	-48.69	3.58	0.06	0.15	0.08	0.13
$6W_{20}$	-97.35	3.10	-97.03	2.66	-101.53	3.09	-48.61	3.65	0.15	0.27	0.13	0.12
$6W_{21}$	-96.01	4.44	-95.55	4.15	-99.57	5.04	-48.62	3.65	0.02	0.02	0.01	0.12
$6W_{22}$	-96.67	3.79	-96.13	3.57	-100.28	4.34	-48.52	3.75	0.0	0.06	0.02	0.10
$6W_{23}$	-99.86	0.60	-99.41	0.29	-104.78	-0.17	-48.13	4.14	9.78	14.27	31.79	0.05
$6W_{24}$	-97.37	3.08	-96.65	3.05	-101.04	3.57	-47.67	4.60	0.16	0.14	0.06	0.02
$6W_{25}$	-97.34	3.12	-96.66	3.04	-101.23	3.34	-47.45	4.81	0.14	0.14	0.09	0.02
$6W_{26}$	-93.94	6.51	-93.83	5.87	-97.89	6.73	-47.45	4.81	0.00	0.00	0.00	0.00
$6W_{27}$	-99.37	1.09	-98.95	0.75	-104.35	0.26	-47.42	4.85	4.53	6.60	15.69	0.02
$6W_{28}$	-96.78	3.68	-96.46	3.24	-101.22	3.39	-47.37	4.89	0.06	0.10	0.08	0.01
$6W_{29}$	-95.26	5.19	-94.62	5.08	-98.64	5.98	-47.01	5.25	0.02	0.00	0.00	0.01
$6W_{30}$	-97.51	2.94	-97.26	2.44	-102.55	2.06	-46.85	5.42	0.19	0.39	0.77	0.00
$6W_{31}$	-96.70	3.76	-96.35	3.35	-101.29	3.33	-46.57	5.70	0.05	0.08	0.09	0.00
$6W_{32}$	-96.72	3.73	-96.42	3.28	-101.39	3.22	-46.23	6.04	0.06	0.10	0.1	0.00
$6W_{33}$	-97.31	3.15	-97.11	2.58	-102.59	2.02	-45.65	6.62	0.12	0.30	0.82	0.00
$6W_{34}$	-92.33	8.12	-92.54	7.16	-96.84	7.78	-45.37	6.89	0.00	0.00	0.00	0.00

$6W_{35}$	-92.65	7.81	-92.90	6.80	-97.66	6.96	-44.07	8.19	0.00	0.00	0.00	0.00
$6W_{36}$	-91.97	8.48	-91.95	7.75	-97.07	7.55	-41.72	10.54	0.00	0.00	0.00	0.00
$6W_{37}$	-87.87	12.59	-88.09	11.61	-92.78	11.83	-39.67	12.12	0.00	0.00	0.00	0.00
$6W_{38}$	-84.45	16.01	-85.41	14.29	-89.49	15.12	-40.15	12.60	0.00	0.00	0.00	0.00

Cartesian coordinates of all structures

$2W_1$

H	2.216830	-0.808042	-0.746483
O	2.284337	-0.332361	0.082431
H	1.385543	0.129162	0.108387
H	-2.217890	-0.805608	0.748086
H	2.216830	-0.808042	-0.746483
O	2.284337	-0.332361	0.082431
H	1.385543	0.129162	0.108387
H	-2.217890	-0.805608	0.748086
O	-2.284173	-0.332632	-0.082472
H	-1.385369	0.128934	-0.108550
F	-0.000048	0.741721	-0.000123

$3W_1$

H	0.806457	1.034170	-0.128041
O	1.617802	1.618035	-0.117015
H	1.575656	1.984172	0.767505
H	-1.936252	0.086126	0.092379
O	-2.931310	0.044527	0.051975
H	-3.058868	-0.659411	-0.585275
H	0.805529	-1.205437	0.053017
O	1.658975	-1.699126	0.025148
H	2.260627	-0.964391	-0.121432
F	-0.357432	0.001921	0.026776

$3W_2$

H	1.337217	1.146593	-0.889418
O	0.803857	1.789630	-0.415174
H	0.499776	1.231276	0.345777
H	0.816623	-1.047899	0.345383
O	1.151620	-1.588047	-0.415905
H	0.329625	-1.730811	-0.892110
H	-1.662650	0.582767	-0.892732
O	-1.953046	-0.200129	-0.417776
H	-1.318347	-0.183142	0.344031
F	-0.002410	-0.001157	1.292212

3W₃

F	0.000644	-1.693300	0.000034
O	-0.000920	2.072115	-0.000178
H	-0.746103	1.454651	0.072184
H	0.744589	1.454992	-0.072065
O	1.936654	-0.124929	-0.100482
H	1.176561	-0.799617	-0.103588
H	2.373344	-0.317268	0.730741
O	-1.936413	-0.126326	0.100528
H	-1.175653	-0.800303	0.103885
H	-2.373107	-0.319628	-0.730408

3W₄

H	-2.521118	-0.184360	-0.415814
O	1.018118	1.725599	0.002593
H	0.460715	0.965724	0.336744
H	0.428489	2.126181	-0.639138
O	1.993821	-1.239358	-0.316225
H	2.228456	-0.315588	-0.447783
H	1.083199	-1.122907	0.036209
O	-0.426186	-0.378557	0.663541
H	-0.609641	-0.567412	1.586787
H	-1.587178	-0.288218	0.070241

4W₁

F	0.881970	0.001435	-0.061545
O	3.472006	0.000450	0.095472
H	3.652625	-0.002840	-0.845430
H	2.480341	0.001336	0.102344
O	-0.759956	-1.946319	-0.029525
H	-0.080919	-1.214961	-0.089549
H	-0.523705	-2.376611	0.793768
O	-2.967525	-0.001825	-0.037807
H	-2.353055	0.747575	-0.049421
H	-2.351819	-0.750207	-0.049389
O	-0.763319	1.946360	-0.029687
H	-0.082981	1.216202	-0.089553
H	-0.527854	2.377269	0.793508

4W₂

F	-0.623728	-0.159071	0.019271
O	-3.232469	-0.159302	0.029815
H	-2.246191	-0.241752	0.032706
H	-3.341048	0.789065	-0.053284
O	1.054605	1.625255	-1.021588
H	1.497374	1.703125	-0.170976
H	0.306043	1.042650	-0.765889
O	1.314650	0.192623	1.815022
H	1.810905	-0.530365	1.419356
H	0.471980	0.106438	1.318069
O	1.457403	-1.580868	-0.833249
H	0.584636	-1.236320	-0.541648
H	1.776332	-0.822873	-1.331766

4W₃

H	2.724232	-0.646146	0.480931
O	2.183235	-1.231715	1.018983
H	1.295363	-0.900834	0.774429
H	-1.289235	0.898459	0.775810
O	-2.174463	1.235388	1.021902
H	-2.720269	0.653720	0.484472
H	1.951204	2.064357	-0.686594
O	2.077540	1.170745	-1.009229
H	1.246832	0.724310	-0.702943
H	-1.964128	-2.063019	-0.679039
O	-2.085241	-1.169849	-1.004895
H	-1.251709	-0.727473	-0.700314
F	-0.000096	-0.004436	0.004350

4W₄

H	-1.492370	-0.313370	0.372496
O	-2.226098	-0.394264	-0.275201
H	-2.132286	0.445049	-0.735598
H	0.443878	2.132368	-0.737447
O	-0.395763	2.224240	-0.277272
H	-0.313030	1.491091	0.370911
H	1.492113	0.312631	0.372221
O	2.225655	0.396136	-0.275577
H	2.134074	-0.442857	-0.736958
H	0.313062	-1.492178	0.370414
O	0.395026	-2.225482	-0.277701

H	-0.444401	-2.132795	-0.738073
F	0.000934	-0.000553	1.145338

4W₅

F	-0.000195	-1.297500	-0.832612
O	-0.000532	1.909372	0.514669
H	-0.755476	1.520513	0.044414
H	0.754178	1.521148	0.043523
O	-2.019009	0.229613	-0.765135
H	-1.263510	-0.415410	-0.898285
H	-2.523960	-0.197278	-0.070172
O	0.001906	-0.979772	1.851139
H	0.001204	-0.018733	1.769779
H	0.001158	-1.243065	0.906985
O	2.017905	0.230841	-0.767056
H	2.523325	-0.195507	-0.072096
H	1.262683	-0.414596	-0.899583

4W₆

F	-0.837236	-0.273842	1.345158
O	-2.266349	-0.125480	-0.895989
H	-1.918185	-0.260330	0.013144
H	-1.809559	0.692702	-1.117746
O	0.567370	-1.687850	-0.140095
H	-0.054905	-1.737945	-0.871345
H	0.012429	-1.187490	0.548118
O	2.510479	0.206615	-0.390144
H	1.856500	-0.529042	-0.380709
H	2.822018	0.212869	0.516999
O	-0.042733	1.917928	0.028855
H	0.810882	1.584142	-0.270880
H	-0.334190	1.199968	0.634982

4W₇

H	2.082629	-1.318316	-1.283503
O	2.064622	-1.169816	-0.336623
H	1.974795	-0.165793	-0.276858
H	0.319478	1.416754	0.157992
O	0.664954	1.411667	0.484548
H	-0.725259	2.179154	1.055133
H	-2.097916	0.519808	-0.540755

O	-2.644528	-0.226176	-0.832639
H	-2.154997	-0.953304	-0.427184
H	-0.588244	-0.482222	1.009567
O	-0.520308	-1.444968	0.913628
H	0.365217	-1.530828	0.521121
F	1.660627	1.307678	-0.227425

4W₈

F	2.442645	0.067166	-0.480822
O	0.846532	1.889134	0.035817
H	1.531527	1.178039	-0.223382
H	1.315530	2.408900	0.690326
O	-3.467752	-0.035933	-0.455800
H	-2.636787	-0.086085	0.062504
H	-3.151760	0.327855	-1.284703
O	-1.026382	-0.068286	0.827242
H	-0.412934	-0.807665	0.660198
H	-0.467328	0.701668	0.610381
O	1.047102	-1.889159	0.162437
H	0.966521	-2.366432	-0.664893
H	1.675423	-1.126828	-0.080589

4W₉

H	1.397152	-1.100035	-0.286402
O	2.181043	-0.611622	-0.641396
H	2.918792	-1.131725	-0.318832
H	0.294793	1.868010	0.329521
O	1.246700	1.998892	0.481436
H	1.630722	1.201326	0.093815
H	-1.759572	0.569143	-0.126732
O	-1.530598	1.552276	-0.144410
H	-1.677663	1.778451	-1.064189
H	0.088912	-1.677178	1.414146
O	0.108784	-1.904436	0.482129
H	-0.806664	-1.538137	0.159446
F	-2.014879	-0.916748	-0.180316

4W₁₀

H	-0.993589	1.175088	-0.474161
O	-1.270890	0.264775	-0.328807
H	-0.444277	-0.111371	0.085093
H	1.168488	1.264022	0.330853
O	1.130161	2.189772	-0.038677
H	1.838429	2.174011	-0.685137

H	-3.820707	-1.246169	-0.603860
O	-3.857211	-0.571126	0.075695
H	-2.947332	-0.210717	0.036699
H	1.099114	-0.596843	1.630136
O	1.077796	-0.346750	0.703285
H	2.057524	-1.028714	0.079558
F	2.822611	-1.523630	-0.410129

4W₁₁

F	-3.093560	-1.159489	-0.278174
O	3.738894	-0.618838	0.160934
H	3.557343	-0.483057	1.092333
H	2.866868	-0.419615	-0.240017
O	1.226765	0.028200	-0.781763
H	1.009481	0.966392	-0.811094
H	0.432020	-0.315724	-0.289619
O	-0.992908	-0.447815	0.590605
H	-0.903364	-0.826858	1.468290
H	-2.175713	-0.871104	0.098902
O	-0.778941	2.146980	0.162298
H	-1.600128	2.325123	-0.300044
H	-0.894946	1.192033	0.428221

5W₁

F	-0.896998	-0.050662	-0.092392
O	3.070011	-0.665984	-0.235571
H	2.369589	-1.158069	0.217423
H	2.554083	0.007418	-0.703581
O	-0.410879	2.157558	1.258324
H	0.191092	1.794753	1.911290
H	-0.696554	1.347173	0.776531
O	-3.360171	-0.816620	-0.629359
H	-3.811355	-0.154213	-0.104008
H	-2.416751	-0.571624	-0.486658
O	0.646562	-1.840434	0.943079
H	0.019066	-1.166983	0.572009
H	0.276924	-2.667939	0.630513
O	1.090196	1.209453	-1.351854
H	0.322775	0.677754	-1.049746
H	0.978359	1.995910	-0.809195

5W₂

F	-0.494285	0.222680	-0.088433
O	1.477190	1.903218	-0.140300
H	0.696534	1.293805	-0.174822
H	1.295952	2.426158	0.642426
O	0.993795	-1.887785	0.112697
H	0.405347	-1.098514	-0.002190
H	0.698444	-2.243592	0.952844
O	3.454537	-0.272443	-0.036733
H	2.752830	-0.937980	0.010189
H	2.935198	0.543377	-0.090310
O	-2.684918	-0.077063	-1.490338
H	-2.492751	-0.883364	-1.971813
H	-1.827845	0.099731	-1.033887
O	-2.622315	0.151539	1.611779
H	-1.762080	0.219967	1.156017
H	-3.199376	0.036572	0.850591

5W₃

F	0.276241	-1.008486	0.003454
O	1.149828	1.085375	-1.328673
H	0.764873	0.277980	-0.916434
H	2.067202	1.008114	-1.053006
O	-1.543506	0.352610	1.333339
H	-0.799461	-0.147343	0.925965
H	-2.293015	-0.175574	1.045298
O	2.805048	-0.967843	0.695338
H	2.705195	-0.598377	1.574403
H	1.865707	-1.101031	0.427179
O	-0.784439	2.877442	0.002654
H	-1.151650	2.142070	0.514735
H	-0.094582	2.430188	-0.509030
O	-1.935414	-2.226289	-0.705716
H	-1.054420	-1.878470	-0.432380
H	-2.028153	-1.851554	-1.583343

5W₄

F	-0.730495	0.650370	-0.117970
O	3.749922	-0.288058	-0.040862
H	3.564326	0.652266	-0.003420
H	2.850292	-0.667456	-0.041006
O	-0.498157	3.262156	-0.079224
H	-0.973034	3.410959	0.739572

H	-0.555338	2.280702	-0.164112
O	-1.922290	-1.317687	-1.458465
H	-1.594137	-0.473047	-1.080073
H	-1.091507	-1.769725	-1.627526
O	-1.603051	-1.158225	1.679482
H	-1.314684	-0.354941	1.201265
H	-2.070032	-1.612198	0.970691
O	1.093789	-1.163441	-0.042443
H	0.721792	-1.607026	0.726281
H	0.475084	-0.390824	-0.127844

5W₅

F	-0.125530	-0.036704	0.244562
O	3.734725	0.079301	-0.272622
H	3.144631	-0.686846	-0.218461
H	3.101611	0.809580	-0.204106
O	-2.460558	-0.287365	1.155429
H	-1.528015	-0.154075	0.805086
H	-2.418374	-1.166645	1.535049
O	-4.134294	0.272693	-1.004541
H	-3.434685	0.523153	-1.611178
H	-3.624687	0.056697	-0.199403
O	1.486893	1.953216	0.031190
H	0.817565	1.219142	0.076879
H	0.372078	2.390050	0.876726
O	1.564435	-1.918911	-0.188252
H	0.884507	-1.222676	0.019912
H	1.285534	-2.229516	-1.051189

5W₆

F	0.935980	0.002041	0.078178
O	-0.481794	-1.992541	-0.738482
H	0.148778	-1.271652	-0.479883
H	-0.506936	-2.533720	0.053295
O	-2.597077	-0.002848	-0.627484
H	-2.012603	0.752247	-0.800266
H	-2.010632	-0.756475	-0.799935
O	-0.487139	1.991896	-0.740135
H	-0.512948	2.534418	0.050695
H	0.145386	1.272945	-0.480803
O	3.567030	0.000882	0.000493
H	3.650405	-0.001885	-0.954166
H	2.587702	0.001603	0.111040

O	-0.999051	0.000540	2.066994
H	-1.712941	-0.000687	1.417433
H	-0.215786	0.001400	1.487896

5W₇

F	-1.807295	0.000137	-0.065167
O	4.585257	-0.000272	0.455552
H	4.941475	-0.000174	-0.434285
H	3.622852	-0.000080	0.276857
O	-0.131120	1.900850	-0.154974
H	-0.842256	1.195014	-0.156493
H	-0.281720	2.350299	0.678376
O	1.967327	0.000152	-0.394415
H	1.359912	-0.756853	-0.314615
H	1.360048	0.757243	-0.314403
O	-0.131154	-1.900616	-0.155256
H	-0.842313	-1.194802	-0.156281
H	-0.281641	-2.350478	0.677883
O	-4.381419	-0.000297	0.332480
H	-3.395124	0.000181	0.250519
H	-4.646712	-0.000110	-0.588150

5W₈

F	0.680172	-0.007290	0.009120
O	-4.265192	-1.085098	0.250142
H	-3.427872	-0.586713	0.178665
H	-4.241784	-1.611473	-0.550572
O	2.685174	-0.884664	1.623762
H	1.857035	-0.557975	1.222561
H	3.166541	-1.123254	0.825745
O	0.126346	2.526648	0.041684
H	0.435103	2.804810	0.905558
H	0.422456	1.582090	0.005263
O	2.591180	-0.920949	-1.510450
H	2.799675	-0.140438	-2.026302
H	1.805503	-0.619822	-0.990813
O	-1.907294	0.256138	-0.308084
H	-1.807969	1.211864	-0.248242
H	-0.971948	-0.030073	-0.180377

5W₉

H	0.102241	1.498030	-0.162015
O	0.106962	2.474149	-0.099392

H	-0.834729	2.662402	-0.087006
H	2.137789	1.412370	1.110630
O	2.264445	0.461394	1.168444
H	1.408996	0.140132	0.822186
H	2.671780	-1.066332	-0.718100
O	2.064219	-1.525167	-1.305890
H	1.220170	-1.122003	-1.028525
H	-1.631087	0.350032	-0.717492
O	-2.573531	0.593021	-0.754861
H	-2.935886	-0.077023	-0.166551
H	-1.526440	-2.627172	0.766770
O	-1.782658	-1.754210	1.068874
H	-1.068985	-1.186523	0.693368
F	-0.019927	-0.219712	-0.125630

5W₁₀

F	-1.412041	0.183343	-0.249845
O	2.731173	-1.495362	1.009984
H	2.871820	-0.570699	0.767751
H	1.938669	-1.684743	0.487916
O	-0.177745	2.342660	0.333071
H	-0.355610	2.427781	1.271250
H	-0.721724	1.545170	0.080153
O	0.514288	-1.262375	-0.885677
H	0.208032	-1.773308	-1.636655
H	-0.296221	-0.717933	-0.617400
O	2.251035	1.039073	-0.510434
H	1.536403	1.619082	-0.198363
H	1.745625	0.300138	-0.880050
O	-3.790558	-0.761534	0.295249
H	-2.931197	-0.351335	0.032664
H	-3.512971	-1.343938	1.003788

5W₁₁

F	1.388281	-0.084285	0.084019
O	-2.644098	-1.405058	0.190138
H	-1.717154	-1.660621	-0.012442
H	-2.691835	-1.537866	1.138779
O	-0.039597	-2.105574	-0.198747
H	0.555418	-1.298867	-0.056057
H	0.266795	-2.456453	-1.036442
O	-2.839612	1.539065	-0.147543
H	-1.896971	1.750174	-0.050034
H	-2.837153	0.572280	-0.128514

O	0.004408	2.077547	0.074039
H	0.536277	1.236903	0.127298
H	0.375721	2.502588	-0.700954
O	3.990564	0.057430	-0.025545
H	3.005033	-0.024482	-0.045799
H	4.136032	0.367625	0.869258

5W₁₂

F	-0.000178	1.021505	0.422662
O	2.896848	-1.376607	-0.342361
H	2.901313	-0.412670	-0.241930
H	1.961659	-1.580887	-0.200867
O	0.000281	-1.505459	0.414536
H	0.000693	-1.730193	1.347348
H	0.000060	-0.502721	0.421952
O	2.464802	1.520607	-0.066963
H	1.506764	1.394213	0.172007
H	2.411714	1.992227	-0.899787
O	-2.465273	1.520120	-0.066768
H	-1.507315	1.393769	0.172217
H	-2.412175	1.994666	-0.897768
O	2.896485	-1.377168	-0.342523
H	-2.901364	-0.413128	-0.243226
H	-1.961140	-1.580763	-0.201275

5W₁₃

F	1.395900	0.000942	0.059281
O	0.356321	2.288851	-0.382231
H	0.860085	2.856265	0.203585
H	0.807539	1.405283	-0.270856
O	3.859360	-0.831211	-0.170470
H	3.827972	-1.070139	-1.097842
H	2.939951	-0.499790	-0.022521
O	-3.017261	-1.359723	-0.880607
H	-2.191727	-1.599210	-0.436087
H	-3.041853	-0.413734	-0.687500
O	-0.615950	-1.282533	0.790667
H	0.222657	-0.815367	0.473122
H	-0.311117	-1.828264	1.517357
O	-2.153982	1.169209	0.492887
H	-1.409829	1.691912	0.151050
H	-1.694679	0.387824	0.834189

5W₁₄

F	1.391979	0.065605	-0.061815
O	3.993628	-0.139221	-0.080754
H	4.176667	0.652101	0.427520
H	3.006200	-0.115876	-0.127390
O	-0.387397	-1.595949	0.338892
H	0.386415	-0.952157	0.178300
H	0.043220	-2.430025	0.532607
O	-2.504524	-0.587952	-1.311333
H	-1.761739	-1.113066	-0.973627
H	-2.800245	-0.173566	-0.490740
O	-2.109829	0.489524	1.497713
H	-1.552157	-0.298580	1.429240
H	-1.565717	1.141276	1.022973
O	-0.473169	1.837791	-0.438864
H	0.320041	1.258007	-0.319281
H	-0.930177	1.407893	-1.168503

5W₁₅

H	0.949013	1.364667	-0.182395
O	1.822019	1.793455	-0.096391
H	2.109675	1.421773	0.743432
H	-1.570812	-0.954055	-0.211845
O	-2.400112	-1.487408	-0.174233
H	-2.248410	-2.042271	0.592729
H	1.000889	-0.747769	-1.113255
O	1.896277	-0.967694	-1.433245
H	2.301834	-0.094878	-1.393903
H	2.028714	-1.255053	1.005472
O	1.543754	-0.804964	1.704648
H	0.763230	-0.499479	1.198179
H	-3.087813	0.689715	-0.026884
O	-2.628663	1.534046	0.028242
H	-1.708848	1.220451	-0.005849
F	-0.267074	0.039713	-0.093095

5W₁₆

F	2.037074	0.743774	0.208030
O	-3.879133	-0.810650	-0.676940
H	-3.412621	-1.025520	-1.486366
H	-3.163840	-0.418561	-0.135858
O	2.692137	-1.402639	-1.101391

H	2.138366	-1.280172	-1.874273
H	2.544459	-0.553724	-0.612714
O	-1.733096	0.280417	0.687620
H	-1.231500	0.990515	0.248849
H	-1.020650	-0.283087	1.038292
O	0.666689	-1.027772	1.501073
H	1.230156	-0.304695	1.120866
H	0.990370	-1.786342	1.007399
O	0.063073	2.131663	-0.509844
H	0.886715	1.608671	-0.264502
H	0.227526	2.990798	-0.118102

5W₁₇

F	-1.770813	0.624048	-0.860574
O	1.581635	-0.118379	0.794476
H	1.134299	0.735910	0.660255
H	0.949410	-0.740269	0.391082
O	4.193639	-0.422969	-0.078651
H	3.300836	-0.292294	0.301205
H	3.984157	-0.662462	-0.983041
O	-3.396899	-0.742019	0.643769
H	2.869943	-0.182726	0.019429
H	-3.146040	-0.372127	1.492056
O	-0.037469	2.144635	0.164234
H	-0.773733	1.591039	-0.236778
H	0.222360	2.713480	-0.562222
O	-0.442171	-1.564791	-0.577068
H	-1.123954	-2.048783	-0.103110
H	-0.929961	-0.730012	-0.807800

5W₁₈

F	1.040394	0.079454	-0.211027
O	-2.466026	-1.572189	0.153571
H	-2.046711	-1.045975	-0.563188
H	-2.048817	-2.430251	0.054716
O	-1.055747	-0.098190	-1.662259
H	-1.245491	0.845235	-1.621908
H	-0.175760	-0.121033	-1.194712
O	-0.214504	2.490795	-0.110212
H	-0.650435	2.161198	0.684846
H	0.445957	1.782094	-0.231926
O	3.397386	-1.047055	-0.070504
H	3.556454	-0.859503	0.855671
H	2.507497	-0.637959	-0.201787

O	-0.701649	0.212471	1.862505
H	0.013326	0.072245	1.208207
H	-1.395246	-0.367796	1.524514

5W₁₉

H	1.018171	0.455910	-0.908711
O	1.013139	1.450690	-1.007909
H	1.850652	1.677831	-0.593910
H	-2.495688	-0.854476	0.213748
O	-3.178885	-0.169391	0.300866
H	-2.674498	0.642687	0.158344
H	-0.193204	-1.712104	-0.171801
O	-1.084845	-2.140693	-0.032512
H	-1.187148	-2.658615	-0.832632
H	2.467068	-0.581704	0.315805
O	3.197046	-0.164066	0.842146
H	2.912218	-0.328575	1.742310
H	-1.005080	1.864030	1.221188
O	-1.283375	2.130282	0.342302
H	-0.478856	1.952998	-0.190789
F	1.164636	-1.034728	-0.501410

5W₂₀

H	-0.234294	-1.100631	0.553807
O	-0.224041	-1.156030	1.529564
H	0.376324	-0.428100	1.741050
H	-1.443871	1.841113	-0.228330
O	-0.562306	1.902970	-0.608857
H	-0.453798	0.984718	-0.956172
H	1.247842	-0.823422	-1.128623
O	2.217751	-0.864448	-0.913267
H	2.294219	-1.714265	-0.475013
H	-2.049889	-0.533839	-0.564085
O	-2.766404	-0.319820	0.062625
H	-2.333047	-0.554140	0.891425
H	2.050596	0.595770	0.443063
O	1.659693	1.178066	1.113173
H	0.948995	1.612326	0.613788
F	-0.333404	-0.645047	-1.150757

5W₂₁

H	-2.008647	-1.703463	-0.097305
O	-2.233719	-1.118702	-0.827131
H	-1.422949	-0.574666	-0.870928
H	2.772991	1.013199	-0.055996
O	2.284937	1.800378	0.207194
H	1.375472	1.495057	0.043650
H	2.001441	-1.707441	-0.088535
O	2.232145	-1.124676	-0.818293
H	1.422670	-0.578972	-0.867118
H	-2.767577	1.020191	-0.055097
O	-2.277866	1.804640	0.213211
H	-1.369055	1.498294	0.047714
H	-0.008875	-1.112263	2.311614
O	-0.005075	-1.544100	1.455564
H	-0.005298	-0.780365	0.825063
F	0.000717	0.321123	-0.337490

5W₂₂

F	1.362628	-0.813561	-0.780856
O	-1.773252	2.030771	0.052199
H	-2.108299	2.293739	-0.806970
H	-0.812589	1.911663	-0.122537
O	-0.672142	-2.261939	-0.276185
H	0.141653	-1.706170	-0.443832
H	-0.834660	-2.653812	-1.135622
O	0.837308	1.665577	-0.617800
H	1.542480	1.847811	0.010829
H	0.990270	0.691154	-0.785667
O	3.028890	0.042710	1.016065
H	2.475812	-0.362865	0.300803
H	2.615409	-0.308674	1.806559
O	-2.871727	-0.653734	0.725601
H	-2.139178	-1.215775	0.425595
H	-2.527167	0.237900	0.579496

5W₂₃

H	2.001310	-0.000064	0.997034
O	1.690987	-0.000145	1.926449
H	0.735936	-0.000154	1.803978
H	-4.016568	0.000057	-0.792850
O	-3.941892	-0.000028	0.162839

H	-2.971430	-0.000001	0.284958
H	1.261397	-1.225768	-0.862512
O	0.567942	-1.948204	-0.786626
H	0.948423	-2.535745	-0.130761
H	0.948395	2.535800	-0.130510
O	0.567908	1.948307	-0.786415
H	1.261373	1.225887	-0.862380
H	-0.697575	0.761248	-0.089373
O	-1.170439	-0.000015	0.296305
H	-0.697566	-0.761229	-0.089458
F	2.167807	0.000071	-0.736504

5W₂₄

F	-1.070302	0.485384	-1.328555
O	0.456455	1.678234	0.139893
H	-0.206053	1.249566	-0.525519
H	0.161618	2.585463	0.230323
O	0.179028	-0.822965	1.656963
H	0.155183	0.100114	1.365428
H	0.177397	-1.295507	0.807202
O	0.480895	-1.599927	-1.112536
H	1.341285	-1.176460	-1.200412
H	-0.144922	-0.868131	-1.336672
O	2.817401	0.174427	0.109028
H	2.468002	-0.343784	0.841602
H	2.133186	0.862276	0.032116
O	-2.913353	-0.076411	0.557549
H	-2.260051	-0.455953	1.152535
H	-2.356328	0.147092	-0.216787

5W₂₅

F	-1.007304	1.398951	0.239726
O	-1.197592	0.464666	0.372597
H	-0.648130	0.050349	-0.367151
H	1.377094	-1.306959	-0.723526
O	2.002671	-1.831699	-0.139445
H	1.571609	-2.685309	-0.073703
H	-3.764970	-0.749098	-0.694828
O	-3.825371	-0.416865	0.202656
H	-2.918820	-0.078765	0.346628
H	0.990827	1.241730	-1.149035
O	1.241401	2.079896	-0.713290
H	1.568053	1.752166	0.133808
H	1.778572	-0.511252	1.258313

O	1.460934	0.245253	1.778508
H	0.514254	0.235818	1.579181
F	0.342496	-0.408626	-1.395291

5W₂₆

F	2.405860	1.263421	-0.570546
O	-4.459886	-0.043767	-0.432716
H	-4.401459	-0.066076	-1.389246
H	-3.516417	-0.079903	-0.182311
O	2.702934	-1.229360	-0.704708
H	2.657188	-0.222422	-0.659530
H	2.477240	-1.407648	-1.619197
O	-1.713948	-0.159927	-0.116304
H	-1.122966	0.590665	0.078708
H	-1.181765	-0.890695	0.232114
O	0.568229	-1.406962	1.183573
H	0.592699	-0.452559	1.348289
H	1.315171	-1.514068	0.567801
O	0.384154	1.457944	0.745224
H	1.248836	1.426075	0.161780
H	0.426874	2.302423	1.195955

5W₂₇

F	-2.140665	1.235299	-0.566584
O	-0.031782	-1.169361	1.086337
H	-0.904007	-1.342207	0.686254
H	0.008516	-0.195318	1.066858
O	-2.541831	-1.201236	-0.223832
H	-2.451419	-0.201100	-0.366856
H	-2.645854	-1.536468	-1.115670
O	2.184271	-1.716786	-0.410309
H	1.390245	-1.621358	0.161355
H	1.798665	-1.806727	-1.284158
O	-0.008030	1.590646	0.554094
H	-0.161588	2.318984	1.158583
H	-0.905230	1.496431	0.043868
O	2.721905	1.251619	-0.356909
H	2.739857	0.286282	-0.326295
H	1.800534	1.444730	-0.119720

5W₂₈

H	-2.227841	-0.511168	-0.602702
O	-3.032166	-0.155494	-0.159591

H	-3.240993	0.611914	-0.695598
H	3.154895	-0.679482	-0.794902
O	2.841061	-0.079679	-0.116113
H	2.098032	-0.604099	0.314952
H	1.516175	1.282355	-0.603332
O	0.668399	1.727500	-0.765238
H	0.203159	1.589492	0.077523
H	-0.121562	-0.071114	1.461575
O	-0.679944	0.725844	1.626981
H	-1.548723	0.438877	1.320983
H	-0.257547	-0.024190	-1.453696
O	-0.655724	-0.892377	-1.292370
H	-0.102454	-1.196341	-0.524770
F	0.821538	-1.271401	0.794512

5W₂₉

H	-0.359995	1.957993	-1.517306
O	-0.308816	1.542590	-0.654896
H	-1.300275	1.326842	-0.407805
H	0.156285	-0.266779	-0.391397
O	0.380832	-1.126580	0.004769
H	-0.500455	-1.497542	0.184199
H	2.304434	-1.333286	-0.504219
O	3.211184	-1.003501	-0.584896
H	3.123969	-0.144962	-0.152681
H	1.203002	1.582778	0.514389
O	1.915486	1.232341	1.076326
H	1.534624	0.380951	1.320937
H	-2.522305	-0.582522	0.249882
O	-2.393585	-1.571836	0.402059
H	-2.944337	-1.963897	-0.277331
F	-2.570640	0.884034	-0.107285

5W₃₀

F	1.960672	1.370812	0.067029
O	2.387798	-1.090105	0.027391
H	2.930082	-1.186151	-0.757108
H	2.250015	-0.088905	0.084250
O	-0.238993	-2.041527	-0.026001
H	-0.596281	-1.539380	-0.770570
H	0.699876	-1.771181	-0.002245
O	-1.911647	-0.211965	1.506188

H	-1.332800	-0.945700	1.245571
H	-1.388137	0.556032	1.226631
O	-1.890046	0.003169	-1.518760
H	-2.414297	-0.180119	-0.730157
H	-1.331181	0.729463	-1.184798
O	-0.419848	1.803165	0.031292
H	-0.490793	2.758344	0.072052
H	0.609356	1.628402	0.052225

5W₃₁

H	1.047078	1.502101	0.277925
O	-1.499919	1.700446	-0.568607
H	-1.892295	0.844359	-0.783193
H	-1.574975	-1.392683	-0.199492
O	-2.415040	-1.187156	-0.674752
H	-3.077458	-1.349585	-0.000654
H	1.062346	1.253110	0.391846
O	1.573135	1.375534	-0.464987
H	0.857523	1.662124	-1.043788
H	2.134733	-0.247750	-0.706747
O	2.419134	-1.191265	-0.671754
H	3.188365	-1.154913	-0.100179
H	-0.074840	-0.636891	1.166840
O	-0.168679	-1.556694	0.787928
H	0.660421	-1.667083	0.302862
F	0.054912	0.895587	1.492439

5W₃₂

F	4.097371	-0.005607	-0.312267
O	-4.595587	0.008314	0.295600
H	-3.623378	-0.022991	0.190969
H	-4.881977	-0.009408	-0.618953
O	0.179407	1.812249	-0.230363
H	0.874708	1.171406	0.109804
H	0.314659	2.591518	0.310977
O	0.233154	-1.842619	-0.029677
H	0.895366	-1.146129	0.268113
H	0.677498	-2.249092	-0.776334
O	1.901298	0.049597	0.650475
H	3.165110	0.027310	0.095849
H	2.041813	0.034761	1.601039
O	-1.930470	-0.059916	-0.403100
H	-1.337419	0.709535	-0.347321
H	-1.305137	-0.797447	-0.287226

5W₃₃

H	0.057788	0.430999	1.138047
O	0.103974	1.354353	0.860251
H	1.021127	1.404362	0.458342
H	-1.288668	1.554776	-0.092310
O	2.182900	1.585739	-0.514932
H	-2.667307	2.170157	0.070854
H	-2.584425	-0.370336	-0.488541
O	-2.627141	-1.329568	-0.363390
H	-1.760214	-1.522714	0.020061
H	2.331234	-0.125052	-0.482778
O	2.140952	-1.138318	-0.698814
H	1.985968	-1.141071	-1.645277
H	0.337658	-2.334669	1.414883
O	0.049155	-1.632945	0.828545
H	0.827008	-1.498437	0.219634
F	2.429724	1.190879	-0.167355

6W₁

H	3.44086100	0.53218000	-0.52325800
O	4.05570600	-0.00130300	0.00053900
H	3.43987600	-0.53400600	0.52393100
H	1.58389300	-1.05437100	2.27240200
O	1.79898800	-1.30823500	1.37305300
H	1.09863100	-0.85277400	0.84754100
H	-1.58702400	2.27310600	1.05324200
O	-1.80167600	1.37376700	1.30751000
H	-1.10028700	0.84850800	0.85333300
H	1.58603700	1.05435200	-2.27162900
O	1.80141200	1.30863800	-1.37246100
H	1.10028400	0.85462600	-0.84671300
H	-3.44088700	0.52244300	0.53240100
O	-4.05561100	-0.00187300	-0.00069000
H	-3.43965000	-0.52478800	-0.53373900
H	-1.58272100	-2.27204800	-1.05402500
O	-1.79879600	-1.37304400	-1.30828300
H	-1.09858300	-0.84665500	-0.85364500
F	-0.00006900	0.00176000	0.00031300

6W₂

F	-0.27255800	-0.27776600	-0.19668300
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O	1.76308700	0.48806300	-1.77827600
H	0.98914800	0.07839700	-1.34134700
H	1.68210100	1.39307900	-1.45982800
O	0.45485300	2.22145200	0.47779100
H	0.02767600	1.37619400	0.23332300
H	1.01601800	1.94098300	1.20583300
O	1.36419300	-0.72446700	1.74113400
H	0.69486000	-0.62754300	1.01576400
H	1.02472100	-1.45322400	2.26326600
O	-4.47941000	0.39284700	0.37650900
H	-3.86002500	-0.26381200	0.00688900
H	-3.89106300	1.12063200	0.58766200
O	-2.53907700	-1.34235600	-0.67436700
H	-1.64668900	-0.94878800	-0.46744300
H	-2.50135300	-1.46993900	-1.62382500
O	3.76041100	-0.72212300	0.02663300
H	3.07589100	-0.79256600	0.70694600
H	3.24927600	-0.36084600	-0.71247900

6W₃

F	0.13956100	-0.16881600	0.25879300
O	-2.42147000	0.27394600	-0.19239600
H	-2.35206600	1.12550100	0.25195200
H	-1.50475800	-0.06539700	-0.08421500
O	-0.52416500	2.19808300	1.28574000
H	0.09356000	2.73311400	0.78154900
H	-0.23242400	1.29265800	1.04811400
O	1.72310500	1.25699000	-1.20247500
H	1.10881700	0.69209200	-0.66797200
H	1.34708100	1.20721900	-2.08323100
O	-4.79401900	-1.15177800	-0.45076900
H	-3.96830800	-0.68020300	-0.23123300
H	-4.69975800	-1.27324900	-1.39685500
O	4.00328500	-0.53235000	-0.56092900
H	3.41865800	-1.11668400	-0.05579600
H	3.38798200	0.16213000	-0.83435500
O	1.89845800	-1.95865900	0.92045200
H	1.88779900	-1.91592100	1.87809300
H	1.17580500	-1.33178000	0.66782700

6W₄

H	1.93452100	0.96263100	0.24915900
O	2.39880900	0.26284900	0.74021700
H	1.67375600	-0.34469700	0.96306200

H	-0.36209800	-1.93495400	0.71155200
O	-0.06533100	-1.14155600	1.16555100
H	-0.57333000	-0.44155900	0.69036600
H	4.40118800	-0.95860700	-1.22020000
O	4.75157700	-0.72848300	-0.35804000
H	3.95927200	-0.37092400	0.08912100
H	-1.90224300	-0.84733900	-1.08010200
O	-2.36946700	-1.68915700	-1.23843800
H	-3.21589100	-1.48699300	-0.82830000
H	-2.93370200	0.65960000	0.23845800
O	-3.84386200	0.48795500	0.57607800
H	-3.68057000	0.32982400	1.50764300
H	0.46574700	2.93678700	-0.27591700
O	0.70579200	2.09096300	-0.65783400
H	-0.12912400	1.55809600	-0.56664400
F	-1.36196400	0.63084100	-0.25538600

6W₅

F	0.03541300	0.54081200	0.25307200
O	-2.01375000	1.81418200	-0.70923800
H	-2.14196400	2.50420700	-0.05604700
H	-1.20155300	1.35389000	-0.38300700
O	-1.46828400	-1.43648100	1.24546300
H	-0.92525400	-2.14500900	0.88940200
H	-0.93017700	-0.65122800	1.01222200
O	2.34450000	1.67009700	0.68219300
H	2.30402700	2.39665500	0.05782600
H	1.44847700	1.26295500	0.59419200
O	-3.81323800	-0.49075900	-0.27720000
H	-3.33496300	0.30881400	-0.53940200
H	-3.15200400	-0.93420500	0.27395300
O	3.84217100	-0.67815800	-0.28879600
H	3.49669900	0.13887500	0.09951500
H	3.02324000	-1.13258200	-0.53032700
O	1.07241100	-1.58019300	-0.84142000
H	0.68353800	-0.75610400	-0.45856700
H	0.70073700	-1.60308300	-1.72541100

6W₆

F	0.13692600	0.31107700	0.20244900
O	2.11435500	1.17714500	-1.25058700
H	1.35553200	0.87818600	-0.69123000
H	1.77129200	1.07913500	-2.14057000
O	3.96148100	-0.84817400	-0.15885600
H	3.24071100	-1.25080500	0.34708200
H	3.49967600	-0.11581500	-0.59142400
O	1.46407400	-1.73403400	1.12731300
H	0.93565300	-0.95016700	0.83941500
H	0.98621900	-2.46540200	0.73240400
O	-1.17514300	2.31260200	1.28823100
H	-0.59502300	3.06354100	1.15198200
H	-0.61894400	1.55615400	0.99060000
O	-4.11621400	-1.70236500	-0.43533200
H	-3.50859300	-0.95916500	-0.61538200
H	-3.82231600	-1.99128600	0.43034100
O	-2.32226700	0.40801300	-0.76062500
H	-1.38710200	0.24352400	-0.50463400
H	-2.49972400	1.20689900	-0.25177700

6W₇

H	-3.37766300	-0.00014000	-0.14421900
O	-4.32976500	-0.00146300	-0.39285700
H	-4.27795400	-0.00421300	-1.34978300
H	3.67644200	-0.00107400	-0.50745800
O	4.64853200	-0.00154800	-0.42166400
H	4.75608800	-0.00120400	0.53092500
H	1.30402000	0.76109000	-0.48638400
O	1.87295700	-0.00009900	-0.26965000
H	1.30349900	-0.76107500	-0.48578500
H	-0.26348400	2.54435300	0.08289500
O	-0.16548400	1.91908600	-0.63810100
H	-0.85182200	1.23226400	-0.42665400
H	0.72502100	0.00089500	1.70333500
O	-0.05498100	0.00100500	2.26946400
H	-0.76962300	0.00129300	1.60735400
H	-0.26458800	-2.54247300	0.08552700
O	-0.16673500	-1.91831000	-0.63645300
H	-0.85261100	-1.23088900	-0.42556000
F	-1.72705600	0.00131100	0.05887800

6W₈

F	-1.28390200	0.05207100	0.26170400
O	0.28198100	-1.85316900	-0.79589300
H	-0.37354000	-1.23600500	-0.40821400
H	0.93401300	-1.93731200	-0.08825400
O	2.01309000	0.30318800	-1.65886400
H	1.39196400	1.02170200	-1.46066200
H	1.42244700	-0.46780400	-1.66495700
O	0.51418800	0.79029600	2.05072400
H	-0.23945200	0.44986500	1.51743400
H	0.63846000	1.66039000	1.66092800
O	-0.10882300	2.05204900	-0.77964000
H	-0.64333800	1.29124900	-0.41595600
H	-0.73528400	2.53231100	-1.32373400
O	2.55408300	-0.94014800	0.99140500
H	1.94660500	-0.37297400	1.49492800
H	2.64500600	-0.44605900	0.16319700
O	-3.85119600	-0.51674300	-0.00879300
H	-3.74109800	-1.40108200	-0.36177200
H	-2.91724200	-0.24670900	0.14022200

6W₉

F	0.53569400	1.01409800	-0.34800000
O	-3.97972000	0.10153100	-0.77024100
H	-3.36443900	0.77681100	-0.45341300
H	-3.56252900	-0.69031400	-0.40674500
O	-1.74885700	1.41842300	0.61954400
H	-1.65301800	2.13793900	1.24552400
H	-0.83537200	1.32794800	0.21129400
O	0.59616300	-1.51178300	-0.49003300
H	0.51407200	-1.70981100	-1.42532100
H	0.57757600	-0.51089900	-0.46138800
O	3.01619400	1.57181200	0.03961300
H	2.04158600	1.42150000	-0.07349500
H	3.25412200	2.03082800	-0.76749700
O	3.52687600	-1.32803600	0.19350900
H	2.59791300	-1.55472900	0.05095800
H	3.49544900	-0.35991000	0.19717000
O	-2.01235200	-1.47516000	0.84922300
H	-1.92170300	-0.52777500	1.02781400

H	-1.15132400	-1.68276600	0.45418300
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6W₁₀

F	2.52316800	-0.11760200	0.26182300
O	0.75847100	-1.52271500	-0.86689800
H	1.51049700	-1.00465000	-0.44839800
H	0.64663300	-2.26187700	-0.26659200
O	1.06704000	1.91250600	0.66721200
H	1.58453000	2.63795300	0.31389300
H	1.68385700	1.12770000	0.57190700
O	-3.66124900	0.69573100	-0.64276900
H	-2.67418500	0.69977500	-0.62298500
H	-3.85325000	0.64853400	-1.58104100
O	5.10249600	-0.53887400	0.35932200
H	4.13144000	-0.36290700	0.40760900
H	5.20191700	-0.79501100	-0.55866900
O	-4.94581200	-1.07926000	1.13045000
H	-4.53953700	-0.45050400	0.50725500
H	-4.18601600	-1.39765500	1.62099100
O	-0.98934800	0.67594100	-0.79077700
H	-0.37496400	1.22929000	-0.27289800
H	-0.49222300	-0.15886400	-0.87980800

6W₁₁

F	1.50444100	0.17669700	0.05414800
O	-0.85728000	1.09441900	-0.41512000
H	-0.56799800	2.00937000	-0.33113900
H	0.00151700	0.62048500	-0.26257700
O	-2.92359500	0.14259100	1.03577400
H	-2.47287000	-0.39293000	1.69217100
H	-2.17966400	0.53260300	0.52046400
O	2.51821700	-1.85630400	1.55930700
H	2.94397500	-2.18280100	0.76118600
H	2.07694200	-1.06354700	1.20042200
O	2.84555700	-1.38427800	-1.55371100
H	2.14908200	-1.72509500	-2.11719900
H	2.35891900	-0.73755700	-0.98772100
O	-4.87871800	-0.99867500	-0.64224300
H	-4.32804500	-1.10889600	-1.41946800
H	-4.25537200	-0.59806400	-0.00999000
O	1.63744800	2.78476200	0.11925800

H	1.68747400	1.79980000	0.16720800
H	2.31304000	2.99624500	-0.52681100

6W₁₂

H	-2.45530900	-1.78773300	-0.06959000
O	-3.30969800	-1.66506800	0.36585000
H	-3.28302400	-0.71803500	0.54542700
H	2.77999200	-1.02598800	0.07144800
O	3.55967500	-1.60100900	0.23696900
H	3.25027400	-2.14064200	0.96605200
H	0.81012400	2.19275400	1.59798800
O	0.35028300	1.37023000	1.77975200
H	0.80923500	0.73465400	1.17805000
H	-0.20609500	2.10733600	-1.16216500
O	0.70938000	2.12912200	-1.45875000
H	1.06927900	1.32408700	-1.04352500
H	-0.56394200	-1.28938500	-1.94586500
O	-0.74374800	-1.19058200	-1.00871800
H	0.13263300	-0.88423500	-0.63049600
H	-1.63365300	0.38950900	-0.35261200
O	-2.01137600	1.12268200	0.15723700
H	-1.33671500	1.26089600	0.84317800
F	1.35456400	-0.16513600	-0.06406700

6W₁₃

H	-1.13557900	2.05504900	-1.93114300
O	-1.67392500	1.78327500	-1.18548300
H	-0.99775700	1.55854300	-0.49441000
H	2.21705500	-1.50737700	-0.71072600
O	3.13165200	-1.21230700	-0.81897300
H	3.09972500	-0.33167300	-0.41718100
H	0.22387200	-0.59124900	0.03461800
O	0.23739000	-1.54628800	-0.22410300
H	-0.05753100	-1.96850700	0.58837900
H	-2.31389200	-0.70394300	1.25516000
O	-1.76092100	-0.53829300	2.02984900
H	-1.12359900	0.10344800	1.67155100
H	-1.72488500	-1.28777300	-0.92931600
O	-2.61658200	-0.91489500	-0.88516700
H	-2.45406000	0.01524500	-1.11180000
H	2.81473100	1.44265800	1.44211700
O	2.60190800	1.36746400	0.51043300
H	1.61546400	1.27630900	0.51812400
F	0.05336500	0.93640200	0.51913100

6W₁₄

H	1.98099400	-0.74463800	1.68971300
O	1.06181000	-0.54529400	1.88791000
H	0.88319100	0.18810000	1.24911700
H	-0.71747800	1.91274700	0.24422300
O	-1.65123200	2.20787900	0.42447100
H	-1.64119200	2.38477300	1.36681300
H	2.32227700	0.86795700	-0.40560300
O	3.12539000	0.36553900	-0.64801200
H	2.76949100	-0.22442200	-1.31833900
H	-1.90754500	-0.36672000	-1.27792200
O	-2.59078200	-0.29891900	-0.59621600
H	-2.42152800	0.58420000	-0.22580600
H	0.02974700	-1.46638200	-1.14214500
O	0.13233900	-0.73490400	-1.76677700
H	0.32931000	0.01973500	-1.17451500
H	-1.55294600	-1.71904300	0.43712500
O	-0.80527300	-2.31277500	0.60218400
H	-0.22075200	-1.79071600	1.17649100
F	0.66315800	1.21135500	0.01692800

6W₁₅

F	0.09939600	1.01856100	-0.23186100
O	1.47717300	-0.53906100	-1.71238700
H	0.79709700	-1.20206000	-1.86013600
H	0.96934800	0.16133400	-1.21690500
O	0.88625900	-0.58373600	1.84569000
H	1.74341700	-0.87855200	1.51187300
H	0.65926400	0.12868900	1.21821600
O	-1.37419300	-1.14618400	-0.06762300
H	-0.96724900	-0.25997900	-0.20865100
H	-0.87278300	-1.43712500	0.70447600
O	3.32095100	-1.19498300	0.19577100
H	2.70824100	-1.01681400	-0.55095500
H	3.95594100	-0.47950100	0.12671600
O	-4.16267400	-1.24161900	-0.07779700
H	-4.32481800	-0.31181700	0.09086700
H	-3.18656300	-1.27631700	-0.08095200
O	-0.36734600	3.59919400	0.01012000
H	-0.42804000	3.61012100	0.96646000
H	-0.18978600	2.64608700	-0.16444800

6W₁₆

F	-0.97643500	0.71908300	-0.06280900
O	1.07468400	2.27963000	0.21988400
H	0.28414100	1.70310300	0.06587000
H	0.91704400	2.61389000	1.10449100
O	3.61402300	0.85558600	0.06989800
H	3.31280600	-0.06296600	0.05599400
H	2.78076200	1.35203800	0.07481500
O	-2.60656200	-0.77808500	1.52191500
H	-3.31563800	-0.63681700	0.88579400
H	-1.94603700	-0.15325100	1.16879000
O	-3.35017300	0.61096800	-1.15426500
H	-3.15618000	0.15458000	-1.97476400
H	-2.44693600	0.76876500	-0.78883700
O	2.57607100	-1.91902700	-0.23402100
H	2.70229900	-2.15159300	-1.15586500
H	1.59955700	-1.87529100	-0.16002500
O	-0.15376100	-1.71785100	-0.27469000
H	-0.40669200	-0.75890900	-0.27167900
H	-0.77147000	-2.07505800	0.37093700

6W₁₇

H	0.13853900	0.19222100	1.08881500
O	0.22981100	-0.59034400	1.70919200
H	0.44405400	-0.19003200	2.55402500
H	-1.48981500	-1.33534700	0.95750800
O	-2.21422600	-1.44455800	0.32477000
H	-2.53755800	-0.53490900	0.22477600
H	-0.07649600	0.01057600	-1.27907500
O	-0.11621700	-0.83765100	-1.76388000
H	-0.85668600	-1.27035900	-1.31646200
H	2.80782100	0.64281700	-0.12677800
O	2.67204700	1.58945600	0.00884100
H	1.70151100	1.64418200	-0.02632100
H	-2.80657200	1.67769900	-1.01699200
O	-2.62832900	1.40193200	-0.11612500
H	-1.63700100	1.45684300	-0.05876500
H	1.58828800	-1.39954700	-0.92319900
O	2.26982200	-1.44473300	-0.23309800
H	1.72493000	-1.35831100	0.56205500
F	-0.07825400	1.23015000	-0.00857600

6W₁₈

F	-1.35376800	-0.06235200	-0.21138100
O	-1.39372300	-2.39387300	-1.38708300
H	-1.44700300	-1.47026600	-1.04106900

H	-2.24046300	-2.76132200	-1.12877800
O	4.34260000	1.50422800	-0.65914400
H	4.01265400	0.75792100	-0.12913100
H	3.53338400	1.86675600	-1.02511400
O	0.73678600	-1.38082600	0.52377000
H	0.49329000	-2.13421100	-0.02484500
H	-0.00553600	-0.75652700	0.31478100
O	-3.25168100	0.57907300	1.45607600
H	-2.78490800	0.58943900	2.29313300
H	-2.55123700	0.27354600	0.82897600
O	-2.18401600	2.46217400	-0.83807000
H	-1.74243500	1.59445800	-0.77880200
H	-2.83794300	2.36144800	-0.14004000
O	3.27286700	-0.58168500	0.92522200
H	3.21186500	-0.39519000	1.86394100
H	2.35957800	-0.87760600	0.70319900

6W₁₉

H	1.47791500	-1.19951700	1.23265300
O	2.30788900	-0.84295200	1.58233600
H	2.22521400	0.09836400	1.36026700
H	-0.66183500	-0.97812900	-0.15032000
O	0.08450500	-1.66626800	-0.15943300
H	-0.38377500	-2.50023900	-0.23048400
H	-1.14924600	1.43558700	-0.05845800
O	-0.70607300	2.33267500	-0.05425200
H	-1.04459900	2.74401400	-0.85125700
H	1.08671300	1.96827900	0.09213700
O	2.01224000	1.66776500	0.16198300
H	2.12473900	1.10498400	-0.61576700
H	-4.38049700	-0.35184000	0.99281200
O	-4.26306300	-0.63826200	0.08595300
H	-3.31793100	-0.40330700	-0.07292200
H	1.57119100	-1.17220500	-1.23569600
O	2.46268000	-0.83954800	-1.43786900
H	2.90496400	-1.02365200	-0.60022600
F	-1.73758600	0.01893000	-0.14361000

6W₂₀

F	-1.99169500	0.17332400	0.17169100
O	-0.01104000	-1.05412400	1.02815400
H	-0.84852700	-0.60977600	0.66540000
H	-0.31240900	-1.49405000	1.82538500
O	-0.91128600	2.41864900	-0.33345500
H	-1.00959900	2.49418300	-1.28424600

H	-1.41371000	1.57999200	-0.12406400
O	2.19133100	-2.31663400	-0.44758900
H	1.40035100	-1.96506900	-0.01301600
H	2.70010500	-1.51675800	-0.63474100
O	-4.27855800	-0.93866200	-0.48217000
H	-3.91420300	-1.59821300	-1.07432900
H	-3.46342900	-0.46631800	-0.19049200
O	3.54371800	0.35135200	-0.70537000
H	4.27783000	0.52436400	-0.11326000
H	2.79146600	0.79466400	-0.25329800
O	1.46259800	1.33217600	0.73054100
H	0.73063300	1.84697300	0.34234200
H	1.01264500	0.50802800	0.98821500

6W₂₁

F	-0.66922900	-0.59380100	0.04457600
O	1.89797900	-0.19473900	0.57297000
H	0.96334200	-0.44531400	0.39376000
H	1.89413900	0.76252600	0.43813300
O	-2.99507800	0.14313000	1.25233000
H	-2.07256100	-0.10569600	1.05509000
H	-3.45429900	-0.51285600	0.71764600
O	-1.09452200	1.81571300	-0.69926300
H	-0.91415500	0.85632600	-0.50075000
H	-1.89511000	1.96421700	-0.18669000
O	1.44113600	2.67465100	-0.15524300
H	0.49026000	2.48332900	-0.30014000
H	1.75921100	2.85235900	-1.04250000
O	4.09145000	-1.71920500	-0.09553100
H	3.30402900	-1.15064600	0.03035800
H	4.09256300	-2.22445900	0.71897500
O	-2.57259800	-2.14941200	-0.80911200
H	-1.77968200	-1.64929200	-0.49415600
H	-2.51160400	-2.04738200	-1.76012800

6W₂₂

F	-1.52849600	-0.10654500	0.03544700
O	0.00824500	1.93076200	-0.20355700
H	-0.44125200	2.55474200	-0.77634200
H	-0.60282400	1.14503100	-0.19623000
O	-3.70212900	-0.36327800	-1.42498200
H	-3.36236800	-1.00755600	-2.04767600
H	-2.92824800	-0.23630700	-0.82864900
O	-0.57731300	0.48807300	2.50298700

H	-0.10273900	1.25032000	2.15640900
H	-1.13924900	0.26794400	1.73469100
O	2.80224500	1.41413000	-0.87684000
H	1.87783700	1.60044400	-0.65373200
H	2.82433700	0.44761300	-0.88842900
O	0.36323400	-1.77102700	0.71131400
H	0.41763600	-1.32984700	1.56801300
H	-0.39154200	-1.27083400	0.31720900
O	2.66734600	-1.54631000	-0.74073100
H	3.28958100	-2.03701100	-0.20112400
H	1.82226800	-1.64443900	-0.24869200

6W₂₃

F	-1.15312100	-1.57503400	-0.27063800
O	0.15766400	-0.95750800	1.73407000
H	-0.38972600	-1.27965000	0.93983100
H	-0.04251700	-1.58458900	2.43107600
O	0.82234900	-0.80184500	-1.87392100
H	0.06386600	-1.16153300	-1.36253100
H	1.57407000	-1.01873400	-1.30908900
O	2.70387400	-0.37030600	0.51353000
H	2.46164000	0.50973100	0.18643600
H	1.92950000	-0.60584900	1.04859600
O	-2.82790800	0.33487900	-0.46665700
H	-2.81437100	0.54076600	-1.40322800
H	-2.24309600	-0.47183800	-0.40839800
O	1.29310900	1.84966800	-0.80225500
H	0.55019100	1.95037800	-0.18295400
H	1.00909700	1.10196200	-1.35348100
O	-0.84740800	1.68915600	1.10792400
H	-1.61947800	1.35941300	0.61694200
H	-0.51453900	0.88289600	1.53102900

6W₂₄

F	-0.97864300	-0.72907300	-0.80382300
O	2.17555900	-0.59706400	0.94041900
H	2.04098400	-1.04865000	0.09307700
H	1.33311200	-0.76261000	1.38834700
O	1.22922100	-1.84055600	-1.53146700
H	0.34850500	-1.41778100	-1.36328400
H	1.01116500	-2.76594800	-1.65172300
O	-0.52704100	1.91485900	-1.01312900
H	-0.61072500	0.93969800	-1.04186300
H	-1.35229700	2.15622600	-0.58310600

O	-3.13836900	0.45042700	0.33643400
H	-2.70545300	0.33273400	1.18699900
H	-2.52701300	-0.04136500	-0.24408200
O	-0.60884800	-1.16222100	1.68614200
H	-0.90897900	-2.06053200	1.83557700
H	-0.76611100	-1.02352900	0.71276000
O	2.05977300	2.30970200	0.38065200
H	2.20487200	1.37884000	0.60456600
H	1.21736200	2.27340300	-0.09526200

6W₂₅

H	-4.43407800	-0.76983600	-0.66996000
O	-4.29456600	-0.79725100	0.27806600
H	-3.34517300	-0.57778300	0.34664800
H	-1.34860700	0.75083000	-0.01662700
O	-1.58287400	-0.15152700	0.26808000
H	-1.00316200	-0.70355500	-0.29036700
H	2.84271800	-0.47113800	-0.20057100
O	3.11050700	-1.27702300	0.27705500
H	2.64160700	-1.13896000	1.10824000
H	-0.21404000	2.92133900	0.15358700
O	-0.42283700	2.30482500	-0.55089700
H	0.44208400	1.83223400	-0.69931800
H	1.30396200	0.60924900	0.98218000
O	1.05404500	0.29584900	1.87388200
H	0.13379800	0.04391200	1.73113500
H	1.02107400	-1.95034100	-0.96475600
O	0.39288100	-1.33536800	-1.35680100
H	0.89251900	-0.48649700	-1.27316600
F	1.66778200	0.84716700	-0.72467900

6W₂₆

F	1.57176900	-0.60107600	-0.03079800
O	-0.86464900	0.17730200	-0.15012900
H	0.05594300	-0.20882100	-0.12538600
H	-0.69423600	1.12738100	-0.06522100
O	2.59876000	-3.01872800	-0.04361200
H	2.27637200	-2.08670900	-0.02131300
H	1.78129900	-3.49999200	-0.18012400
O	0.21315500	2.89815100	0.19021400
H	0.27305400	3.24963900	1.08053100
H	1.11262000	2.52904100	0.03848100

O	-2.80181000	-0.87892700	1.44534600
H	-2.71259000	-0.47233600	2.30851000
H	-2.02866600	-0.52644300	0.95171400
O	2.59802200	1.64977100	-0.09064400
H	3.11388900	1.65438300	-0.89865600
H	2.24298400	0.69822800	-0.04176200
O	-3.41910500	-0.36426600	-1.46161600
H	-2.48160500	-0.16416200	-1.32206400
H	-3.67997300	-0.59695100	-0.56400800

6W₂₇

H	1.07408600	2.52561200	-1.33073800
O	1.04765400	1.64748200	-0.94793200
H	0.25433100	1.67590600	-0.30743300
H	1.75569200	-1.18088100	-0.98699400
O	1.06581500	-1.11984300	-1.66482900
H	0.94374300	-0.15720700	-1.68797000
H	-2.97192600	0.72533600	-1.20909500
O	-2.83286700	0.30653400	-0.35816000
H	-2.11022300	0.86269700	0.05100900
H	-0.22322600	0.35410900	1.61981800
O	0.19453200	-0.45957200	1.97190600
H	-0.27913200	-1.14756600	1.47883500
H	-0.50128600	-1.81718400	-0.70832800
O	-1.20472200	-2.03951800	-0.07742300
H	-1.86884600	-1.34935400	-0.23843900
H	1.90492700	-0.37008900	1.23594800
O	2.66141100	-0.23287400	0.63305400
H	2.39094500	0.57868100	0.18130800
F	-0.86929500	1.60914100	0.60546100

6W₂₈

H	-3.43149500	-0.25218600	-0.07269900
O	-4.35786100	-0.30392200	-0.38100300
H	-4.24634200	-0.30275100	-1.33310100
H	1.11400500	-1.80183800	-0.59227000
O	0.41451300	-2.05699400	0.03379000
H	0.73974100	-1.66133800	0.85833800
H	-1.06018600	-0.82612100	0.07038400
O	-1.67006900	-0.10169700	0.29657000
H	-1.22796800	0.69488300	-0.05430300
H	1.48210800	0.41735400	1.38411800
O	1.04304900	-0.11316700	2.09125400
H	0.11936200	0.14198200	2.00008300
H	0.70798300	1.80186200	-0.39128500

O	-0.22306300	2.13860100	-0.55979100
H	-0.26497700	2.94481300	-0.04280100
H	2.37995000	-0.02471900	-0.92536300
O	2.54624600	-0.86627700	-1.44129600
H	3.45670600	-1.07613400	-1.22737200
F	2.02317700	1.15242800	0.00112000

6W₂₉

H	1.23946300	1.98015300	-0.47003500
O	0.97577500	2.89468300	-0.73976600
H	1.60343600	3.44306000	-0.26665000
H	-3.49876900	-0.81074700	0.49442800
O	-3.62058000	-0.24196400	1.26157500
H	-2.79656900	0.26481600	1.24392300
H	-0.12629500	0.71143300	0.41748500
O	-1.09714400	0.95703800	0.37752400
H	-1.03800700	1.86603800	0.06273000
H	-1.64539000	-0.33780300	-0.69746200
O	-1.95153500	-1.14937000	-1.15282100
H	-1.77882200	-0.96301600	-2.07795600
H	0.18019400	-2.04636000	-0.94475900
O	1.12599900	-1.91642200	-1.06801700
H	1.25299200	-1.01199600	-0.71573500
H	2.83901000	-1.89583300	0.76308400
O	3.17311100	-1.17993800	1.31147000
H	2.59397000	-0.45261300	1.01489600
F	1.36997600	0.48229500	0.13959200

6W₃₀

H	-0.09073200	2.95489800	0.53763600
O	-0.49861300	2.32622800	-0.06028800
H	-0.84522800	1.60742700	0.55715400
H	0.04912000	-1.79291400	-0.29315500
O	-0.26456000	-1.71892200	-1.21381700
H	-1.19074900	-1.45058300	-1.09106400
H	0.62477500	1.30695300	-1.12128900
O	1.22716100	0.66297800	-1.53899600
H	0.68751300	-0.14995300	-1.57746900
H	-3.01515800	0.24758100	-0.94608000
O	-2.78136000	-0.54931700	-0.46564800
H	-2.29082900	-0.18423000	0.32361800
H	1.40916700	-0.85079900	1.35676300
O	0.59350900	-1.35485600	1.47168700
H	-0.10534400	-0.66489500	1.55944300

H	2.44883100	0.31368700	-0.33573600
O	3.05351300	0.03645300	0.38973900
H	3.61668700	-0.61172600	-0.03723900
F	-1.32614000	0.45044900	1.37844500

6W₃₁

F	1.96878300	0.63834100	1.22271500
O	-1.51265400	-0.32187500	-0.13536400
H	-1.02521100	-0.59380500	0.66519800
H	-1.02739500	-0.82805400	-0.80778100
O	-4.24739200	0.24398700	-0.12434500
H	-4.11049100	1.19244700	-0.15991700
H	-3.33051700	-0.08633100	-0.12930000
O	0.44452200	-1.21769800	1.60567800
H	0.51806400	-1.50060700	2.51826500
H	1.11834900	-0.43937200	1.51048400
O	0.22734000	2.19832100	-0.17116900
H	0.86140800	1.78746100	0.44991000
H	-0.46196200	1.52372500	-0.21526700
O	2.39070500	0.34154100	-1.34102700
H	2.41478800	0.42177600	-0.35661500
H	1.82100100	1.08932400	-1.55351800
O	0.63304300	-1.88362000	-1.23778000
H	0.71912400	-2.00439000	-0.28158300
H	1.29928600	-1.19248700	-1.41226200

6W₃₂

H	-3.00929600	0.47497000	-0.02782000
O	-2.94387600	1.43455000	0.07448800
H	-1.98806300	1.58236500	0.01522000
H	-1.83555100	-1.59840400	-0.18118000
O	-2.81605300	-1.52131000	-0.13484900
H	-3.02838300	-2.01059900	0.66200500
H	0.23771100	-1.32664300	0.72263200
O	-0.09828700	-1.70240200	-0.10590000
H	0.35284300	-1.11860500	-0.76052500
H	2.02362400	0.01545400	1.39329800
O	1.18558900	0.06593400	1.88084000
H	0.73115600	0.79410100	1.43098500
H	3.60205400	-1.06626800	-0.28280800
O	3.31620200	-0.17421100	-0.07818900
H	2.55426300	-0.03529400	-0.71117700
H	0.43280600	1.17858800	-0.73960600
O	-0.04672500	1.81273800	-0.11849200

H	0.21352100	2.67974800	-0.43526500
F	1.21539000	0.12313400	-1.46988200

6W₃₃

H	1.78751500	-1.19406200	-0.45082900
O	1.28479200	-1.58841200	-1.20207500
H	1.19941300	-0.80622500	-1.76242400
H	-1.78760200	1.41455800	-0.22149800
O	-1.04673700	1.96065000	0.07720900
H	-0.69058200	1.44905100	0.82320000
H	-0.70148000	-1.17947100	0.99795200
O	-1.08309900	-1.71916200	0.28260100
H	-0.31682000	-1.81383800	-0.31874300
H	-2.34941500	-0.75514700	-0.38263800
O	-3.03437800	-0.09795700	-0.64826800
H	-3.78235600	-0.32711500	-0.09385300
H	1.11865000	0.06442400	1.47368900
O	0.18875800	0.17902200	1.93096800
H	0.38395800	0.25694100	2.86619700
H	1.88971500	1.01272300	-0.63942400
O	1.46538600	1.41107500	-1.42209300
H	0.62351900	1.72232900	-1.05842000
F	2.26974600	-0.11176700	0.73556300

6W₃₄

F	2.43196800	-1.93675300	0.30062400
O	0.58867800	1.19235700	-0.08674000
H	1.34202300	0.88902500	-0.63278700
H	0.58864000	0.53690900	0.63378400
O	0.44940100	-1.17605500	1.43286000
H	0.54093800	-1.40084300	2.36011800
H	1.30852900	-1.56620400	0.97129500
O	2.69748900	-0.08811900	-1.37375600
H	2.53987200	-0.52401200	-2.21291400
H	2.66892100	-0.84983300	-0.71137500
O	-4.44487200	-0.95233200	-0.40950700
H	-4.41071800	-1.60426600	-1.11142100
H	-3.49691200	-0.77638600	-0.26110100
O	-1.68326000	-0.68473800	-0.28069300
H	-1.08576800	-1.07566600	0.38320300
H	-1.16746500	0.08983300	-0.54194300
O	-0.10025100	3.84205800	0.44549200
H	-1.03803500	3.69553500	0.30985500
H	0.26478300	2.95131400	0.28642300

6W₃₅

F	2.80266700	1.00356200	-0.64003900
O	0.90164200	1.59912200	0.68260800
H	1.73823500	1.37438100	0.06640500
H	1.25839400	2.22233000	1.31905500
O	0.50529700	-1.17810100	1.05280300
H	1.28063900	-1.45266500	0.52715700
H	0.58963600	-0.20742600	1.04246900
O	-1.92264300	-2.10485200	0.26910900
H	-1.02619200	-1.76698400	0.49515000
H	-2.23656000	-2.44944900	1.10688500
O	-3.48097200	0.02267100	-1.01745200
H	-2.87534100	0.75939900	-0.85582600
H	-2.99236700	-0.72712500	-0.64806600
O	-1.72190800	2.12329200	0.06679100
H	-0.75749500	1.97130400	0.16476800
H	-2.04733300	1.94859300	0.95217700
O	2.76779300	-1.51674700	-0.58890600
H	2.87053400	-0.51758500	-0.62956200
H	2.58017700	-1.74990400	-1.49987700

6W₃₆

H	2.84003400	-0.38653900	0.12080700
O	3.01899100	0.61572200	0.39657800
H	3.23267100	0.56716900	1.32993300
H	-2.88883500	-1.06469800	-0.40234200
O	-2.60558900	-0.76323000	-1.27426400
H	-1.66423700	-1.01038500	-1.24108600
H	1.14689200	2.29717700	-1.21707200
O	0.85974900	1.86650800	-0.40928500
H	1.69478600	1.45900500	-0.04354100
H	-1.02677300	1.89210200	0.08786700
O	-1.97015000	1.74693500	0.25346000
H	-2.22469500	1.13228800	-0.44998700
H	0.94978500	-1.39800300	-0.34787200
O	0.02445500	-1.00566300	-0.38932300
H	0.22733100	-0.06495400	-0.47311800
H	-1.18199500	-1.10444700	1.15237900
O	-1.98319800	-0.91188700	1.66958400
H	-2.03890100	0.04776000	1.56962700
F	2.46443000	-1.63928400	-0.22884500

6W₃₇

F	-5.04696500	-1.17834000	-0.36507200
O	1.52553500	-0.58504200	0.64528700
H	1.42577500	-0.20252300	1.51895000
H	-1.62158000	-0.28951800	-0.04424300
O	6.34520100	0.31842900	0.31252400
H	6.33054100	1.20417700	-0.05365400
H	5.48628000	-0.03551600	0.02269600
O	-0.77210300	-0.02344800	-0.51193100
H	0.65989300	-0.37893100	0.19879400
H	-0.96816400	0.90133600	-0.70259800
O	3.86306000	-0.48777500	-0.72512200
H	3.02034900	-0.46147900	-0.22109500
H	3.78465200	-1.29327400	-1.23966700
O	-3.07256400	-0.30912600	0.67078200
H	-3.08370100	-0.57498500	1.59345700
H	-4.19774800	-0.82755200	0.08111000
O	-2.75745200	2.20150200	-0.08282900
H	-2.94266900	1.30085100	0.30246200
H	-3.52437100	2.34614900	-0.64023700

6W₃₈

F	-1.65767000	-1.79761100	-0.27081600
O	1.99240400	0.74884800	-1.39970000
H	2.13594400	1.59743800	-0.97297400
H	1.14867900	0.45426600	-0.96791400
O	3.97822200	-0.80688200	-0.27441900
H	4.79442400	-0.43729800	-0.61507400
H	3.28831200	-0.33679700	-0.78526600
O	-0.11365700	0.11305800	0.09189400
H	-0.67834900	-0.72407700	-0.05395100
H	-0.78931700	0.80678500	0.12744000
O	-3.73729500	-0.58636700	0.06407600
H	-2.88703100	-1.15797100	-0.10384000
H	-4.09497900	-0.94830000	0.87639900
O	-2.53254500	1.81806000	-0.02383600
H	-2.74093300	2.10402000	-0.91531500
H	-3.04909100	0.98145900	0.06278900
O	2.12684300	0.41982300	1.91239400
H	2.77704300	-0.07213900	1.39861400
H	1.30254800	0.25879000	1.42315800