Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information Available

The Self-Assembly Mechanism of the Lindqvist Anion $[W_6O_{19}]^{2-}$ in Aqueous Solution: A Density Functional Theory Study

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The material enclosed in the supporting information is organized as following:

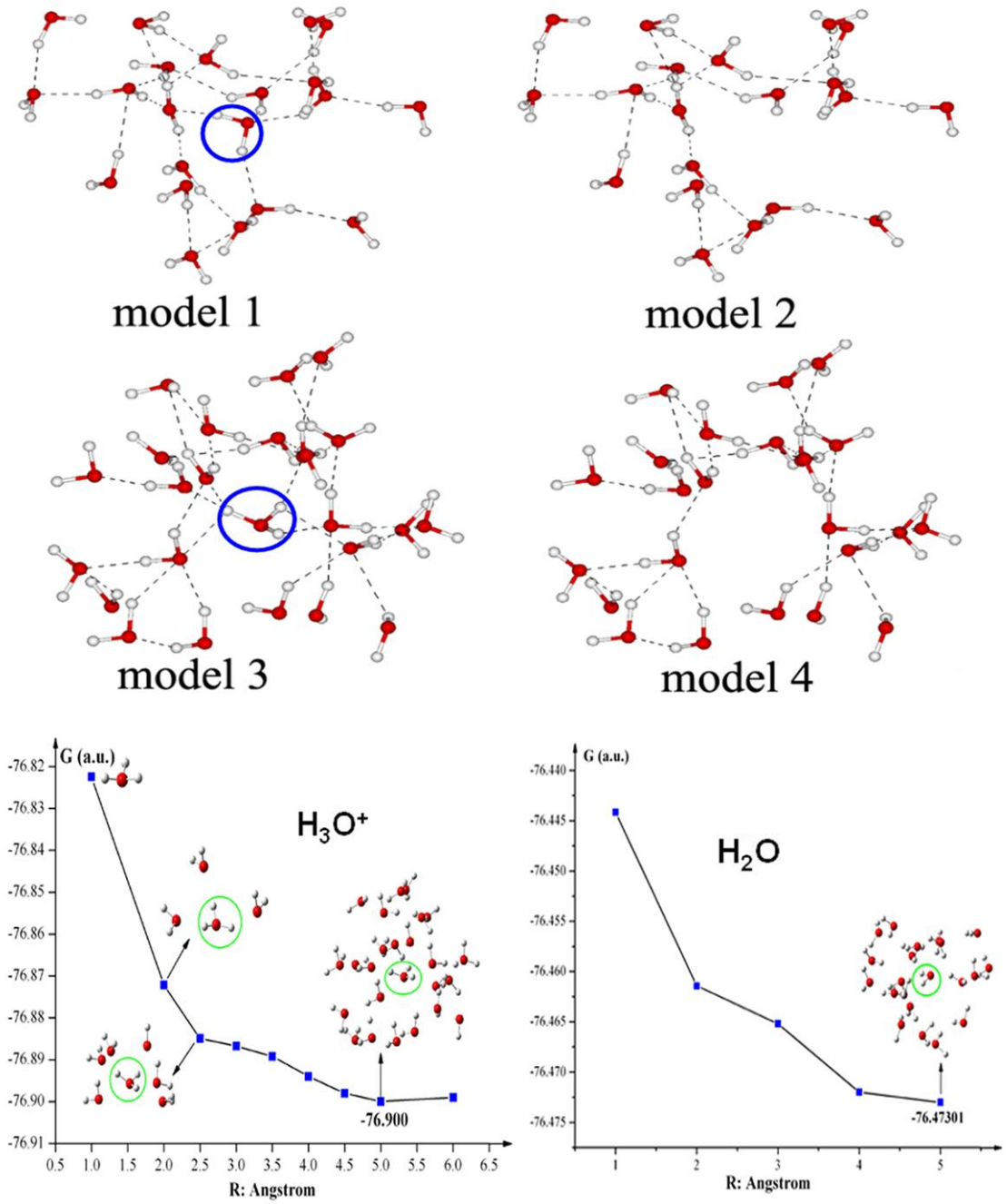

Figure S1. Ball-and-stick representations of the selected models for H_2O with 20 water surrounding (models 1 and 2) and H_3O^+ with 24 water surrounding (models 3 and 4) within the radius of 5 Å from the center molecule, and the trends of the Gibbs free energy as the radius changes (The test models for H_2O and H_3O^+ here were selected by setting a H_2O or H_3O^+ as the center and defining different radius from system 1 and 2 respectively. The energy of the H_3O^+ shows a significant fluctuation from 1.0 Å to 2.5 Å, which correspond to the model with a bare H_3O^+, three water, and six water surrounding, respectively. This is in agreement with the previous report, that is the first hydration shell of the proton is composed of at least four water molecules. From 3 Å to 6Å, little change can be found, especially for 4.5-6Å. Finally, we selected the model within the radius of 5 Å to evaluate the energy of the H_3O^+ in the aqueous solution. The same approach was performed to H_2O case.).

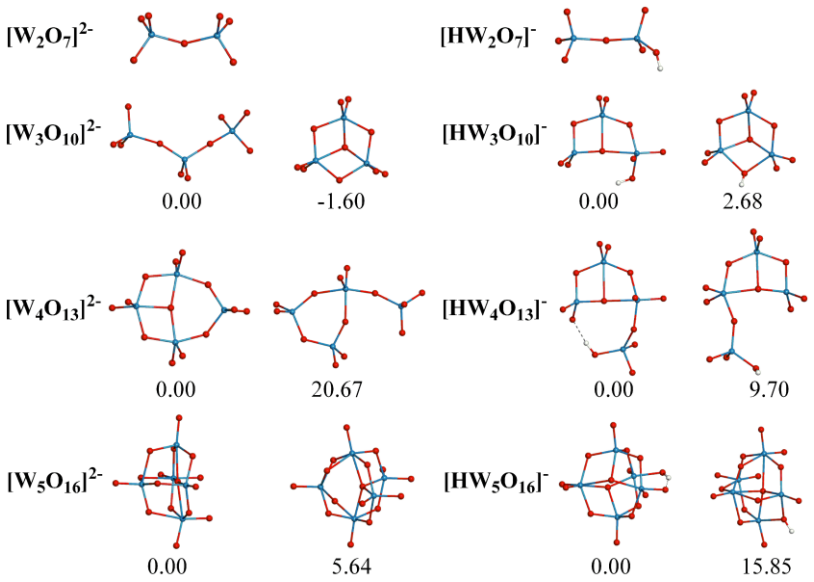

Figure S2. Relative stable building blocks and relative energies (kcal/mol) optimized at PCM/B3LYP/[LANL2DZ(W)/6-31g*(O)/6-31g**(H)] level.

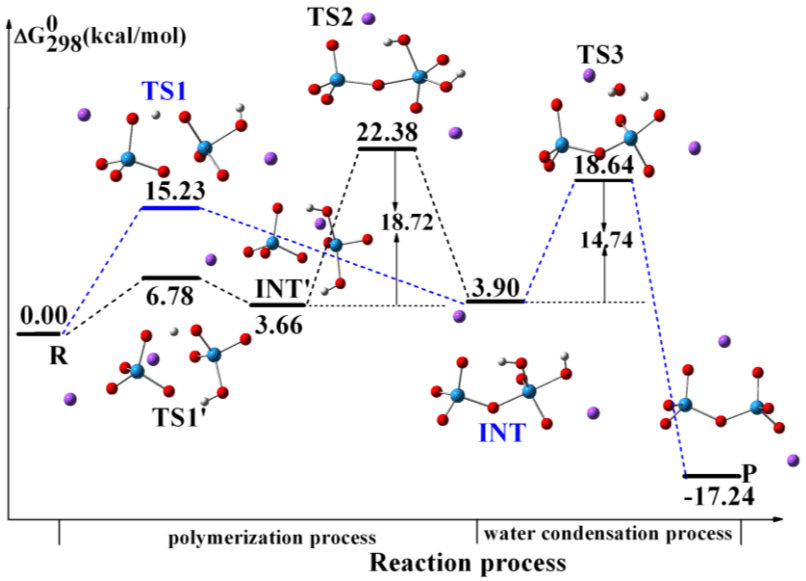

Figure S3. DFT calculated relative Gibbs free energies at PCM/B3LYP/[LANL2DZ(W)/6-311++g*(O)/6-311++g**(H)]//PCM/B3LYP/[LANL2DZ(W)/6-31g*(O)/6-31g**(H)] level for formation process of $[W_2O_7]^{2-}$ with considering the counterions Na^+.

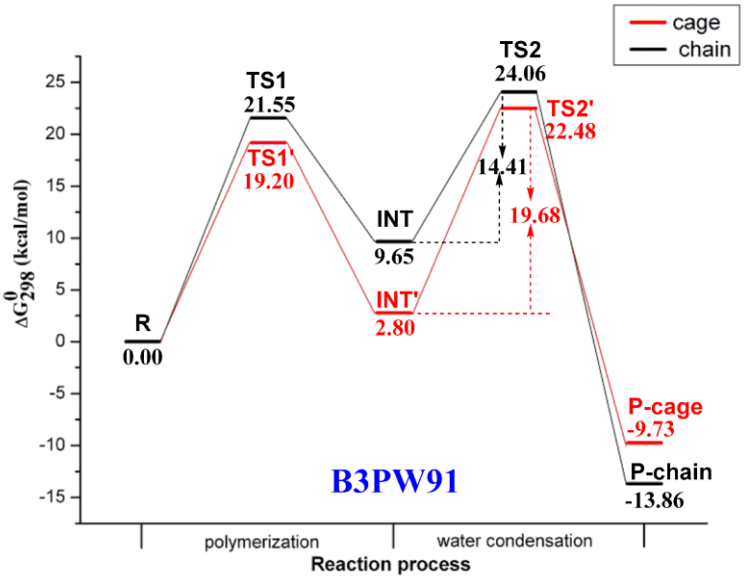

Figure S4. DFT calculated relative Gibbs free energies at PCM/B3PW91/[LANL2DZ(W)/6-311++g*(O) /6-311++g**(H)]// PCM/B3PW91/[LANL2DZ(W)/6-31g*(O)/6-31g**(H)] level for formation process of $[W_3O_{10}]^{2-}$.

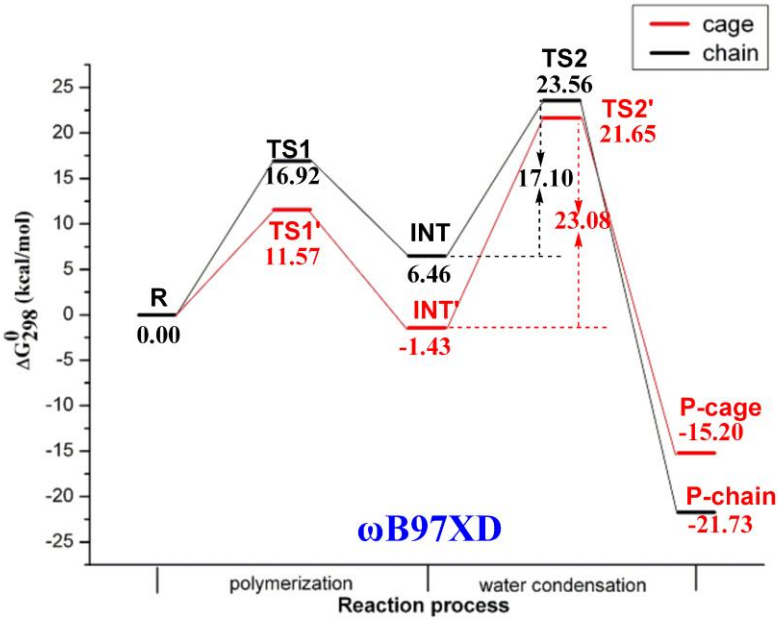

Figure S5. DFT calculated relative Gibbs free energies at PCM/ωB97XD/LANL2DZ(W)/6-311++g*(O) /6-311++g**(H)]//PCM/B3LYP/[LANL2DZ(W)/6-31g*(O)/6-31g**(H)] level for formation process of $[W_3O_{10}]^{2-}$. (Figure S5, page 4)

Optimized coordinates (xyz)

$[W_2O_7]^{2-}$-TS1

12

W	-1.957934	0.020790	0.008574
O	-2.867583	1.059942	-1.084914
O	-2.942200	-0.354910	1.420996
O	-1.436897	-1.527111	-0.847899
O	-0.386482	0.776306	0.474112
H	-0.259179	-1.535131	-0.822219
W	1.882951	-0.016589	0.015269
O	2.027027	-0.278287	1.736377
O	0.963500	-1.403456	-0.747065
O	1.763871	1.866794	-0.444099
O	3.496700	-0.255152	-0.599737
H	0.864421	2.151200	-0.204340

$[W_2O_7]^{2-}$-TS1'

12

O	0.339043	-0.827709	0.166725
W	-1.796556	-0.061362	0.007411
O	-1.920527	-1.156210	-1.357840
W	1.941645	-0.017951	0.002020
O	2.821896	-0.619316	-1.398164
O	2.924661	-0.232701	1.445327
O	1.470928	1.761027	-0.229480
O	-3.589251	0.668824	-0.226440
O	-0.938015	1.549954	-0.115312
O	-2.011765	-0.790490	1.590978
H	0.344293	1.773617	-0.188853
H	-3.856587	1.268484	0.484583

$[W_2O_7]^{2-}$-INT'

12

O	0.180214	-0.622464	0.259394
W	-1.814729	0.011194	0.015732
O	-2.307807	0.141768	1.678613
W	1.925568	-0.028673	-0.000694
O	2.653716	-0.846301	-1.384939
O	2.919032	-0.293161	1.433143
O	1.791450	1.716481	-0.325671
O	-1.903853	-1.901460	-0.402509
O	-0.976444	1.688956	-0.414791
O	-3.250641	0.340981	-0.917941
H	0.001737	1.795162	-0.334356
H	-1.049130	-2.300143	-0.18082

$[W_2O_7]^{2-}$-TS2

12

O	-0.185900	-0.591167	0.041343
W	1.830250	-0.057506	-0.056281
O	2.048290	-1.780935	-0.313590
W	-1.960586	-0.031677	-0.000627
O	-2.807241	-0.574438	1.451455
O	-2.782140	-0.644828	-1.440086
O	-1.903481	1.743398	-0.052092
O	2.385913	0.048513	1.772709
O	0.965223	1.717426	-0.190527
O	3.170325	0.559511	-0.989974
H	-0.003128	1.819636	-0.096426
H	2.520054	0.960086	2.073713

$[W_2O_7]^{2-}$-INT

12

O	0.157915	-0.644264	0.052060

W	-1.760402	-0.104011	0.010569
O	-2.206015	-1.347564	-1.139599
W	1.932445	-0.017996	-0.011301
O	2.675247	-0.397537	-1.563964
O	2.874299	-0.727349	1.297919
O	1.856667	1.739728	0.188266
O	-3.349645	0.964951	-0.412430
O	-1.014698	1.732534	-0.014408
O	-2.180340	-0.658136	1.608081
H	-0.048724	1.842416	0.093189
H	-3.189852	1.887218	-0.166456

$[W_2O_7]^{2-}$-TS3

12

O	0.101004	-0.615987	0.390474
W	-1.750314	-0.134467	0.020043
O	-2.252557	-1.607672	-0.772731
W	1.877655	-0.044294	-0.002253
O	2.535166	-1.018765	-1.309456
O	2.902682	-0.213659	1.415584
O	1.857726	1.648654	-0.507440
O	-2.610323	1.120831	-1.070450
O	-0.921067	1.987891	0.222164
O	-2.557547	-0.146104	1.563511
H	-0.020039	2.084319	-0.137245
H	-1.843869	1.902489	-0.632438

$[W_2O_7]^{2-}$-TS1'-2Na

14

O	0.221703	-1.053263	-0.188248
W	-1.626131	0.032551	0.212675
O	-2.416166	-1.054125	-0.947719

W	1.936615	-0.472819	-0.078077
O	2.968764	-1.289290	-1.225586
O	2.570102	-0.705035	1.535716
O	1.778644	1.363413	-0.479853
O	-3.322385	1.058776	0.287437
O	-0.641824	1.515321	-0.167581
O	-1.584441	-0.523780	1.873460
H	0.715377	1.566677	-0.366339
H	-3.289497	1.881269	0.792516
Na	-4.528330	-0.119965	-1.258031
Na	2.983156	3.268665	-0.186279

$[W_2O_7]^{2-}$-INT-2Na

14

O	0.151227	-0.883881	0.002090
W	-1.578140	0.028367	0.194335
O	-2.573544	-1.408383	-0.030860
W	1.990707	-0.450555	-0.074413
O	2.827196	-1.570635	-1.132415
O	2.688215	-0.526879	1.531519
O	2.086001	1.212518	-0.721622
O	-3.182827	1.086585	-0.342365
O	-0.787126	1.450977	-0.927145
O	-1.520210	0.407328	1.887461
H	0.189365	1.455760	-0.980171
H	-2.927654	1.952923	-0.686662
Na	-4.620798	-0.611319	-0.864219
Na	2.320514	3.310610	0.015065

$[W_2O_7]^{2-}$-TS3-2Na

14

O	0.224350	-0.798331	-0.465318

W	-1.474671	-0.135122	0.118520
O	-2.363911	-1.546708	0.624672
W	2.055198	-0.267554	-0.080962
O	3.158983	-0.873991	-1.300005
O	2.537789	-0.914581	1.474177
O	2.189790	1.495894	-0.023855
O	-2.852204	0.638466	-0.906837
O	-0.884325	1.842226	-1.113359
O	-1.235351	0.833957	1.547364
H	-0.368678	1.652363	-1.909066
H	-2.099679	1.455003	-1.246268
Na	-4.595752	-0.819934	-0.441981
Na	0.351062	2.754044	0.594830

$[W_3O_{10}]^{2-}$-TS1

15

W	3.026523	-0.584110	0.038119
W	-0.071267	1.332632	-0.000910
W	-3.157300	-0.676009	-0.000110
O	3.157435	-1.036900	1.743507
O	-3.810551	-0.650230	1.632348
O	0.312343	1.830282	-1.633578
O	1.433161	0.949276	0.884768
O	-1.316112	-0.113883	-0.001670
O	-3.245383	-2.320223	-0.616861
O	-0.801342	2.706780	0.793278
O	-4.147942	0.363312	-1.014157
O	4.341012	-1.812043	-0.733594
O	1.573062	-1.126652	-0.833645
O	3.856749	0.882128	-0.493417
H	4.131765	-2.740766	-0.561184

$[W_3O_{10}]^{2-}$-INT

15

W	2.956009	-0.488388	0.018158
W	0.210426	1.030770	-0.014130
W	-3.266647	-0.457186	0.001400
O	4.068245	-0.501675	1.374000
O	-3.487059	-0.730473	1.730310
O	0.141224	2.145829	-1.359853
O	2.146528	1.242362	0.351175
O	-1.518484	0.138903	-0.375458
O	-3.570857	-1.970155	-0.854119
O	-0.302720	1.842064	1.454312
O	-4.436214	0.746367	-0.540538
O	2.813508	-2.451003	-0.078129
O	0.962615	-0.750610	-0.272871
O	3.871342	-0.165901	-1.435157
H	1.910724	-2.670235	-0.350986

$[W_3O_{10}]^{2-}$-TS1'

15

W	-2.024871	-0.505762	-0.002963
W	0.538498	1.969696	-0.007368
W	1.556477	-1.377343	-0.013444
O	-2.118846	-0.409571	-1.747063
O	0.249998	-2.492857	-0.532989
O	0.679951	2.416056	1.689648
O	-1.162031	2.076648	-0.536994
O	1.682739	0.486887	-0.557024
O	1.895580	-1.621519	1.691277
O	1.351900	3.264820	-0.872674
O	2.985581	-1.987854	-0.829148
O	-2.237150	-2.349193	0.398632

O	-0.413561	-0.114912	0.749325
O	-3.391598	0.272212	0.755651
H	-1.368197	-2.733476	0.090251

$[W_3O_{10}]^{2-}$-TS2

19

W	-2.753975	0.045256	0.043890
W	0.243635	-1.287065	-0.129210
W	3.164150	0.745493	0.042721
O	-4.009064	-0.988796	0.700278
O	3.463544	1.372519	1.655106
O	1.036167	-2.443079	-1.141449
O	-1.541728	-1.297549	-0.731537
O	1.271667	0.285761	-0.196849
O	3.620000	1.971648	-1.125461
O	0.316561	-1.954310	1.466414
O	4.173482	-0.667880	-0.197928
O	-3.942880	1.777316	1.107490
O	-1.498597	0.633565	1.159301
O	-3.194691	0.989112	-1.399468
H	-3.355736	2.043702	1.830878
H	-3.968662	2.551752	0.473044
O	-3.800740	3.531456	-0.869687
H	-4.674562	3.750044	-1.221616
H	-3.532742	2.703821	-1.339687

$[W_3O_{10}]^{2-}$-INT'

15

O	-0.010065	-0.274674	-0.205525
W	1.986896	-0.837320	0.008757
W	0.038613	1.789720	-0.013775
W	-2.023329	-0.812016	0.010631

O	3.459844	-1.001328	-0.921559
O	-1.366410	-2.482707	0.073781
O	0.048994	2.748593	-1.479850
O	1.890491	1.107749	-0.029472
O	-1.761117	1.272583	0.149535
O	-2.963674	-0.787967	-1.475625
O	0.203282	2.882567	1.353007
O	-3.149995	-0.801287	1.366105
O	2.389382	-1.128725	1.681802
O	1.210744	-2.512263	-0.522277
H	0.226954	-2.568793	-0.334743

$[W_3O_{10}]^{2-}$-TS2'

19

W	1.590822	-0.426924	-0.414809
W	-1.381046	-1.378009	0.196589
W	-0.906954	1.695505	0.019022
O	2.308351	-0.483156	-2.007064
O	0.623624	1.407294	-1.019499
O	-1.643381	-2.395926	1.581311
O	0.295679	-1.851494	-0.713960
O	-2.273265	0.333791	0.439998
O	-0.570657	2.771509	1.349955
O	-2.420331	-1.997052	-1.069774
O	-1.887021	2.627425	-1.096505
O	2.707373	1.276064	0.435862
O	0.066885	-0.035711	0.882561
O	2.738863	-1.276157	0.612669
H	2.553700	2.180967	0.139401
H	3.516281	1.134351	1.010632
O	4.557594	0.262054	1.916446
H	5.422769	0.207921	1.487192

H	4.068653	-0.534692	1.607391

Chain route-$[W_4O_{13}]^{2-}$-TS1

19

O	-0.034035	0.372157	-0.016665
W	-0.169017	2.185797	-0.301411
W	0.056422	-1.589852	-0.659198
W	3.292949	-0.304169	0.481222
W	-3.240690	-0.421418	0.493017
O	-0.335627	3.083883	1.184067
O	0.254868	-3.222837	-0.082668
O	-2.749160	1.274895	0.562499
O	1.496544	2.657554	-1.022994
O	1.969946	-1.176850	-0.550922
O	-1.824012	-1.499820	-0.165833
O	-4.630105	-0.581017	-0.572515
O	4.785721	-1.214221	0.347016
O	2.831895	-0.245673	2.171874
O	-3.691670	-0.960055	2.105156
O	-1.271202	2.764331	-1.518349
O	-0.092369	-1.693134	-2.380159
O	3.557101	1.360860	-0.109653
H	2.321721	2.232906	-0.615400

Chain route-$[W_4O_{13}]^{2-}$-INT

19

O	-0.610953	0.028873	-0.185019
W	-1.198150	2.011983	-0.436895
W	0.442442	-1.745919	-0.777595
W	3.017862	0.408146	0.508652
W	-2.301739	-0.813285	0.728471
O	-0.908927	3.142390	0.851705

O	1.296213	-3.230473	-0.439548
O	-2.696453	1.032185	0.446391
O	0.442741	2.184125	-1.412613
O	2.003504	-0.595930	-0.749359
O	-1.151939	-2.292235	0.164303
O	-3.824165	-1.520057	0.234207
O	4.725546	0.090582	0.248527
O	2.619653	0.038672	2.178210
O	-2.199222	-0.933036	2.463690
O	-2.204542	2.792754	-1.624640
O	0.042194	-1.837945	-2.461041
O	2.672892	2.119103	0.186515
H	1.276957	2.139510	-0.885465

Chain route-$[W_4O_{13}]^{2-}$-TS2

23

O	0.629995	0.005989	0.198909
W	0.960874	1.969611	-0.019311
W	-0.287693	-1.946857	0.787302
W	-3.043477	0.097286	-0.556120
W	2.479310	-0.744637	-0.540223
O	0.184665	2.649862	-1.403355
O	-0.893597	-3.549628	0.517479
O	2.546514	1.211060	-0.744784
O	-0.716101	2.092558	1.286850
O	-1.946076	-1.005060	0.533370
O	1.458849	-2.283795	0.040839
O	3.921249	-0.978704	0.397894
O	-4.701337	-0.460807	-0.518039
O	-2.495772	0.114243	-2.218104
O	2.866932	-1.216187	-2.166009
O	1.632510	3.302930	0.896908

O	-0.036761	-1.865990	2.495258
O	-2.949650	1.747430	0.124825
H	-1.634309	1.989336	0.835116
H	-0.692590	2.938606	1.832152
O	-0.281246	4.335718	2.559842
H	0.592845	4.325813	2.120848
H	-0.094414	4.169460	3.494799

Cage route-$[W_4O_{13}]^{2-}$-TS1

19

O	0.917195	-0.033306	0.823267
W	2.956590	-0.198760	0.509926
W	0.228130	-1.510355	-0.483402
W	0.622880	1.691173	-0.347214
O	3.565831	-0.500868	2.107620
O	2.482345	1.693586	0.278659
O	-0.527257	-2.518107	0.709417
O	2.135702	-1.822081	-0.256969
O	-0.330580	0.282622	-1.218596
O	-0.485830	2.560598	0.695227
O	0.084373	-2.374154	-1.996657
O	0.879148	2.716485	-1.741499
O	4.344026	-0.194097	-0.556435
O	-2.692094	-1.156100	-0.660512
W	-3.618376	-0.004252	0.309622
O	-5.324717	-0.169812	-0.072305
O	-3.152699	1.823203	-0.047966
O	-3.362517	-0.368873	2.009063
H	-2.265974	2.129621	0.240459

Cage route-$[W_4O_{13}]^{2-}$-INT

19

O	0.059668	0.479697	0.027457
W	1.601381	1.640538	-0.482131
W	-1.360560	1.785517	0.481144
W	2.347251	-1.785613	0.272663
O	1.874348	2.121044	-2.136030
O	2.504646	-0.121108	-0.598074
O	-2.598245	2.614122	-0.440359
O	0.138205	2.885466	-0.057587
O	2.074537	-1.556555	1.986006
O	1.019117	-2.787458	-0.401950
O	-1.510993	2.235445	2.157043
O	3.858381	-2.647905	0.059079
O	2.811389	2.397680	0.529495
O	-2.445599	0.069041	0.618955
W	-2.574216	-1.540216	-0.281825
O	-4.170484	-2.186735	-0.024251
O	-1.353650	-2.787727	0.358270
O	-2.344772	-1.292684	-1.987912
H	-0.357743	-2.795316	0.029889

Cage route-$[W_4O_{13}]^{2-}$-TS2

23

O	0.714508	0.035018	-0.089942
W	-0.315119	-1.874541	0.588265
W	2.660551	-0.796758	-0.383178
W	-3.342770	0.053133	-0.442992
O	-0.853950	-3.522437	0.643550
O	-1.854846	-1.132654	-0.269165
O	3.163107	-1.230422	-1.985284
O	1.490345	-2.284664	0.062228
O	-2.745364	1.693932	-0.816238
O	-4.430799	-0.452698	-1.714208

O	3.977423	-1.186009	0.681104
O	-4.229931	0.122848	1.062636
O	-0.317586	-1.389622	2.247209
O	2.881227	1.148516	-0.421418
W	1.190040	1.954019	-0.037914
O	1.641074	3.065012	1.229360
O	-0.784173	2.161166	0.733040
O	0.866543	2.852868	-1.481475
H	-1.588723	2.067983	0.109858
H	-0.813135	3.029123	1.247629
O	-0.861835	4.414520	2.053777
H	-1.198287	5.116310	1.477838
H	0.094294	4.570497	2.093914

$[W_5O_{16}]^{2-}$-TS1

23

O	-0.904549	1.950270	-1.607604
O	1.297170	-0.442524	2.836636
W	-0.048274	-0.890463	1.834207
W	-3.006529	-0.596899	-0.753558
W	-0.925278	2.025703	0.143228
W	1.683473	-1.823261	-0.772589
W	2.318426	1.299775	-0.371046
O	-2.909132	1.073967	-0.085177
O	-0.972001	0.782349	1.658781
O	-1.951849	-1.572344	0.259766
O	2.844337	-0.352088	-1.282485
O	2.779289	2.380313	-1.662132
O	0.713519	-2.206683	-2.164634
O	-1.076737	-1.756511	2.942481
O	-4.634281	-1.201590	-0.675139
O	-1.655624	3.524901	0.607116

O	2.930414	-3.047302	-0.682524
O	3.546577	1.432813	0.847635
O	0.703307	-2.365874	0.803996
O	-2.433645	-0.659774	-2.567337
O	0.913918	2.434064	0.412457
O	0.795497	-0.059699	-0.045062
H	-1.504186	-0.413539	-2.712075

$[W_5O_{16}]^{2-}$-INT

23

O	-0.498170	2.202630	-1.741640
O	1.337427	-0.292601	2.807388
W	-0.123020	-0.670495	1.944575
W	-2.921959	-0.475191	-0.744736
W	-0.660898	2.151274	-0.000422
W	1.324863	-2.009027	-0.683864
W	2.392543	1.030709	-0.443487
O	-2.545048	1.266828	-0.383281
O	-0.896763	1.030728	1.659549
O	-2.187795	-1.364046	0.570893
O	2.693384	-0.771911	-1.203092
O	2.842990	1.919416	-1.869331
O	0.200947	-2.245426	-2.015285
O	-1.137603	-1.354587	3.184406
O	-4.639220	-0.735590	-0.726758
O	-1.259341	3.702930	0.476378
O	2.313529	-3.446871	-0.658780
O	3.750721	1.132423	0.635693
O	0.410315	-2.300393	0.971553
O	-2.194748	-1.097493	-2.370086
O	1.213136	2.351363	0.373775
O	0.649892	-0.061942	-0.088790

H	-1.282309	-1.501646	-2.313585

$[W_5O_{16}]^{2-}$-TS2

27

O	2.904181	-0.113339	-1.827993
O	-0.601786	-1.931659	1.133486
W	-0.197965	-0.373186	1.952722
W	0.632650	2.054327	0.020423
W	2.511983	-0.502645	-0.180864
W	-2.786487	0.277264	-0.250500
W	-0.286349	-2.040408	-1.072908
O	2.370934	1.591484	0.162348
O	1.615659	-0.451291	1.801854
O	-0.031949	1.712494	1.685500
O	-2.140234	-1.258554	-1.068633
O	0.019759	-1.661619	-2.736743
O	-2.117134	1.732317	-1.007912
O	-0.489966	-0.591316	3.639491
O	0.622806	3.797537	-0.035636
O	4.027417	-0.984867	0.497138
O	-4.519712	0.378064	-0.227610
O	-0.677710	-3.722883	-1.101720
O	-2.151574	0.222683	1.453513
O	0.216689	2.158728	-2.088697
O	1.573186	-2.127427	-0.469506
O	0.217994	0.131661	-0.366092
H	-0.714538	1.838466	-2.144899
H	0.240918	3.123128	-2.425626
O	0.385645	4.664695	-2.634182
H	-0.447636	5.069808	-2.914600
H	0.464008	4.858944	-1.680332

$[W_6O_{19}]^{2-}$-TS1

27

W	0.961402	2.233126	-0.762329
W	-0.006894	-0.657484	-2.117168
W	2.659203	-0.702556	-0.185709
W	0.703811	0.811454	2.168618
W	-0.171449	-2.101934	0.797967
W	-3.967006	0.264416	0.023744
O	2.811016	0.912227	-0.958683
O	0.404184	1.145852	-2.347073
O	-3.178205	0.093143	-1.548258
O	-5.698295	0.440348	-0.222245
O	1.469494	2.209907	1.096962
O	-0.912038	1.466248	2.275689
O	1.377898	1.098168	3.733248
O	2.601867	-0.258997	1.561534
O	1.647373	-1.349331	-2.024493
O	0.052025	-1.087377	2.336657
O	-0.935258	-1.879732	-0.942075
O	1.527931	-2.478951	0.360228
O	-0.820188	-3.596236	1.346398
O	4.171304	-1.506720	-0.445837
O	1.876984	3.534718	-1.437564
O	-0.619851	2.910071	-0.549845
O	0.503968	0.012142	0.002909
O	-0.620947	-1.125653	-3.654187
O	-3.358617	1.822339	0.948014
O	-3.650034	-1.170786	0.994158
H	-2.455917	1.789308	1.336629

$[W_6O_{19}]^{2-}$-INT

27

W	0.874971	-0.258761	2.252645
W	2.288866	-0.816942	-0.779031
W	-0.663957	-2.157207	-0.038083
W	-3.080482	0.502878	0.403952
W	-0.486718	0.388314	-2.121712
W	1.093440	2.255386	0.142924
O	-0.067846	-1.935084	1.736520
O	2.448008	-1.123289	1.013115
O	2.666201	0.950631	-0.781090
O	2.159103	3.610452	-0.047337
O	-0.584872	0.494182	2.909915
O	-2.798666	1.448604	1.986781
O	-4.782340	0.478849	0.110392
O	-2.488347	-1.169362	0.639342
O	0.980323	-2.478658	-0.759006
O	-2.214191	1.088348	-1.075174
O	1.120662	-0.443404	-2.461840
O	-1.282294	-1.319025	-1.657942
O	-1.115007	0.677192	-3.700235
O	-1.398017	-3.716019	-0.050496
O	1.736785	-0.740786	3.674356
O	1.731371	1.390383	1.753145
O	0.271378	0.014829	0.027563
O	3.654016	-1.592493	-1.518185
O	-0.330960	2.967004	0.842737
O	0.290618	2.042364	-1.655440
H	-1.900198	1.230829	2.411582

$[W_6O_{19}]^{2-}$-TS2

31

W	-0.555958	2.374085	-0.263528
W	-2.527962	-0.383871	-0.579269

W	0.355632	-0.236244	-2.178427
W	3.045381	-0.283022	0.327770
W	0.004342	-2.291583	0.350938
W	-0.813381	0.296866	2.276889
O	0.170444	1.628550	-1.951732
O	-2.359957	1.401806	-0.921328
O	-2.671695	-0.296395	1.222883
O	-1.634627	0.346421	3.798440
O	1.057040	2.802715	0.350721
O	3.075173	1.523708	1.246360
O	4.669991	-0.808233	0.165614
O	2.445088	0.048358	-1.305062
O	-1.409753	-0.619152	-2.375300
O	2.047988	-1.659387	0.877109
O	-1.705829	-2.280501	-0.310827
O	0.747924	-1.955794	-1.398611
O	0.329418	-3.959944	0.613312
O	0.991032	-0.374976	-3.771490
O	-1.202874	3.908561	-0.710739
O	-1.274322	2.001837	1.471114
O	-0.305762	-0.013174	0.011036
O	-4.097174	-0.820214	-1.161851
O	0.838695	0.714324	2.667393
O	-0.434475	-1.641852	2.059248
H	2.134251	1.891164	1.304133
H	3.547182	2.316612	0.698890
O	3.706456	3.500099	-0.072783
H	4.111482	3.338999	-0.938342
H	2.748863	3.638134	-0.236335

$[HW_2O_7]^-$-TS2

16

O	0.316399	-0.738332	-0.087004
W	-1.611722	-0.384986	0.055019
O	-1.981533	-1.109606	1.572866
W	2.041543	0.062881	-0.027675
O	2.927249	-0.148229	-1.529502
O	2.994557	-0.570019	1.303919
O	1.704344	1.784966	0.246311
O	-1.798989	-1.786153	-1.248733
O	-0.992821	1.469133	0.503122
O	-3.140726	0.434444	-0.432196
H	-0.025382	1.686185	0.472771
H	-1.011720	-2.334582	-1.376900
O	-2.888171	2.793655	-0.280621
H	-1.952855	2.463695	0.100179
H	-2.731286	3.256026	-1.119054
H	-3.207963	1.725607	-0.485749

$[HW_2O_7]^-$-TS2'

16

O	-0.206119	-0.527108	-0.497198
W	1.631617	-0.377930	-0.056290
O	2.382377	0.773138	-1.228832
W	-2.007887	-0.021946	-0.012551
O	-2.956017	-1.397153	0.524550
O	-2.817209	0.740775	-1.365770
O	-1.854465	1.138406	1.307591
O	2.135906	-1.929606	-0.631914
O	1.003784	1.238297	1.151652
O	2.809298	-0.493247	1.457713
H	0.045865	1.317707	1.335528
O	2.014184	2.976431	-0.337712
H	1.508720	2.465689	0.414893

H	2.253392	1.915464	-0.930289
H	1.361036	3.498180	-0.827978
H	2.581032	0.234332	2.061431

$[HW_3O_{10}]^-$-TS1

16

O	-0.596766	0.121068	0.283788
W	-2.212462	-0.669375	0.009061
W	0.417454	2.039051	-0.027164
W	1.831380	-1.292783	0.002040
O	-3.417259	-0.138829	1.146613
O	0.529566	-2.505606	-0.782655
O	0.987051	2.453274	1.578166
O	-1.211197	2.703445	-0.134969
O	1.802877	0.452881	-0.495880
O	1.675749	-1.399132	1.727482
O	1.318310	3.051989	-1.147611
O	3.411846	-1.881685	-0.403008
O	-2.780670	-0.286471	-1.592447
O	-2.012632	-2.549593	0.187881
H	-1.150774	-2.827336	-0.203613
H	0.804215	-3.033510	-1.546572

$[HW_3O_{10}]^-$-INT

16

O	-0.020604	-0.308914	0.195862
W	2.045672	-0.773140	-0.005403
W	-0.017507	1.762666	0.002571
W	-2.016414	-0.774279	-0.012871
O	3.421505	-0.897773	-1.066555
O	-1.303577	-2.595445	0.349221
O	-0.062172	2.860077	-1.355221
O	1.822103	1.167661	-0.144839

O	-1.874601	1.169057	-0.014976
O	-2.555825	-1.076044	-1.632430
O	0.026019	2.722707	1.453900
O	-3.388598	-0.895316	1.052411
O	2.647971	-0.975792	1.611787
O	1.295056	-2.481316	-0.444662
H	0.355170	-2.601617	-0.159686
H	-1.282924	-2.837847	1.285760

$[HW_3O_{10}]^-$-TS2

20

O	-0.063439	-0.258640	-0.021032
W	1.914343	-1.234093	0.048593
W	0.574614	1.775544	-0.172358
W	-1.985944	0.021742	0.245341
O	3.433377	-1.713209	-0.634334
O	-1.889487	-2.219054	0.087699
O	0.674234	2.400238	-1.782868
O	2.169642	0.694470	-0.070115
O	-1.395584	1.811935	0.119528
O	-3.308029	-0.068621	-0.883701
O	1.020897	3.070104	0.895149
O	-2.628438	-0.114127	1.847684
O	2.019091	-1.608255	1.735694
O	0.868623	-2.639528	-0.726331
H	-0.091229	-2.561601	-0.566603
H	-1.898535	-2.658863	0.952385
H	-2.688496	-2.570173	-0.450999
O	-3.910527	-2.963052	-1.302385
H	-3.796511	-2.507781	-2.150556
H	-4.671029	-2.515981	-0.900845

$[HW_4O_{13}]^-$-TS2

20

O	0.512699	-0.094823	-0.564649
W	0.518748	1.997429	0.018359
W	0.465161	-1.809436	0.072307
W	-3.873386	-0.134869	-0.034069
W	3.217280	-0.218861	-0.028814
O	0.855686	3.631449	-0.440443
O	0.001119	-2.947471	-1.150410
O	2.418689	1.445110	0.281022
O	-1.155446	1.833848	-0.906964
O	-2.387746	-0.685904	-0.839477
O	2.355623	-1.891033	0.423678
O	4.748462	-0.173206	0.767501
O	-4.553766	-1.368474	1.008375
O	-5.047717	0.301984	-1.262082
O	3.568750	-0.297076	-1.718108
O	0.020153	2.078519	1.667733
O	-0.463757	-2.053358	1.518379
O	-3.383290	1.397114	1.017707
H	-1.461867	0.904830	-1.046302
H	-2.711289	1.946307	0.572315

$[HW_4O_{13}]^-$-INT

20

O	0.732728	-0.024498	-0.197165
W	0.947731	2.122905	-0.030180
W	-0.208137	-1.834743	-0.083762
W	-3.334513	0.171696	0.048668
W	2.741054	-0.598751	0.054460
O	1.431640	3.692282	-0.596312
O	-0.624809	-3.093481	-1.208372

O	2.694689	1.348799	0.200750
O	-0.634036	2.000415	-1.185190
O	-1.804288	-0.671020	-0.560319
O	1.680717	-2.231486	0.085143
O	3.798463	-0.917095	1.399781
O	-3.924340	-0.461095	1.547642
O	-4.606900	-0.013970	-1.118326
O	3.679963	-0.814953	-1.388898
O	0.331529	2.391202	1.564175
O	-0.769993	-2.350126	1.468772
O	-2.959768	2.009071	0.292268
H	-0.827295	1.064307	-1.369909
H	-2.191366	2.301396	-0.261374

$[HW_4O_{13}]^-$-TS2

24

O	-0.193222	0.236460	0.831557
W	-0.571493	1.835871	-0.042309
W	0.106867	-1.807974	0.622925
W	3.223526	-0.271210	-0.411970
W	-3.083777	-0.460647	-0.394593
O	-1.281095	3.247829	0.707971
O	0.007776	-2.472733	2.207236
O	-2.145616	1.101449	-0.902167
O	1.242898	2.395612	1.160329
O	1.978446	-1.255398	0.593418
O	-1.844095	-1.715337	0.158998
O	-3.996035	-1.110010	-1.717576
O	4.321803	-1.387854	-1.140450
O	4.169822	0.579621	0.758034
O	-4.194158	-0.161833	0.903014
O	0.398274	2.276346	-1.427096

O	0.336510	-3.163800	-0.434351
O	2.804675	0.949410	-1.797063
H	1.342789	1.829533	1.939488
H	1.194579	3.362626	1.450786
O	0.717458	4.883619	1.678785
H	-0.189587	4.685209	1.371265
H	1.093701	5.458136	0.996418
H	2.011953	1.530468	-1.682953

$[HW_5O_{16}]^-$-TS1

24

W	-2.930961	-0.952194	-0.262943
W	-0.628081	-0.010624	1.980085
W	0.453178	-2.111697	-1.045431
W	3.337198	-0.241433	0.093380
W	-0.404891	3.141529	-0.777771
O	2.298811	-1.660437	-0.582541
O	-0.838863	-0.790677	3.508168
O	0.155664	-1.238641	0.930130
O	-1.475066	-1.680009	-1.161257
O	0.685984	-2.124943	-2.757317
O	0.410856	-3.775962	-0.625582
O	-3.928711	-0.153086	-1.428372
O	-2.338293	0.208441	1.127764
O	3.013585	0.178717	1.897819
O	0.534322	1.307161	2.195638
O	5.014034	-0.651114	0.001734
O	3.101662	1.157419	-0.893029
O	0.730799	3.645928	0.685665
O	-2.034330	3.746956	-0.518318
O	0.232744	3.825830	-2.262722
O	-0.443684	1.377446	-0.870909

H	0.749787	2.945228	1.373222
H	2.198194	0.705329	2.102164
O	-3.882623	-2.215978	0.435984

$[HW_5O_{16}]^-$-INT

24

W	2.524206	0.316163	-0.710578
W	1.268992	-1.267642	1.681282
W	-0.238764	2.254684	0.056131
W	-2.636554	0.040637	0.587459
W	-0.838916	-1.289659	-1.653207
O	-1.791478	1.646189	1.128359
O	2.022944	-1.210474	3.247622
O	0.729405	0.387097	1.231986
O	1.280495	1.741856	-1.022388
O	-0.985243	3.399783	-1.000285
O	0.496150	3.249203	1.269684
O	3.478015	0.152600	-2.139778
O	2.535768	-1.411381	0.276681
O	-2.474142	-0.932613	2.191043
O	-0.120836	-2.374316	1.692079
O	-4.286300	0.508687	0.489457
O	-2.541201	-1.450812	-0.537685
O	-0.602032	-3.121709	-1.181886
O	0.879063	-0.794838	-1.721256
O	-1.381974	-1.333963	-3.281483
O	-1.279483	0.498621	-0.912526
H	-0.509881	-3.252276	-0.216193
H	-1.698274	-1.551649	2.194563
O	3.586458	1.145380	0.383020

$[HW_5O_{16}]^-$-TS2

28

W	-2.743357	0.217322	0.273372
W	-0.937000	-1.814889	-1.298522
W	-0.065335	2.171507	-0.706081
W	2.587886	0.276327	-0.111750
W	0.547820	-0.599237	2.140287
O	1.701702	1.426282	-1.292840
O	-1.444131	-2.375375	-2.856201
O	-0.703402	-0.034700	-1.360684
O	-1.684138	1.825827	0.266935
O	0.436914	3.640537	0.044427
O	-0.626835	2.692180	-2.254835
O	-3.877577	0.370495	1.562602
O	-2.407252	-1.698964	-0.093745
O	2.849017	-1.281033	-1.361429
O	0.617439	-2.569358	-0.853130
O	4.026317	1.124109	0.248693
O	2.418241	-0.873088	1.332350
O	0.546621	-2.495770	2.238515
O	-1.174841	-0.281592	1.829948
O	0.836313	-0.093082	3.751912
O	1.001669	0.941021	0.938288
H	0.644778	-2.929750	1.368488
H	2.085410	-1.945972	-1.284481
O	-3.706398	0.531115	-1.131103
H	3.667899	-1.555769	-1.995738
O	4.716473	-1.931701	-2.813233
H	5.470234	-2.279381	-2.312828
H	5.061618	-1.200573	-3.347888

$[HW_6O_{19}]^-$-TS1

28

W	0.266509	1.750457	-0.263934
W	-0.076909	-0.359574	2.046572
W	-2.979668	1.595631	-0.298554
W	-2.681890	-1.626742	0.282656
W	-0.277690	-1.261127	-1.684885
O	-3.724989	-0.070205	0.428785
O	-0.006373	0.051871	3.711208
O	-1.189192	1.025688	0.997290
O	-1.342901	2.468667	-0.938569
O	-3.929516	1.785260	-1.728320
O	-3.628964	2.752184	0.801462
O	1.264415	3.137521	-0.409981
O	1.173331	0.878664	1.163973
O	-1.780243	-1.446185	1.877080
O	0.969027	-1.739515	1.807655
O	-3.846172	-2.861412	0.520049
O	-1.309980	-2.580895	-0.679068
O	1.269586	-2.120877	-1.039666
O	0.559024	0.511995	-1.652646
O	-0.364528	-1.709175	-3.325664
O	-1.940627	-0.368186	-1.269190
H	1.372519	-2.172704	-0.058721
O	4.290235	1.050332	-1.057199
W	5.300032	0.004847	-0.065166
O	4.784415	0.135592	1.611398
O	5.224112	-1.828605	-0.671689
O	6.973423	0.520719	-0.203765
H	4.346405	-2.233215	-0.721444

$[HW_6O_{19}]^-$-INT

28

W	1.126786	-0.721374	1.379846

W	-0.809335	-2.164737	-0.873569
W	-2.153697	-0.108692	1.558182
W	-2.385060	0.650755	-1.606673
W	-0.114717	2.174824	0.217012
O	-3.303305	0.625461	-0.047473
O	-1.483307	-3.756458	-0.913204
O	-0.662551	-0.056316	-0.192327
O	-0.519009	-0.399380	2.442995
O	-3.313823	0.051342	2.822903
O	-2.352276	-1.744974	0.880063
O	2.063920	-1.146393	2.745200
O	0.376233	-2.296115	0.714062
O	-2.158204	-1.171853	-1.951426
O	0.429325	-2.199264	-2.075608
O	-3.524022	1.158422	-2.784464
O	-1.313325	2.190235	-1.340182
O	1.268302	1.967225	-1.418486
O	1.195383	1.245048	1.196179
O	0.232448	3.829856	0.492279
O	-1.480511	1.868501	1.391815
H	0.995066	2.283110	-2.290505
O	2.491898	-0.770272	0.049065
W	4.104667	0.064400	-0.583003
O	4.694623	-0.791796	-1.986229
O	3.712164	1.749419	-1.038124
O	5.373310	0.088720	0.614321
H	2.307119	1.942532	-1.313090

$[HW_6O_{19}]^-$-TS2

28

W	-0.619536	-0.146298	-2.017139
W	-0.026512	-2.345423	0.282731

W	2.473119	-0.261496	-0.847970
W	0.490091	2.399151	-0.069548
W	1.259214	0.052708	2.133810
W	-3.364364	0.088491	0.453224
O	1.359253	-0.050439	-2.339406
O	-0.357409	-1.974581	-1.616268
O	-1.694553	-2.273101	0.755417
O	-4.586398	-1.128305	0.755069
O	-0.458149	1.803529	-1.557738
O	-1.593213	3.172485	0.678078
O	0.720259	4.092006	-0.179986
O	2.122233	1.806223	-0.581098
O	2.157706	-1.982064	-0.495440
O	0.664704	1.850150	1.765422
O	0.739494	-1.744456	2.019210
O	2.816371	0.037669	1.209964
O	1.748934	0.193349	3.772442
O	4.079127	-0.176310	-1.468047
O	-1.061568	-0.127957	-3.671968
O	-2.289312	-0.171302	-1.178686
O	0.384895	-0.138223	0.084086
O	0.358484	-4.029352	0.297065
O	-4.170535	1.617241	0.153724
O	-2.427487	0.392347	1.905453
H	-1.492260	3.835869	1.376528
H	-2.299308	2.565046	0.967130

The complete reference 19.

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