Supporting Information for:

Assessment of the Accuracy of Density Functionals for the Prediction of the Relative Energies of Low-Lying Isomers Water Hexamers

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Table S1. Cartesian Coordinates (Å) for MP2/aug´-cc-pVTZ Optimized Geometries

bag

O	-1.021998	1.608318	-0.456678
O	-0.094094	-1.928019	0.493961
O	1.621813	1.696837	-0.207570
O	2.340853	-0.867718	0.060479
O	-1.335648	0.181853	1.956564
O	-1.331460	-0.850965	-1.805075
H	1.486938	-1.336848	0.231505
H	1.950152	0.765154	-0.162978
H	-0.034787	1.695742	-0.376042
H	-0.530521	-1.352198	1.145180
H	-0.582961	-1.741144	-0.326943
H	-1.328990	0.062498	-1.465517
H	-1.401914	0.792714	1.201738
H	-1.326789	2.461744	-0.778163
H	-2.217520	-0.997128	-2.146353
H	-2.199557	0.194882	2.376682
H	1.966189	2.111332	0.588698
H	2.784035	-1.379201	-0.621253

boat

O	0.117613	1.552002	0.864931
H	0.963251	1.520430	0.354199
H	0.279396	2.151449	1.599045
O	-0.026563	-1.369287	0.919209
H	-0.047968	-0.420972	1.118927
H	-0.875920	-1.529241	0.463859
O	-2.331117	1.360418	-0.433665
H	-1.466018	1.543880	-0.018808
H	-2.343909	1.884708	-1.238766
O	-2.472465	-1.406461	-0.434029
H	-2.546787	-0.433786	-0.500267
H	-3.280214	-1.690609	0.002142
O	2.419101	1.204125	-0.466685
H	2.492309	0.220567	-0.499730
H	2.557399	1.499342	-1.370620
O	2.286417	-1.480732	-0.445130
H	1.425830	-1.570951	0.031306
H	2.898736	-2.055343	0.021662

book

O	0.117613	1.552002	0.864931
H	0.963251	1.520430	0.354199
H	0.279396	2.151449	1.599045

O	-0.026563	-1.369287	0.919209
H	-0.047968	-0.420972	1.118927
H	-0.875920	-1.529241	0.463859
O	-2.331117	1.360418	-0.433665
H	-1.466018	1.543880	-0.018808
H	-2.343909	1.884708	-1.238766
O	-2.472465	-1.406461	-0.434029
H	-2.546787	-0.433786	-0.500267
H	-3.280214	-1.690609	0.002142
O	2.419101	1.204125	-0.466685
H	2.492309	0.220567	-0.499730
H	2.557399	1.499342	-1.370620
O	2.286417	-1.480732	-0.445130
H	1.425830	-1.570951	0.031306
H	2.898736	-2.055343	0.021662

cage
O	0.864297	-1.713818	-0.473367
H	1.685273	-1.201591	-0.301982
H	1.149970	-2.586897	-0.756299
O	-0.730697	0.405669	-1.636684
H	-0.264780	-0.435767	-1.507301
H	-1.610695	0.246805	-1.244929
O	0.590124	1.738583	0.250431
H	0.067494	1.372619	-0.512684
H	0.498694	2.694291	0.201321
O	-0.702299	-0.494721	1.659451
H	-0.201238	-1.096535	1.085954
H	-0.282609	0.363229	1.492787
O	2.795840	0.113442	0.079925
H	2.149178	0.841756	0.181125
H	3.296432	0.102464	0.900406
O	-2.890180	0.015279	0.063048
H	-2.256884	-0.248085	0.763095
H	-3.647524	-0.567756	0.156079

prism
O	-1.502169	-0.191359	1.434927
H	-0.601054	-0.596972	1.553718
H	-2.006698	-0.422327	2.219847
O	-1.744575	-0.382348	-1.309144
H	-1.888941	-0.479653	-0.347624
H	-2.516835	-0.766765	-1.733766
O	-0.560409	2.017830	-0.121984
H	-0.947720	1.533567	0.625228
H	-0.989831	1.592736	-0.877419

O	0.964803	-1.165765	1.439987
H	0.979557	-1.522041	0.527833
H	1.542224	-0.393692	1.344373
O	0.974705	-1.401503	-1.335970
H	0.065161	-1.118951	-1.522886
H	1.470709	-0.570933	-1.277710
O	2.002280	1.057824	-0.124502
H	1.141637	1.532266	-0.140121
H	2.674716	1.735342	-0.237995

ring

O	0.000000	2.696547	0.139502
H	-0.128610	3.230175	0.927789
H	-0.842514	2.202380	0.025953
O	-2.335278	-1.348274	0.139502
H	-1.486060	-1.830828	0.025953
H	-2.733108	-1.726467	0.927789
O	2.335278	1.348274	-0.139502
H	2.733108	1.726467	-0.927789
H	1.486060	1.830828	-0.025953
O	0.000000	-2.696547	-0.139502
H	0.842514	-2.202380	-0.025953
H	0.128610	-3.230175	-0.927789
O	2.335278	-1.348274	0.139502
H	2.861718	-1.503708	0.927789
H	2.328574	-0.371551	0.025953
O	-2.335278	1.348274	-0.139502
H	-2.861718	1.503708	-0.927789
H	-2.328574	0.371551	-0.025953

Table S2. Cartesian Coordinates (Å) for BLYP/MG3S Optimized Geometries

bag

O	-0.867072	1.719742	-0.355420
O	-0.279106	-1.970403	0.378257
O	1.810317	1.591218	-0.175817
O	2.271050	-1.057809	0.102081
O	-1.381999	0.168563	2.000506
O	-1.384248	-0.628522	-1.915192
H	1.361502	-1.468253	0.209685
H	2.035356	0.614453	-0.117662
H	0.140063	1.729674	-0.294657
H	-0.679283	-1.392898	1.067204
H	-0.721784	-1.680889	-0.452595
H	-1.302256	0.264009	-1.504849
H	-1.347569	0.829745	1.271657
H	-1.129881	2.620454	-0.603047
H	-2.309424	-0.709737	-2.195142
H	-2.294669	0.179378	2.328846
H	2.191481	1.984864	0.625402
H	2.704928	-1.553122	-0.610161

boat

O	-1.617227	-2.055146	-0.371675
O	-2.682763	0.464410	-0.244994
O	-0.934110	2.410109	0.570527
O	2.682753	-0.464431	-0.245006
O	0.934116	-2.410069	0.570698
O	1.617230	2.055125	-0.371826
H	-2.043691	1.169284	0.053401
H	0.004298	2.284750	0.260034
H	2.003018	1.136445	-0.330857
H	-0.004294	-2.284727	0.260204
H	-2.003026	-1.136470	-0.330749
H	0.881644	-2.529325	1.531717
H	-0.881628	2.529451	1.531535
H	3.057114	-0.793620	-1.077314
H	-3.057134	0.793537	-1.077321
H	2.043688	-1.169285	0.053452
H	2.319507	2.650710	-0.068039
H	-2.319497	-2.650729	-0.067867

book

O	0.103223	1.551319	0.882282
H	0.961823	1.533423	0.364751
H	0.241380	2.165616	1.620655

O	-0.006979	-1.427809	0.967893
H	-0.024506	-0.471572	1.180339
H	-0.848085	-1.574910	0.468472
O	-2.383530	1.381240	-0.424237
H	-1.502643	1.553624	-0.009553
H	-2.379683	1.863905	-1.265720
O	-2.447192	-1.425071	-0.471705
H	-2.536040	-0.439801	-0.514193
H	-3.240698	-1.738131	-0.009338
O	2.434390	1.245488	-0.464083
H	2.491011	0.246578	-0.511118
H	2.515224	1.557786	-1.379044
O	2.291812	-1.465207	-0.484442
H	1.436661	-1.574996	0.026507
H	2.951771	-2.001203	-0.017429

cage
O	0.865487	-1.682753	-0.609504
H	1.701734	-1.184287	-0.402530
H	1.136650	-2.541776	-0.969709
O	-0.728825	0.608686	-1.623032
H	-0.258948	-0.250896	-1.588372
H	-1.614622	0.415520	-1.228248
O	0.624784	1.706084	0.434807
H	0.094872	1.430344	-0.378194
H	0.566319	2.673010	0.490150
O	-0.768853	-0.673444	1.656791
H	-0.254829	-1.226715	1.030338
H	-0.337146	0.203206	1.589451
O	2.861871	0.093100	0.063578
H	2.204201	0.812989	0.243597
H	3.346969	-0.033686	0.894496
O	-2.935094	0.029512	0.033537
H	-2.305326	-0.310886	0.721074
H	-3.634829	-0.636298	-0.051474

prism
O	-1.468796	-0.271499	1.459406
H	-0.529530	-0.621044	1.584953
H	-1.975133	-0.527958	2.245959
O	-1.714715	-0.565729	-1.313232
H	-1.843234	-0.644467	-0.336453
H	-2.463993	-1.020081	-1.729862
O	-0.769183	2.051168	-0.159891
H	-1.090214	1.534783	0.610507
H	-1.155754	1.563382	-0.912995

O	1.086309	-1.091539	1.490442
H	1.127318	-1.470989	0.574785
H	1.586263	-0.258019	1.376353
O	1.117641	-1.413393	-1.315952
H	0.174129	-1.224373	-1.507390
H	1.538219	-0.529539	-1.288280
O	1.888381	1.238797	-0.174970
H	0.987208	1.660142	-0.192761
H	2.527631	1.955708	-0.311246

ring

O	0.000000	2.723584	0.122139
H	-0.098635	3.234214	0.940893
H	-0.849399	2.210348	0.023986
O	-2.358693	-1.361792	0.122139
H	-1.489518	-1.840775	0.023986
H	-2.751594	-1.702528	0.940893
O	2.358693	1.361792	-0.122139
H	2.751594	1.702528	-0.940893
H	1.489518	1.840775	-0.023986
O	0.000000	-2.723584	-0.122139
H	0.849399	-2.210348	-0.023986
H	0.098635	-3.234214	-0.940893
O	2.358693	-1.361792	0.122139
H	2.850229	-1.531686	0.940893
H	2.338917	-0.369573	0.023986
O	-2.358693	1.361792	-0.122139
H	-2.850229	1.531686	-0.940893
H	-2.338917	0.369573	-0.023986

Table S3. Cartesian Coordinates (Å) for BLYP/6-31+G(d,p) Optimized Geometries

bag

O	-0.895908	1.705511	-0.322424
O	-0.214024	-1.969182	0.336690
O	1.747304	1.612262	-0.137267
O	2.274418	-0.993100	0.087869
O	-1.393979	0.082778	1.949591
O	-1.351699	-0.612965	-1.881958
H	1.371604	-1.442636	0.190472
H	2.007463	0.632841	-0.103645
H	0.122199	1.727311	-0.255899
H	-0.645063	-1.429071	1.045285
H	-0.678609	-1.684186	-0.490877
H	-1.299368	0.288965	-1.471778
H	-1.379653	0.781733	1.247569
H	-1.172872	2.609096	-0.562408
H	-2.252796	-0.705709	-2.240616
H	-2.290417	0.087340	2.331113
H	2.139613	2.010836	0.661721
H	2.749006	-1.478950	-0.610940

boat

O	-1.585653	-2.044999	-0.349220
O	-2.658899	0.437958	-0.253041
O	-0.947659	2.372314	0.560252
O	2.658902	-0.437962	-0.253007
O	0.947670	-2.372286	0.560377
O	1.585633	2.044976	-0.349415
H	-2.024298	1.153879	0.056127
H	0.000820	2.263031	0.248935
H	1.984740	1.122439	-0.322639
H	-0.000821	-2.263016	0.249090
H	-1.984754	-1.122457	-0.322521
H	0.904155	-2.522705	1.522022
H	-0.904109	2.522747	1.521894
H	3.047180	-0.772502	-1.082151
H	-3.047139	0.772434	-1.082229
H	2.024299	-1.153867	0.056195
H	2.295057	2.658314	-0.086272
H	-2.295077	-2.658308	-0.086012

book

O	0.087831	1.535678	0.863249
H	0.956356	1.528649	0.343205
H	0.216585	2.143583	1.614605

O	0.009638	-1.421620	0.938020
H	-0.031191	-0.463822	1.165519
H	-0.837444	-1.586481	0.441111
O	-2.380076	1.350472	-0.407165
H	-1.492654	1.538675	0.003350
H	-2.417875	1.869522	-1.231080
O	-2.413570	-1.420343	-0.463191
H	-2.527757	-0.431133	-0.511872
H	-3.215783	-1.764453	-0.029571
O	2.397553	1.247659	-0.457106
H	2.479876	0.241258	-0.502525
H	2.502867	1.572048	-1.370139
O	2.295698	-1.430507	-0.466955
H	1.427813	-1.560681	0.036408
H	2.962611	-1.977872	-0.013825

cage

O	0.851078	-1.663677	-0.608439
H	1.704572	-1.177406	-0.404624
H	1.096860	-2.538005	-0.962098
O	-0.720207	0.621303	-1.586793
H	-0.260529	-0.250696	-1.575587
H	-1.622536	0.430418	-1.212875
O	0.643820	1.691030	0.436938
H	0.098776	1.421370	-0.381163
H	0.598159	2.662631	0.502206
O	-0.774149	-0.677615	1.624880
H	-0.248869	-1.224390	0.992444
H	-0.325952	0.198360	1.594989
O	2.832342	0.073966	0.060571
H	2.184575	0.811495	0.248000
H	3.358097	-0.041851	0.873319
O	-2.911856	0.032218	0.027036
H	-2.294867	-0.317736	0.731538
H	-3.656511	-0.591989	-0.039695

prism

O	-1.484601	-0.239180	1.429977
H	-0.546364	-0.617623	1.568770
H	-2.013737	-0.474384	2.213952
O	-1.701580	-0.509929	-1.314309
H	-1.857518	-0.605103	-0.335960
H	-2.449353	-0.939964	-1.768215
O	-0.690097	2.045819	-0.156376
H	-1.053214	1.545792	0.613478
H	-1.095503	1.578757	-0.919440

O	1.017080	-1.113582	1.479354
H	1.073223	-1.497876	0.558641
H	1.561586	-0.299550	1.383027
O	1.079552	-1.414496	-1.298558
H	0.142002	-1.194958	-1.514401
H	1.539832	-0.544247	-1.286250
O	1.915000	1.174862	-0.149588
H	1.024316	1.634833	-0.171315
H	2.591895	1.866378	-0.266294

ring

O	0.000000	2.689391	0.127015
H	-0.105776	3.217024	0.939457
H	-0.857771	2.175486	0.019320
O	-2.329081	-1.344695	0.127015
H	-1.455140	-1.830594	0.019320
H	-2.733137	-1.700117	0.939457
O	2.329081	1.344695	-0.127015
H	2.733137	1.700117	-0.939457
H	1.455140	1.830594	-0.019320
O	0.000000	-2.689391	-0.127015
H	0.857771	-2.175486	-0.019320
H	0.105776	-3.217024	-0.939457
O	2.329081	-1.344695	0.127015
H	2.838913	-1.516907	0.939457
H	2.312911	-0.344892	0.019320
O	-2.329081	1.344695	-0.127015
H	-2.838913	1.516907	-0.939457
H	-2.312911	0.344892	-0.019320

Table S4. Cartesian Coordinates (Å) for B3LYP/MG3S Optimized Geometries

bag

O	-0.901454	1.702162	-0.369863
O	-0.219322	-1.961647	0.391852
O	1.763706	1.620860	-0.162193
O	2.294791	-1.006710	0.077545
O	-1.387533	0.145747	1.968051
O	-1.385705	-0.670557	-1.871411
H	1.410819	-1.433717	0.202815
H	2.019221	0.665557	-0.125330
H	0.090602	1.725926	-0.303432
H	-0.630591	-1.405243	1.075168
H	-0.675598	-1.704318	-0.428382
H	-1.314346	0.218634	-1.479912
H	-1.366869	0.799691	1.247674
H	-1.177243	2.584529	-0.630568
H	-2.288460	-0.760390	-2.185076
H	-2.276282	0.164038	2.330271
H	2.143855	2.018475	0.625378
H	2.749021	-1.512025	-0.600457

boat

O	-1.608556	-2.068483	-0.291578
O	-2.657804	0.446316	-0.310240
O	-0.963060	2.395979	0.561099
O	2.657780	-0.446365	-0.310307
O	0.963052	-2.395912	0.561315
O	1.608594	2.068460	-0.291648
H	-2.048943	1.149977	0.010033
H	-0.026883	2.291018	0.279684
H	1.987905	1.160623	-0.306675
H	0.026877	-2.290962	0.279884
H	-1.987911	-1.160663	-0.306573
H	0.944176	-2.551160	1.508293
H	-0.944185	2.551381	1.508053
H	3.011043	-0.765388	-1.144150
H	-3.011132	0.765272	-1.144082
H	2.048930	-1.149992	0.010061
H	2.318529	2.654827	-0.021866
H	-2.318453	-2.654892	-0.021784

book

O	0.111359	1.548909	0.875795
H	0.958037	1.525180	0.365631
H	0.252728	2.137913	1.621207

O	-0.019080	-1.406356	0.933094
H	-0.038829	-0.460983	1.144110
H	-0.857117	-1.567712	0.457850
O	-2.358554	1.374618	-0.426527
H	-1.490964	1.543472	-0.010379
H	-2.370261	1.878984	-1.243344
O	-2.470252	-1.410920	-0.452139
H	-2.547844	-0.437560	-0.506446
H	-3.265830	-1.717665	-0.010676
O	2.429254	1.228928	-0.466326
H	2.497815	0.244556	-0.503181
H	2.542415	1.540902	-1.367259
O	2.299727	-1.470541	-0.459271
H	1.443077	-1.577178	0.021459
H	2.937151	-2.027015	-0.005981

cage

O	0.864424	-1.707606	-0.528571
H	1.689675	-1.205716	-0.348188
H	1.125927	-2.575624	-0.845149
O	-0.728612	0.502377	-1.632260
H	-0.266828	-0.346185	-1.549164
H	-1.612338	0.341343	-1.250188
O	0.620107	1.731182	0.336082
H	0.096163	1.410067	-0.445479
H	0.547287	2.688674	0.349500
O	-0.745312	-0.570150	1.660264
H	-0.244618	-1.155676	1.070397
H	-0.315310	0.291173	1.551478
O	2.837707	0.094365	0.069692
H	2.195228	0.820545	0.205764
H	3.345238	0.027586	0.882320
O	-2.924271	0.021076	0.043377
H	-2.296518	-0.266898	0.738682
H	-3.656246	-0.599243	0.051355

prism

O	-1.480796	-0.270076	1.449388
H	-0.562517	-0.635790	1.564081
H	-1.988371	-0.520260	2.224940
O	-1.724274	-0.476300	-1.318185
H	-1.855575	-0.576335	-0.355736
H	-2.474439	-0.892061	-1.750286
O	-0.696791	2.035146	-0.119064
H	-1.041624	1.530577	0.634563
H	-1.091612	1.585051	-0.878019

O	1.044978	-1.139196	1.453013
H	1.077771	-1.508389	0.547097
H	1.571986	-0.332523	1.359953
O	1.065943	-1.383782	-1.345402
H	0.141145	-1.160139	-1.533970
H	1.519634	-0.530121	-1.288437
O	1.925794	1.178468	-0.135752
H	1.045063	1.613660	-0.146451
H	2.579706	1.872250	-0.249724

ring

O	0.000000	2.705829	0.146979
H	-0.111194	3.227967	0.944734
H	-0.840303	2.207793	0.028737
O	-2.343317	-1.352914	0.146979
H	-1.491853	-1.831620	0.028737
H	-2.739904	-1.710280	0.944734
O	2.343317	1.352914	-0.146979
H	2.739904	1.710280	-0.944734
H	1.491853	1.831620	-0.028737
O	0.000000	-2.705829	-0.146979
H	0.840303	-2.207793	-0.028737
H	0.111194	-3.227967	-0.944734
O	2.343317	-1.352914	0.146979
H	2.851098	-1.517687	0.944734
H	2.332156	-0.376172	0.028737
O	-2.343317	1.352914	-0.146979
H	-2.851098	1.517687	-0.944734
H	-2.332156	0.376172	-0.028737

Table S5. Cartesian Coordinates (Å) for B3LYP/6-31+G(d,2p) Optimized Geometries

bag

O	-0.906488	1.701971	-0.333205
O	-0.193070	-1.964622	0.347463
O	1.737924	1.625156	-0.125513
O	2.289432	-0.978714	0.077641
O	-1.412182	0.076435	1.929578
O	-1.356033	-0.633680	-1.862485
H	1.405266	-1.423995	0.190516
H	2.008311	0.666771	-0.102719
H	0.092152	1.729282	-0.260018
H	-0.629194	-1.436262	1.043697
H	-0.656945	-1.697173	-0.470606
H	-1.299370	0.257755	-1.462177
H	-1.387236	0.762553	1.233559
H	-1.182254	2.593210	-0.576913
H	-2.238294	-0.709581	-2.241687
H	-2.295184	0.106046	2.313491
H	2.140182	2.022396	0.655630
H	2.765904	-1.483380	-0.590612

boat

O	-1.604590	-2.058093	-0.247231
O	-2.631398	0.440793	-0.328195
O	-0.965218	2.386748	0.537337
O	2.631372	-0.440841	-0.328271
O	0.965218	-2.386682	0.537569
O	1.604630	2.058069	-0.247315
H	-2.026303	1.153913	-0.003515
H	-0.017335	2.286255	0.274610
H	1.983806	1.144573	-0.287304
H	0.017343	-2.286221	0.274801
H	-1.983797	-1.144610	-0.287215
H	0.963088	-2.575459	1.482285
H	-0.963112	2.575692	1.482019
H	2.985191	-0.761401	-1.165445
H	-2.985325	0.761294	-1.165347
H	2.026293	-1.153925	-0.003477
H	2.328322	2.641599	0.003695
H	-2.328269	-2.641655	0.003741

book

O	0.102012	1.541908	0.860842
H	0.955629	1.523536	0.349438
H	0.243627	2.129706	1.611922

O	-0.010583	-1.404160	0.909967
H	-0.044064	-0.456377	1.127792
H	-0.856042	-1.572392	0.440001
O	-2.355178	1.354734	-0.413877
H	-1.482596	1.536023	-0.001340
H	-2.394168	1.891579	-1.213061
O	-2.451517	-1.407754	-0.445231
H	-2.543256	-0.430888	-0.503792
H	-3.259401	-1.727667	-0.028592
O	2.406894	1.228786	-0.461680
H	2.491569	0.239370	-0.495523
H	2.546415	1.542480	-1.362099
O	2.304202	-1.449652	-0.444687
H	1.437167	-1.567143	0.028112
H	2.938475	-2.019131	0.004468

cage
O	0.852373	-1.684373	-0.558436
H	1.688880	-1.194149	-0.367250
H	1.106348	-2.551916	-0.892919
O	-0.720812	0.553547	-1.603205
H	-0.266255	-0.305895	-1.548544
H	-1.613746	0.381147	-1.235783
O	0.633925	1.711003	0.376052
H	0.099530	1.411968	-0.416206
H	0.565723	2.671989	0.412088
O	-0.756043	-0.610129	1.635523
H	-0.243826	-1.182163	1.035121
H	-0.311018	0.251773	1.564062
O	2.817377	0.077373	0.066525
H	2.180746	0.811262	0.225782
H	3.363283	0.015392	0.858527
O	-2.904601	0.021069	0.031740
H	-2.284036	-0.285661	0.732878
H	-3.663377	-0.571665	0.046648

prism
O	-1.484724	-0.245495	1.432351
H	-0.565819	-0.627284	1.555386
H	-1.999333	-0.483264	2.211875
O	-1.716278	-0.458612	-1.315695
H	-1.858999	-0.555336	-0.349342
H	-2.471113	-0.867654	-1.754108
O	-0.655829	2.035317	-0.122643
H	-1.021870	1.533840	0.628718
H	-1.065297	1.598879	-0.886671

O	1.008088	-1.145766	1.450841
H	1.049551	-1.511300	0.537908
H	1.560371	-0.350201	1.368037
O	1.047173	-1.392979	-1.326491
H	0.124382	-1.156296	-1.530729
H	1.514608	-0.541245	-1.282929
O	1.935331	1.147944	-0.132196
H	1.058873	1.603909	-0.144482
H	2.604563	1.832680	-0.242995

ring

O	0.000000	2.681870	0.149242
H	-0.119300	3.213219	0.944138
H	-0.846952	2.183776	0.026715
O	-2.322567	-1.340935	0.149242
H	-1.467730	-1.825370	0.026715
H	-2.723079	-1.709926	0.944138
O	2.322567	1.340935	-0.149242
H	2.723079	1.709926	-0.944138
H	1.467730	1.825370	-0.026715
O	0.000000	-2.681870	-0.149242
H	0.846952	-2.183776	-0.026715
H	0.119300	-3.213219	-0.944138
O	2.322567	-1.340935	0.149242
H	2.842379	-1.503293	0.944138
H	2.314682	-0.358406	0.026715
O	-2.322567	1.340935	-0.149242
H	-2.842379	1.503293	-0.944138
H	-2.314682	0.358406	-0.026715

**Table S6. Cartesian Coordinates (Å) for PBE/MG3S
Optimized Geometries**

bag

O	-0.856167	1.666265	-0.395547
O	-0.270504	-1.919194	0.426841
O	1.759300	1.556171	-0.202375
O	2.219906	-1.030071	0.102138
O	-1.321402	0.227625	1.969119
O	-1.353760	-0.674942	-1.861416
H	1.303314	-1.434879	0.230866
H	1.981818	0.572518	-0.126337
H	0.159393	1.678449	-0.330396
H	-0.655407	-1.306300	1.095916
H	-0.711588	-1.643238	-0.411542
H	-1.269399	0.227468	-1.469592
H	-1.301886	0.859926	1.212769
H	-1.118065	2.557311	-0.670236
H	-2.289100	-0.775177	-2.090744
H	-2.238954	0.213916	2.277945
H	2.104707	1.950447	0.612650
H	2.616183	-1.507277	-0.641388

boat

O	-1.565885	-1.971983	-0.452725
O	-2.632561	0.477100	-0.214657
O	-0.868490	2.319596	0.622807
O	2.632546	-0.477143	-0.214713
O	0.868484	-2.319532	0.623013
O	1.565915	1.971953	-0.452823
H	-1.972165	1.162682	0.097423
H	0.053229	2.188006	0.254234
H	1.963800	1.055853	-0.371423
H	-0.053225	-2.187976	0.254402
H	-1.963794	-1.055892	-0.371339
H	0.764613	-2.342636	1.585173
H	-0.764638	2.342868	1.584966
H	2.989603	-0.830040	-1.042865
H	-2.989690	0.829942	-1.042802
H	1.972159	-1.162692	0.097460
H	2.259242	2.583598	-0.166273
H	-2.259199	-2.583643	-0.166176

book

O	0.101694	1.517809	0.874103
H	0.962582	1.494944	0.347788
H	0.242012	2.141080	1.601998

O	-0.004189	-1.401397	0.970245
H	-0.015374	-0.444135	1.179683
H	-0.841682	-1.535224	0.455390
O	-2.330240	1.354213	-0.418245
H	-1.449828	1.521445	0.004675
H	-2.299398	1.806782	-1.273760
O	-2.372019	-1.398401	-0.473431
H	-2.458845	-0.409924	-0.507524
H	-3.154106	-1.707109	0.007307
O	2.372355	1.219262	-0.459224
H	2.415115	0.213220	-0.507185
H	2.413503	1.525203	-1.377153
O	2.222648	-1.432878	-0.488943
H	1.371278	-1.533831	0.042008
H	2.892749	-1.941308	-0.009273

cage

O	0.847466	-1.648935	-0.588569
H	1.680186	-1.136125	-0.382894
H	1.129997	-2.507332	-0.936182
O	-0.722978	0.577852	-1.594250
H	-0.247929	-0.278909	-1.549445
H	-1.601882	0.382209	-1.177239
O	0.604631	1.671358	0.405614
H	0.072493	1.375007	-0.408718
H	0.547732	2.637529	0.438340
O	-0.740768	-0.641264	1.631899
H	-0.231797	-1.196778	1.002628
H	-0.313316	0.235797	1.542075
O	2.802431	0.097901	0.060748
H	2.133058	0.814598	0.227910
H	3.247269	-0.040986	0.910151
O	-2.872966	0.029139	0.043681
H	-2.227582	-0.301023	0.726523
H	-3.530762	-0.672399	-0.066133

prism

O	-1.427124	-0.287571	1.429331
H	-0.473372	-0.625357	1.544913
H	-1.925456	-0.565610	2.211199
O	-1.667223	-0.570377	-1.285736
H	-1.785661	-0.649341	-0.305249
H	-2.412826	-1.035002	-1.693101
O	-0.789107	2.001612	-0.152900
H	-1.096103	1.473788	0.616231
H	-1.164990	1.498720	-0.901065

O	1.081705	-1.058823	1.454481
H	1.122512	-1.423464	0.528811
H	1.561538	-0.213981	1.337132
O	1.117837	-1.369247	-1.291280
H	0.170270	-1.192026	-1.476339
H	1.519195	-0.476475	-1.256770
O	1.824829	1.235128	-0.168326
H	0.911337	1.637865	-0.186160
H	2.446229	1.965109	-0.304161

ring

O	0.000000	2.670670	0.091752
H	-0.086724	3.180246	0.910441
H	-0.851553	2.148257	0.014378
O	-2.312868	-1.335335	0.091752
H	-1.434669	-1.811595	0.014378
H	-2.710812	-1.665228	0.910441
O	2.312868	1.335335	-0.091752
H	2.710812	1.665228	-0.910441
H	1.434669	1.811595	-0.014378
O	0.000000	-2.670670	-0.091752
H	0.851553	-2.148257	-0.014378
H	0.086724	-3.180246	-0.910441
O	2.312868	-1.335335	0.091752
H	2.797535	-1.515018	0.910441
H	2.286221	-0.336662	0.014378
O	-2.312868	1.335335	-0.091752
H	-2.797535	1.515018	-0.910441
H	-2.286221	0.336662	-0.014378

Table S7. Cartesian Coordinates (Å) for PBE/aug-cc-pVTZ Optimized Geometries

bag
O	-0.847695	1.670552	-0.352446
O	-0.274309	-1.919400	0.376138
O	1.763539	1.551017	-0.178024
O	2.214566	-1.031685	0.110038
O	-1.343901	0.173082	1.959317
O	-1.337953	-0.619213	-1.879001
H	1.293497	-1.440557	0.215899
H	1.985606	0.563769	-0.108475
H	0.170674	1.683801	-0.288023
H	-0.672190	-1.326413	1.057987
H	-0.710172	-1.622276	-0.459774
H	-1.261273	0.273083	-1.458322
H	-1.311271	0.825747	1.218339
H	-1.111239	2.569439	-0.601844
H	-2.271033	-0.714356	-2.123676
H	-2.266998	0.156460	2.254546
H	2.129411	1.944039	0.629634
H	2.631016	-1.507563	-0.624461

boat
O	-1.564443	-1.985289	-0.431145
O	-2.630617	0.454879	-0.188659
O	-0.890708	2.340138	0.573285
O	2.630607	-0.454902	-0.188683
O	0.890711	-2.340094	0.573463
O	1.564453	1.985264	-0.431282
H	-1.972408	1.157536	0.097228
H	0.044152	2.206892	0.233187
H	1.965072	1.067825	-0.347313
H	-0.044147	-2.206873	0.233351
H	-1.965075	-1.067852	-0.347214
H	0.810034	-2.424646	1.535324
H	-0.810030	2.424798	1.535137
H	3.024475	-0.796677	-1.005785
H	-3.024513	0.796595	-1.005772
H	1.972405	-1.157536	0.097276
H	2.255453	2.599022	-0.140699
H	-2.255440	-2.599047	-0.140552

book
O	0.104356	1.527461	0.858968
H	0.969923	1.497638	0.335473
H	0.244693	2.157699	1.581950

O	-0.010240	-1.392765	0.963066
H	-0.019582	-0.434381	1.171883
H	-0.854301	-1.525920	0.454436
O	-2.322590	1.347674	-0.415180
H	-1.438261	1.523162	0.001330
H	-2.306372	1.808613	-1.267667
O	-2.372617	-1.394550	-0.467294
H	-2.458231	-0.403745	-0.503940
H	-3.156462	-1.701018	0.014031
O	2.375532	1.206962	-0.454157
H	2.416944	0.198151	-0.501460
H	2.434137	1.513417	-1.371897
O	2.216200	-1.437957	-0.480739
H	1.360097	-1.535639	0.048723
H	2.882278	-1.952592	-0.000176

cage
O	0.841069	-1.637084	-0.613250
H	1.677695	-1.130131	-0.397052
H	1.122325	-2.492034	-0.972654
O	-0.724186	0.616917	-1.573436
H	-0.250023	-0.242271	-1.548557
H	-1.604274	0.410844	-1.158408
O	0.617389	1.662741	0.435485
H	0.076234	1.384473	-0.382859
H	0.568624	2.629539	0.484082
O	-0.745048	-0.677009	1.611867
H	-0.231057	-1.215481	0.969336
H	-0.314811	0.201718	1.547613
O	2.793429	0.088846	0.057095
H	2.124650	0.804916	0.244135
H	3.252529	-0.060520	0.898156
O	-2.866820	0.032222	0.042682
H	-2.222101	-0.318404	0.719411
H	-3.526456	-0.665711	-0.086746

prism
O	1.459337	-0.474955	-1.328262
H	0.532859	-0.897764	-1.397066
H	1.995399	-0.844516	-2.045725
O	1.677811	-0.266389	1.397007
H	1.810828	-0.503085	0.443183
H	2.424703	-0.650136	1.881286
O	0.687738	2.026973	-0.238013
H	1.028169	1.346007	-0.862139
H	1.081554	1.737283	0.607202

O	-0.981766	-1.422599	-1.243202
H	-1.041313	-1.516970	-0.246985
H	-1.548603	-0.642689	-1.395092
O	-1.085316	-1.108453	1.463029
H	-0.148278	-0.875526	1.648213
H	-1.503778	-0.245599	1.245079
O	-1.896086	1.190187	-0.029227
H	-0.995829	1.616925	-0.111713
H	-2.529454	1.917955	0.063100

ring
O	0.000000	2.662815	0.093630
H	-0.089479	3.176955	0.910246
H	-0.855225	2.141875	0.013985
O	-2.306066	-1.331408	0.093630
H	-1.427306	-1.811584	0.013985
H	-2.706584	-1.665969	0.910246
O	2.306066	1.331408	-0.093630
H	2.706584	1.665969	-0.910246
H	1.427306	1.811584	-0.013985
O	0.000000	-2.662815	-0.093630
H	0.855225	-2.141875	-0.013985
H	0.089479	-3.176955	-0.910246
O	2.306066	-1.331408	0.093630
H	2.796064	-1.510986	0.910246
H	2.282531	-0.330291	0.013985
O	-2.306066	1.331408	-0.093630
H	-2.796064	1.510986	-0.910246
H	-2.282531	0.330291	-0.013985

Table S8. Cartesian Coordinates (Å) for PBE1W/MG3S Optimized Geometries

bag
O	-0.873438	1.693078	-0.394841
O	-0.269730	-1.951610	0.424206
O	1.777856	1.583634	-0.196369
O	2.250347	-1.038282	0.098879
O	-1.341993	0.216971	1.991576
O	-1.367432	-0.678365	-1.885562
H	1.342446	-1.447786	0.226404
H	2.003752	0.606963	-0.128129
H	0.134635	1.707223	-0.329820
H	-0.658757	-1.349692	1.096911
H	-0.713127	-1.676783	-0.410110
H	-1.289833	0.222174	-1.494989
H	-1.325994	0.854836	1.243278
H	-1.135008	2.584762	-0.666455
H	-2.296481	-0.775425	-2.138955
H	-2.253090	0.216505	2.318100
H	2.131126	1.975572	0.615893
H	2.655447	-1.521758	-0.635245

boat
O	-1.586767	-2.011729	-0.428667
O	-2.664188	0.473676	-0.236696
O	-0.897690	2.353734	0.620831
O	2.664160	-0.473746	-0.236806
O	0.897674	-2.353651	0.621092
O	1.586830	2.011700	-0.428713
H	-2.014985	1.161900	0.077956
H	0.025980	2.228218	0.268502
H	1.981403	1.097995	-0.365135
H	-0.025972	-2.228179	0.268686
H	-1.981383	-1.098043	-0.365070
H	0.806190	-2.396162	1.583480
H	-0.806259	2.396505	1.583212
H	3.015965	-0.821084	-1.069091
H	-3.016142	0.820965	-1.068938
H	2.014973	-1.161925	0.077977
H	2.284228	2.617012	-0.139956
H	-2.284149	-2.617083	-0.139956

book
O	0.104642	1.537609	0.886469
H	0.961127	1.516419	0.364760
H	0.245275	2.160671	1.613992

O	-0.007441	-1.422318	0.977644
H	-0.021244	-0.468010	1.191702
H	-0.843830	-1.558383	0.468292
O	-2.355334	1.374910	-0.427069
H	-1.478107	1.542219	-0.004797
H	-2.327903	1.836673	-1.277335
O	-2.412873	-1.411248	-0.474885
H	-2.498596	-0.426256	-0.513869
H	-3.200354	-1.717795	-0.002444
O	2.407840	1.234019	-0.462584
H	2.454222	0.234257	-0.512095
H	2.462563	1.541676	-1.378807
O	2.253640	-1.453759	-0.494081
H	1.405167	-1.558321	0.029625
H	2.917895	-1.976857	-0.022970

cage

O	0.861310	-1.664928	-0.618600
H	1.692493	-1.160745	-0.407080
H	1.142351	-2.517680	-0.980103
O	-0.729948	0.611505	-1.610771
H	-0.257846	-0.245291	-1.582301
H	-1.609082	0.411998	-1.205488
O	0.612599	1.691221	0.435073
H	0.083750	1.413511	-0.378813
H	0.554681	2.656246	0.484877
O	-0.754287	-0.678882	1.645096
H	-0.243283	-1.225109	1.012442
H	-0.326943	0.197988	1.575755
O	2.838776	0.097612	0.066211
H	2.176078	0.812826	0.242601
H	3.295418	-0.043792	0.908409
O	-2.909647	0.027514	0.041949
H	-2.273327	-0.314739	0.721616
H	-3.584721	-0.657551	-0.063578

prism

O	-1.446440	-0.285597	1.450797
H	-0.501281	-0.623567	1.569896
H	-1.943242	-0.555618	2.236008
O	-1.695011	-0.579072	-1.302025
H	-1.817437	-0.659628	-0.325708
H	-2.436237	-1.048118	-1.711413
O	-0.792209	2.033033	-0.154883
H	-1.102321	1.509852	0.613676
H	-1.172032	1.536884	-0.903733

O	1.096107	-1.073536	1.478083
H	1.136246	-1.446580	0.560127
H	1.581464	-0.233887	1.359800
O	1.123824	-1.394464	-1.307193
H	0.179274	-1.211912	-1.492741
H	1.532644	-0.506789	-1.280181
O	1.853713	1.250292	-0.179010
H	0.946277	1.656566	-0.192952
H	2.476782	1.977545	-0.318937

ring

O	0.000000	2.703373	0.106700
H	-0.092797	3.207353	0.927711
H	-0.847559	2.185462	0.019197
O	-2.341190	-1.351687	0.106700
H	-1.468886	-1.826738	0.019197
H	-2.731251	-1.684042	0.927711
O	2.341190	1.351687	-0.106700
H	2.731251	1.684042	-0.927711
H	1.468886	1.826738	-0.019197
O	0.000000	-2.703373	-0.106700
H	0.847559	-2.185462	-0.019197
H	0.092797	-3.207353	-0.927711
O	2.341190	-1.351687	0.106700
H	2.824048	-1.523312	0.927711
H	2.316445	-0.358723	0.019197
O	-2.341190	1.351687	-0.106700
H	-2.824048	1.523312	-0.927711
H	-2.316445	0.358723	-0.019197

Table S9. Cartesian Coordinates (Å) for PBE1W/6-311+G(2d,2p) Optimized Geometries

bag

O	-0.876929	1.681854	-0.414465
O	-0.277075	-1.943819	0.448548
O	1.771914	1.579556	-0.212174
O	2.241886	-1.038073	0.107061
O	-1.325077	0.247527	1.998088
O	-1.354814	-0.701258	-1.886357
H	1.332635	-1.444249	0.239863
H	1.993175	0.601862	-0.131651
H	0.132075	1.699035	-0.349801
H	-0.660642	-1.328902	1.113133
H	-0.717919	-1.675730	-0.389707
H	-1.284270	0.203163	-1.502576
H	-1.318390	0.872955	1.238839
H	-1.139105	2.569693	-0.698176
H	-2.284776	-0.808487	-2.132717
H	-2.236403	0.241001	2.324313
H	2.111891	1.975760	0.603814
H	2.632487	-1.512389	-0.640954

boat

O	-1.572981	-2.002839	-0.462246
O	-2.666081	0.470236	-0.219282
O	-0.889597	2.341261	0.636542
O	2.666060	-0.470293	-0.219363
O	0.889584	-2.341185	0.636775
O	1.573027	2.002810	-0.462321
H	-2.011867	1.154765	0.094500
H	0.027224	2.213767	0.265709
H	1.972174	1.091952	-0.380332
H	-0.027221	-2.213730	0.265888
H	-1.972164	-1.091997	-0.380254
H	0.780594	-2.354435	1.598319
H	-0.780637	2.354717	1.598086
H	3.017205	-0.822299	-1.050134
H	-3.017331	0.822189	-1.050031
H	2.011859	-1.154783	0.094529
H	2.263334	2.614143	-0.168584
H	-2.263270	-2.614203	-0.168534

book

O	0.100695	1.529964	0.889838
H	0.956990	1.513508	0.366296
H	0.239149	2.156624	1.614777

O	-0.002914	-1.424470	0.986059
H	-0.015118	-0.469702	1.199452
H	-0.836865	-1.556678	0.470720
O	-2.356752	1.373976	-0.427276
H	-1.479348	1.540553	-0.004437
H	-2.320349	1.822167	-1.284591
O	-2.397616	-1.411868	-0.479774
H	-2.485540	-0.426512	-0.515518
H	-3.179913	-1.718731	0.001257
O	2.401719	1.237912	-0.460929
H	2.444015	0.237144	-0.513089
H	2.441598	1.544733	-1.378333
O	2.244897	-1.447058	-0.502650
H	1.399997	-1.552384	0.028151
H	2.915149	-1.958374	-0.026825

cage
O	0.852216	-1.649347	-0.646692
H	1.685610	-1.150978	-0.427792
H	1.131515	-2.500211	-1.013995
O	-0.730058	0.647415	-1.601518
H	-0.256968	-0.209384	-1.593321
H	-1.605287	0.436891	-1.191539
O	0.613149	1.677837	0.466312
H	0.085596	1.416481	-0.354758
H	0.562146	2.642582	0.528324
O	-0.752935	-0.709452	1.637742
H	-0.243144	-1.239178	0.989598
H	-0.327773	0.169752	1.584003
O	2.836551	0.092907	0.063154
H	2.172563	0.804148	0.253027
H	3.281025	-0.073041	0.907517
O	-2.901334	0.027790	0.042955
H	-2.264643	-0.327616	0.716260
H	-3.561348	-0.666647	-0.092950

prism
O	-1.439407	-0.297803	1.448318
H	-0.491421	-0.630941	1.566663
H	-1.934242	-0.574860	2.232418
O	-1.686206	-0.592326	-1.300405
H	-1.807229	-0.675948	-0.323743
H	-2.424309	-1.066903	-1.709284
O	-0.812367	2.028996	-0.152841
H	-1.113474	1.499839	0.615406
H	-1.186919	1.529093	-0.902001

O	1.104404	-1.068567	1.474500
H	1.147459	-1.434295	0.553119
H	1.579164	-0.222101	1.360931
O	1.137676	-1.383219	-1.306807
H	0.190479	-1.213180	-1.491701
H	1.533993	-0.489653	-1.279881
O	1.836699	1.264952	-0.177051
H	0.926082	1.665220	-0.191939
H	2.454022	1.997464	-0.315703

ring

O	0.000000	2.704209	0.089828
H	-0.082331	3.209029	0.911610
H	-0.846847	2.181563	0.018620
O	-2.341914	-1.352105	0.089828
H	-1.465866	-1.824173	0.018620
H	-2.737935	-1.675816	0.911610
O	2.341914	1.352105	-0.089828
H	2.737935	1.675816	-0.911610
H	1.465866	1.824173	-0.018620
O	0.000000	-2.704209	-0.089828
H	0.846847	-2.181563	-0.018620
H	0.082331	-3.209029	-0.911610
O	2.341914	-1.352105	0.089828
H	2.820266	-1.533214	0.911610
H	2.312713	-0.357391	0.018620
O	-2.341914	1.352105	-0.089828
H	-2.820266	1.533214	-0.911610
H	-2.312713	0.357391	-0.018620

Table S10. Cartesian Coordinates (Å) for M06-L/MG3S Optimized Geometries

bag

O	-1.336302	1.216607	-0.847886
O	0.267594	-1.644201	1.000958
O	1.265297	1.769494	-0.572687
O	2.499918	-0.602995	-0.150205
O	-1.051770	0.734508	1.907594
O	-1.410073	-1.568760	-1.289204
H	1.752888	-1.072461	0.287612
H	1.773788	0.930037	-0.493401
H	-0.372772	1.446971	-0.820256
H	-0.143174	-0.906187	1.477599
H	-0.340749	-1.803233	0.261535
H	-1.503555	-0.601327	-1.271537
H	-1.381272	1.007400	1.036550
H	-1.750761	1.898516	-1.377526
H	-2.300386	-1.913165	-1.361062
H	-1.817416	0.723763	2.482546
H	1.425231	2.226382	0.254644
H	2.780864	-1.173910	-0.865270

boat

O	-1.765467	-1.914262	-0.396361
O	-2.650064	0.677153	-0.276743
O	-0.727730	2.409418	0.633669
O	2.650073	-0.677144	-0.276678
O	0.727748	-2.409401	0.633765
O	1.765427	1.914242	-0.396574
H	-1.966894	1.295571	0.056448
H	0.175787	2.242592	0.294307
H	2.085391	0.988109	-0.372277
H	-0.175791	-2.242569	0.294461
H	-2.085426	-0.988125	-0.372142
H	0.631839	-2.486960	1.582762
H	-0.631764	2.486940	1.582663
H	2.956613	-1.068480	-1.094922
H	-2.956524	1.068416	-1.095052
H	1.966899	-1.295553	0.056521
H	2.520164	2.448559	-0.150854
H	-2.520190	-2.448551	-0.150543

book

O	0.136957	1.596957	0.831319
H	0.984561	1.535797	0.332390

H	0.302542	2.194701	1.560741
O	-0.047009	-1.307788	0.910437
H	-0.071498	-0.357387	1.084999
H	-0.891230	-1.492508	0.461289
O	-2.342099	1.354855	-0.430298
H	-1.473842	1.549134	-0.034427
H	-2.356826	1.833874	-1.259001
O	-2.520504	-1.424277	-0.421421
H	-2.581594	-0.453453	-0.487777
H	-3.292803	-1.690325	0.078180
O	2.459245	1.174549	-0.478177
H	2.523787	0.192960	-0.485564
H	2.574728	1.442211	-1.389996
O	2.307126	-1.532120	-0.413508
H	1.434326	-1.582935	0.038540
H	2.898124	-2.069482	0.113803

cage

O	-0.904608	-1.733201	0.405667
H	-1.703572	-1.184497	0.259813
H	-1.217758	-2.607217	0.639827
O	0.799800	0.201369	1.685063
H	0.302896	-0.604732	1.485136
H	1.654316	0.074224	1.236768
O	-0.514341	1.765979	-0.052663
H	-0.004159	1.317769	0.669144
H	-0.368465	2.705790	0.057266
O	0.583872	-0.374420	-1.682858
H	0.119549	-1.022808	-1.134623
H	0.208055	0.470709	-1.398809
O	-2.780124	0.188013	-0.120917
H	-2.123762	0.909909	-0.103269
H	-3.150479	0.208008	-1.004184
O	2.873320	0.014483	-0.173546
H	2.204515	-0.198794	-0.853855
H	3.615516	-0.566142	-0.339182

prism

O	1.557189	-0.344725	-1.401367
H	0.667867	-0.778613	-1.463320
H	2.067972	-0.662770	-2.145812
O	1.768536	-0.103062	1.347026
H	1.937725	-0.355009	0.421250
H	2.540035	-0.373138	1.846025
O	0.456475	1.976304	-0.149094
H	0.877312	1.434696	-0.832258

H	0.895995	1.668394	0.652979
O	-0.913052	-1.358515	-1.265748
H	-0.914417	-1.595308	-0.318727
H	-1.513046	-0.601261	-1.270949
O	-0.914462	-1.199818	1.527978
H	-0.019956	-0.854314	1.658594
H	-1.451944	-0.417981	1.344515
O	-2.087493	0.961952	-0.033371
H	-1.242882	1.457732	-0.078941
H	-2.782208	1.620481	-0.016750

ring

O	0.000000	2.722699	0.143203
H	-0.119536	3.217535	0.953777
H	-0.834648	2.222622	0.025658
O	-2.357927	-1.361350	0.143203
H	-1.507523	-1.834137	0.025658
H	-2.726699	-1.712289	0.953777
O	2.357927	1.361350	-0.143203
H	2.726699	1.712289	-0.953777
H	1.507523	1.834137	-0.025658
O	0.000000	-2.722699	-0.143203
H	0.834648	-2.222622	-0.025658
H	0.119536	-3.217535	-0.953777
O	2.357927	-1.361350	0.143203
H	2.846235	-1.505246	0.953777
H	2.342171	-0.388485	0.025658
O	-2.357927	1.361350	-0.143203
H	-2.846235	1.505246	-0.953777
H	-2.342171	0.388485	-0.025658

Table S11. Cartesian Coordinates (Å) for M06-L/aug-cc-pVTZ Optimized Geometries

bag

O	1.460309	-0.908346	-0.985669
O	-0.436724	1.504204	1.171339
O	-0.971236	-1.923179	-0.585163
O	-2.514941	0.229438	-0.033937
O	1.312890	-0.681657	1.807152
O	0.894594	1.818856	-1.296703
H	-1.837448	0.764176	0.443164
H	-1.596887	-1.171750	-0.456222
H	0.557809	-1.316941	-0.912856
H	0.118451	0.803994	1.550534
H	0.065203	1.791388	0.390001
H	1.196864	0.893364	-1.324839
H	1.625639	-0.821205	0.897572
H	1.946865	-1.464750	-1.595144
H	1.676682	2.347237	-1.460449
H	2.103267	-0.552021	2.333033
H	-0.981006	-2.384631	0.255648
H	-2.834573	0.796611	-0.736583

boat

O	-1.812461	-1.849714	-0.413602
O	-2.602835	0.756925	-0.267301
O	-0.638069	2.422406	0.638801
O	2.602829	-0.756937	-0.267284
O	0.638084	-2.422371	0.638946
O	1.812449	1.849691	-0.413779
H	-1.897915	1.353957	0.066019
H	0.260728	2.226634	0.295941
H	2.100389	0.911105	-0.379237
H	-0.260718	-2.226617	0.296092
H	-2.100403	-0.911127	-0.379129
H	0.537517	-2.482377	1.589294
H	-0.537485	2.482466	1.589144
H	2.897543	-1.161703	-1.083994
H	-2.897542	1.161630	-1.084043
H	1.897915	-1.353952	0.066080
H	2.581565	2.356074	-0.151324
H	-2.581572	-2.356080	-0.151101

book

O	0.125902	1.574620	0.845677
H	0.968865	1.526890	0.333585
H	0.293082	2.178969	1.569816

O	-0.039121	-1.322085	0.911674
H	-0.063961	-0.372704	1.097429
H	-0.880182	-1.495406	0.448447
O	-2.343221	1.348113	-0.412859
H	-1.472945	1.536994	-0.014746
H	-2.347942	1.823970	-1.244239
O	-2.487009	-1.425038	-0.444219
H	-2.557578	-0.452088	-0.494364
H	-3.254985	-1.703017	0.056866
O	2.427779	1.192244	-0.495528
H	2.503680	0.209291	-0.493717
H	2.501934	1.445977	-1.416283
O	2.310665	-1.506513	-0.407433
H	1.437699	-1.568344	0.047416
H	2.912374	-2.021275	0.131296

cage

O	0.877947	-1.729550	-0.423256
H	1.685103	-1.190936	-0.271427
H	1.182339	-2.610605	-0.644452
O	-0.794868	0.243721	-1.665493
H	-0.304199	-0.571210	-1.480912
H	-1.650067	0.110090	-1.216079
O	0.543880	1.767674	0.078337
H	0.020494	1.332678	-0.644690
H	0.421035	2.711301	-0.031974
O	-0.588471	-0.379319	1.672432
H	-0.124949	-1.015108	1.106280
H	-0.209202	0.470603	1.404362
O	2.774143	0.153979	0.112601
H	2.123088	0.883331	0.109877
H	3.131684	0.147670	1.002275
O	-2.873879	0.012979	0.166935
H	-2.201699	-0.205462	0.844729
H	-3.583646	-0.618220	0.289566

prism

O	1.518701	-0.365982	-1.405766
H	0.621184	-0.788926	-1.457834
H	2.017199	-0.700356	-2.152083
O	1.771816	-0.132659	1.328917
H	1.923816	-0.375567	0.395949
H	2.549086	-0.420467	1.809804
O	0.496142	1.977913	-0.159057
H	0.898519	1.420045	-0.842069
H	0.943923	1.668763	0.638903

O	-0.956075	-1.354100	-1.255708
H	-0.948855	-1.580551	-0.304449
H	-1.544626	-0.586889	-1.257290
O	-0.913869	-1.188191	1.528676
H	-0.009791	-0.859800	1.646463
H	-1.435938	-0.392371	1.355545
O	-2.053123	0.996479	-0.009873
H	-1.195404	1.472240	-0.063421
H	-2.727845	1.676207	0.012960

ring

O	0.000000	2.713502	0.120506
H	-0.115590	3.221812	0.923893
H	-0.836933	2.209742	0.018807
O	-2.349961	-1.356751	0.120506
H	-1.495226	-1.829676	0.018807
H	-2.732376	-1.711009	0.923893
O	2.349961	1.356751	-0.120506
H	2.732376	1.711009	-0.923893
H	1.495226	1.829676	-0.018807
O	0.000000	-2.713502	-0.120506
H	0.836933	-2.209742	-0.018807
H	0.115590	-3.221812	-0.923893
O	2.349961	-1.356751	0.120506
H	2.847966	-1.510802	0.923893
H	2.332159	-0.380066	0.018807
O	-2.349961	1.356751	-0.120506
H	-2.847966	1.510802	-0.923893
H	-2.332159	0.380066	-0.018807

Table S12. Cartesian Coordinates (Å) for PWB6K/MG3S Optimized Geometries

bag

O	-0.974991	1.685122	-0.432388
O	-0.099008	-1.969001	0.450607
O	1.687626	1.689328	-0.143915
O	2.361873	-0.921486	-0.005522
O	-1.369154	0.145061	1.925416
O	-1.439074	-0.786383	-1.761272
H	1.522560	-1.378487	0.169761
H	1.995738	0.768354	-0.151867
H	-0.003876	1.736563	-0.350388
H	-0.508551	-1.421964	1.122073
H	-0.595972	-1.773235	-0.345714
H	-1.370382	0.110323	-1.426008
H	-1.392270	0.774448	1.202411
H	-1.267672	2.535753	-0.732564
H	-2.331115	-0.900747	-2.059999
H	-2.225824	0.158696	2.330410
H	2.030057	2.066960	0.656019
H	2.809123	-1.417796	-0.677538

boat

O	-1.452406	-2.199330	-0.201379
O	-2.658742	0.241638	-0.396665
O	-1.170810	2.321154	0.564253
O	2.658763	-0.241656	-0.396604
O	1.170811	-2.321120	0.564373
O	1.452378	2.199318	-0.201597
H	-2.141532	0.979944	-0.045145
H	-0.238424	2.301754	0.310446
H	1.881274	1.335889	-0.281735
H	0.238416	-2.301740	0.310596
H	-1.881278	-1.335899	-0.281634
H	1.192179	-2.490700	1.496521
H	-1.192140	2.490691	1.496410
H	2.985563	-0.528001	-1.239127
H	-2.985509	0.527937	-1.239217
H	2.141543	-0.979945	-0.045060
H	2.130432	2.819251	0.029299
H	-2.130476	-2.819208	0.029613

book

O	0.117874	1.572275	0.860362
H	0.949472	1.538137	0.359263
H	0.268203	2.137350	1.607136

O	-0.025580	-1.368681	0.898281
H	-0.053774	-0.434904	1.099146
H	-0.855686	-1.552758	0.449400
O	-2.362667	1.361173	-0.424712
H	-1.509815	1.537084	-0.016225
H	-2.394430	1.878175	-1.218626
O	-2.508978	-1.422226	-0.431354
H	-2.582996	-0.464586	-0.495673
H	-3.295360	-1.723162	0.004152
O	2.434402	1.216353	-0.480936
H	2.522377	0.250496	-0.494251
H	2.578582	1.512138	-1.369954
O	2.338611	-1.489032	-0.419978
H	1.479564	-1.583381	0.021430
H	2.944569	-2.053486	0.040899

cage
O	-0.875787	-1.736705	0.458302
H	-1.688045	-1.239068	0.295937
H	-1.128240	-2.611132	0.723640
O	0.768946	0.365779	1.625872
H	0.310706	-0.462982	1.493723
H	1.640550	0.236244	1.243104
O	-0.622939	1.772826	-0.182490
H	-0.090811	1.391225	0.541049
H	-0.536999	2.715363	-0.126789
O	0.683418	-0.451217	-1.634552
H	0.202441	-1.062580	-1.077121
H	0.261993	0.392143	-1.480899
O	-2.826200	0.098799	-0.103812
H	-2.203345	0.831916	-0.158058
H	-3.317804	0.100553	-0.914447
O	2.942492	0.011041	-0.105077
H	2.299097	-0.218166	-0.785772
H	3.691020	-0.557694	-0.220306

prism
O	1.515928	-0.346418	-1.428219
H	0.631643	-0.755871	-1.492351
H	2.019851	-0.637800	-2.176537
O	1.774967	-0.207063	1.340751
H	1.909518	-0.412882	0.410803
H	2.534747	-0.521908	1.812883
O	0.540321	2.005762	-0.092067
H	0.934706	1.472371	-0.781643
H	0.964894	1.690919	0.702001

O	-0.969332	-1.323206	-1.303332
H	-0.975956	-1.598193	-0.380110
H	-1.553795	-0.567959	-1.299204
O	-0.951823	-1.244513	1.492721
H	-0.064066	-0.922406	1.643731
H	-1.483155	-0.464454	1.346154
O	-2.036441	1.051590	0.013718
H	-1.190499	1.518313	-0.027613
H	-2.716838	1.710645	0.053309

ring

O	0.000000	2.706019	0.168983
H	-0.120001	3.226447	0.952048
H	-0.826850	2.221338	0.036357
O	-2.343481	-1.353009	0.168983
H	-1.510310	-1.826742	0.036357
H	-2.734184	-1.717148	0.952048
O	2.343481	1.353009	-0.168983
H	2.734184	1.717148	-0.952048
H	1.510310	1.826742	-0.036357
O	0.000000	-2.706019	-0.168983
H	0.826850	-2.221338	-0.036357
H	0.120001	-3.226447	-0.952048
O	2.343481	-1.353009	0.168983
H	2.854186	-1.509299	0.952048
H	2.337160	-0.394596	0.036357
O	-2.343481	1.353009	-0.168983
H	-2.854186	1.509299	-0.952048
H	-2.337160	0.394596	-0.036357

Table S13. Cartesian Coordinates (Å) for MPWB1K/MG3S Optimized Geometries

bag

O	-0.939010	1.698480	-0.404851
O	-0.142901	-1.962710	0.424675
O	1.726141	1.659748	-0.146916
O	2.342732	-0.960323	0.019334
O	-1.384319	0.141140	1.934895
O	-1.438237	-0.736976	-1.795827
H	1.489138	-1.400899	0.179722
H	2.012498	0.729284	-0.147132
H	0.035497	1.733757	-0.329317
H	-0.552531	-1.416164	1.099062
H	-0.624767	-1.745527	-0.377380
H	-1.353659	0.152858	-1.441807
H	-1.382383	0.783212	1.220567
H	-1.219150	2.559791	-0.690592
H	-2.340056	-0.835577	-2.074643
H	-2.255010	0.152945	2.312378
H	2.085919	2.036947	0.647161
H	2.789258	-1.465498	-0.648500

boat

O	-1.524601	-2.154008	-0.216120
O	-2.656612	0.325617	-0.370635
O	-1.092106	2.366205	0.551409
O	2.656610	-0.325642	-0.370628
O	1.092110	-2.366166	0.551571
O	1.524599	2.153993	-0.216289
H	-2.107952	1.050250	-0.033308
H	-0.159391	2.313668	0.295829
H	1.926525	1.274255	-0.280443
H	0.159393	-2.313648	0.295993
H	-1.926526	-1.274274	-0.280338
H	1.104553	-2.541249	1.484275
H	-1.104542	2.541342	1.484104
H	2.990867	-0.619866	-1.209063
H	-2.990876	0.619781	-1.209088
H	2.107953	-1.050250	-0.033245
H	2.219899	2.752482	0.025305
H	-2.219903	-2.752480	0.025512

book

O	0.123130	1.569248	0.866687
H	0.955956	1.532937	0.363655
H	0.272555	2.147447	1.605233

O	-0.028390	-1.372601	0.916259
H	-0.049057	-0.437920	1.120907
H	-0.861858	-1.546153	0.465426
O	-2.350838	1.368381	-0.433995
H	-1.496564	1.543159	-0.023865
H	-2.375246	1.877945	-1.234543
O	-2.500776	-1.414849	-0.433119
H	-2.571866	-0.455228	-0.498525
H	-3.290659	-1.711842	0.001722
O	2.436885	1.209467	-0.475489
H	2.511489	0.240394	-0.499369
H	2.576332	1.511183	-1.364704
O	2.313022	-1.492335	-0.437087
H	1.459425	-1.583145	0.020301
H	2.925230	-2.057264	0.017715

cage

O	0.868126	-1.730361	-0.468548
H	1.684266	-1.235703	-0.304237
H	1.117643	-2.605865	-0.738409
O	-0.769057	0.383882	-1.621277
H	-0.312010	-0.448276	-1.494037
H	-1.642754	0.253336	-1.238819
O	0.631043	1.767844	0.192434
H	0.093697	1.392045	-0.533624
H	0.550271	2.712587	0.141157
O	-0.685505	-0.455391	1.634305
H	-0.205588	-1.063026	1.069077
H	-0.265941	0.391300	1.483577
O	2.830473	0.088428	0.101669
H	2.206170	0.822692	0.158721
H	3.304271	0.073898	0.924539
O	-2.944259	0.009076	0.104139
H	-2.295982	-0.220761	0.782824
H	-3.680601	-0.580050	0.207450

prism

O	-1.513369	-0.322444	1.431280
H	-0.627504	-0.733698	1.500231
H	-2.016863	-0.601061	2.186380
O	-1.777001	-0.217848	-1.335876
H	-1.907905	-0.411023	-0.400889
H	-2.537216	-0.545587	-1.801164
O	-0.530682	2.006615	0.068066
H	-0.924505	1.478640	0.764383
H	-0.961859	1.686324	-0.721932

O	0.964151	-1.308093	1.317961
H	0.967800	-1.594419	0.396047
H	1.548909	-0.551297	1.299232
O	0.945085	-1.268077	-1.474065
H	0.053488	-0.951333	-1.624481
H	1.473444	-0.481804	-1.340369
O	2.039172	1.045583	-0.030438
H	1.192070	1.515010	0.003087
H	2.721289	1.704360	-0.075942

ring

O	0.000000	2.707705	0.159955
H	-0.117841	3.229415	0.944112
H	-0.828328	2.219999	0.033291
O	-2.344941	-1.353853	0.159955
H	-1.508412	-1.827352	0.033291
H	-2.737835	-1.716761	0.944112
O	2.344941	1.353853	-0.159955
H	2.737835	1.716761	-0.944112
H	1.508412	1.827352	-0.033291
O	0.000000	-2.707705	-0.159955
H	0.828328	-2.219999	-0.033291
H	0.117841	-3.229415	-0.944112
O	2.344941	-1.353853	0.159955
H	2.855676	-1.512654	0.944112
H	2.336740	-0.392647	0.033291
O	-2.344941	1.353853	-0.159955
H	-2.855676	1.512654	-0.944112
H	-2.336740	0.392647	-0.033291

Table S14. Cartesian Coordinates (Å) for M05-2X/MG3S Optimized Geometries

bag

O	-1.283101	1.352762	-0.746156
O	0.245704	-1.765359	0.829948
O	1.315870	1.812140	-0.411488
O	2.503294	-0.595322	-0.114042
O	-1.172530	0.487265	1.949503
O	-1.398439	-1.392624	-1.462464
H	1.748336	-1.109875	0.245886
H	1.807674	0.962873	-0.389457
H	-0.315282	1.548083	-0.675478
H	-0.179591	-1.100657	1.388884
H	-0.335680	-1.841582	0.059696
H	-1.454216	-0.432257	-1.345227
H	-1.429226	0.876252	1.101607
H	-1.675137	2.077050	-1.233475
H	-2.288202	-1.706541	-1.617178
H	-1.965452	0.424689	2.480440
H	1.501835	2.236075	0.426844
H	2.898560	-1.124990	-0.804950

boat

O	-1.803644	-1.946687	-0.154689
O	-2.563130	0.665582	-0.453039
O	-0.788994	2.485733	0.569037
O	2.563240	-0.665582	-0.452863
O	0.788972	-2.485719	0.569027
O	1.803526	1.946669	-0.154891
H	-1.942644	1.318616	-0.074615
H	0.141718	2.318406	0.327618
H	2.072172	1.014678	-0.271577
H	-0.141758	-2.318378	0.327686
H	-2.072192	-1.014683	-0.271512
H	0.801608	-2.648644	1.511325
H	-0.801571	2.648493	1.511364
H	2.782970	-0.983576	-1.327919
H	-2.782714	0.983511	-1.328156
H	1.942694	-1.318589	-0.074496
H	2.577389	2.421190	0.144463
H	-2.577442	-2.420996	0.145168

book

O	0.147786	1.565862	0.878885
H	0.987215	1.518869	0.371141
H	0.304372	2.135425	1.631716

O	-0.048581	-1.363199	0.890134
H	-0.070941	-0.420230	1.091904
H	-0.890594	-1.548067	0.444682
O	-2.322541	1.392528	-0.450210
H	-1.466467	1.554228	-0.022070
H	-2.306588	1.865274	-1.281491
O	-2.553072	-1.395243	-0.410672
H	-2.597651	-0.427600	-0.485423
H	-3.350401	-1.670896	0.039603
O	2.455717	1.188653	-0.472808
H	2.525797	0.210896	-0.489222
H	2.587743	1.486246	-1.372128
O	2.311110	-1.515553	-0.432261
H	1.441238	-1.593198	0.014370
H	2.912927	-2.095335	0.032377

cage

O	0.898045	-1.757500	-0.426954
H	1.699578	-1.221466	-0.272579
H	1.182501	-2.639315	-0.665010
O	-0.798955	0.257058	-1.649004
H	-0.316258	-0.562738	-1.483863
H	-1.664224	0.136997	-1.226427
O	0.567954	1.791223	0.056239
H	0.038454	1.344212	-0.649426
H	0.451628	2.734807	-0.050745
O	-0.604183	-0.358382	1.658955
H	-0.144295	-1.009428	1.114399
H	-0.211639	0.487491	1.410771
O	2.792976	0.138964	0.136306
H	2.156191	0.873935	0.118015
H	3.199997	0.153492	1.002149
O	-2.915626	-0.011849	0.164329
H	-2.247226	-0.196396	0.847828
H	-3.666408	-0.577700	0.335915

prism

O	-1.536656	-0.269243	1.435270
H	-0.637814	-0.675591	1.517760
H	-2.042619	-0.527646	2.204885
O	-1.763116	-0.260154	-1.343189
H	-1.909128	-0.421185	-0.396355
H	-2.528490	-0.590173	-1.812865
O	-0.527808	1.994872	-0.018241
H	-0.926089	1.495393	0.706337
H	-0.949255	1.621215	-0.799710

O	0.939020	-1.242630	1.372104
H	0.955514	-1.584141	0.461545
H	1.524010	-0.477670	1.313854
O	0.973329	-1.315010	-1.427483
H	0.074050	-1.013161	-1.603530
H	1.493644	-0.513254	-1.299321
O	2.042802	1.028982	-0.038950
H	1.189641	1.505515	-0.039041
H	2.735967	1.686166	-0.089647

ring

O	0.000000	2.713942	0.170320
H	-0.120065	3.228844	0.967172
H	-0.833197	2.222193	0.034395
O	-2.350343	-1.356971	0.170320
H	-1.507877	-1.832666	0.034395
H	-2.736228	-1.718401	0.967172
O	2.350343	1.356971	-0.170320
H	2.736228	1.718401	-0.967172
H	1.507877	1.832666	-0.034395
O	0.000000	-2.713942	-0.170320
H	0.833197	-2.222193	-0.034395
H	0.120065	-3.228844	-0.967172
O	2.350343	-1.356971	0.170320
H	2.856293	-1.510443	0.967172
H	2.341074	-0.389527	0.034395
O	-2.350343	1.356971	-0.170320
H	-2.856293	1.510443	-0.967172
H	-2.341074	0.389527	-0.034395

Table S15. Cartesian Coordinates (Å) for M06-2X/MG3S Optimized Geometries

bag

O	1.632286	-0.697436	-1.008753
O	-0.619705	1.216748	1.262976
O	-0.821501	-1.622524	-0.849602
O	-2.600661	0.404819	-0.423076
O	0.778536	-1.321019	1.575146
O	1.378253	2.050926	-0.546106
H	-1.978682	0.823540	0.207509
H	-1.526416	-0.944711	-0.848513
H	0.693775	-1.014089	-1.096939
H	-0.209152	0.393077	1.557505
H	0.061307	1.654085	0.728008
H	1.599672	1.145870	-0.819862
H	1.397399	-1.187186	0.840851
H	2.139627	-1.137662	-1.692493
H	2.205152	2.480719	-0.325494
H	1.286599	-1.642430	2.321325
H	-0.755542	-1.916323	0.065416
H	-2.891413	1.092996	-1.022000

boat

O	-1.459569	-2.181999	-0.229882
O	-2.656912	0.259881	-0.374308
O	-1.146367	2.323875	0.567149
O	2.656901	-0.259927	-0.374362
O	1.146362	-2.323806	0.567368
O	1.459596	2.181974	-0.229985
H	-2.123623	1.001933	-0.023650
H	-0.206142	2.291975	0.300662
H	1.887788	1.303901	-0.289504
H	0.206143	-2.291940	0.300855
H	-1.887775	-1.303934	-0.289407
H	1.153069	-2.490771	1.510343
H	-1.153091	2.490946	1.510106
H	2.974547	-0.548900	-1.230818
H	-2.974658	0.548778	-1.230752
H	2.123620	-1.001934	-0.023596
H	2.143604	2.799577	0.028916
H	-2.143572	-2.799614	0.029005

book

O	0.160433	1.566236	0.858485
H	1.004394	1.506291	0.353714
H	0.323369	2.137961	1.610178

O	-0.057148	-1.328450	0.878588
H	-0.080552	-0.382605	1.074555
H	-0.903423	-1.518106	0.440062
O	-2.296862	1.381084	-0.445495
H	-1.436307	1.549119	-0.024885
H	-2.281151	1.843299	-1.284449
O	-2.551463	-1.383489	-0.400115
H	-2.592154	-0.413603	-0.470862
H	-3.346774	-1.652768	0.060848
O	2.448132	1.159305	-0.470516
H	2.510504	0.178295	-0.484736
H	2.572448	1.449858	-1.374851
O	2.288216	-1.522210	-0.419976
H	1.414155	-1.585945	0.025968
H	2.885021	-2.091606	0.066683

cage

O	0.894777	-1.751631	-0.420134
H	1.692695	-1.207416	-0.261798
H	1.190008	-2.632203	-0.655417
O	-0.808275	0.209948	-1.635994
H	-0.320464	-0.606292	-1.458217
H	-1.671172	0.090665	-1.205377
O	0.548686	1.791206	-0.003862
H	0.014753	1.314395	-0.690878
H	0.433642	2.730681	-0.152658
O	-0.553004	-0.322881	1.643808
H	-0.100962	-0.980938	1.098104
H	-0.173499	0.522293	1.367722
O	2.746886	0.148210	0.156998
H	2.113143	0.886633	0.103546
H	3.109329	0.171179	1.044004
O	-2.885585	-0.015760	0.200400
H	-2.200877	-0.187258	0.873131
H	-3.634471	-0.574473	0.408113

prism

O	-1.537691	1.150654	-0.879239
H	-0.648390	1.516588	-0.630380
H	-2.048484	1.864133	-1.263568
O	-1.781234	-0.783900	1.079935
H	-1.928892	-0.004785	0.515591
H	-2.559455	-0.891004	1.628733
O	-0.424336	-1.421288	-1.356397
H	-0.852877	-0.575517	-1.549838
H	-0.868578	-1.709690	-0.549947

O	0.883593	1.843147	-0.096187
H	0.882265	1.439019	0.790664
H	1.507278	1.278601	-0.571764
O	0.890407	-0.056554	1.936607
H	0.001941	-0.418014	1.816576
H	1.448262	-0.530686	1.306390
O	2.094682	-0.697355	-0.620912
H	1.255159	-1.053920	-0.977657
H	2.808405	-1.192362	-1.025249

ring

O	0.000000	2.694124	0.174434
H	-0.117249	3.193462	0.983242
H	-0.835556	2.202952	0.035359
O	-2.333180	-1.347062	0.174434
H	-1.490034	-1.825088	0.035359
H	-2.706995	-1.698272	0.983242
O	2.333180	1.347062	-0.174434
H	2.706995	1.698272	-0.983242
H	1.490034	1.825088	-0.035359
O	0.000000	-2.694124	-0.174434
H	0.835556	-2.202952	-0.035359
H	0.117249	-3.193462	-0.983242
O	2.333180	-1.347062	0.174434
H	2.824244	-1.495190	0.983242
H	2.325590	-0.377864	0.035359
O	-2.333180	1.347062	-0.174434
H	-2.824244	1.495190	-0.983242
H	-2.325590	0.377864	-0.035359

Table S16. Cartesian Coordinates (Å) for MPW1K/MG3S Optimized Geometries

bag

O	-0.894964	1.687001	-0.377325
O	-0.201999	-1.942293	0.397019
O	1.741311	1.610598	-0.153111
O	2.281397	-0.990068	0.063548
O	-1.378826	0.146738	1.938081
O	-1.384740	-0.678049	-1.834439
H	1.410960	-1.413614	0.197944
H	1.999566	0.668456	-0.125521
H	0.084474	1.707948	-0.307010
H	-0.608141	-1.391615	1.071997
H	-0.658036	-1.695925	-0.413368
H	-1.303486	0.202289	-1.453123
H	-1.353625	0.789528	1.223161
H	-1.165613	2.556946	-0.645253
H	-2.282364	-0.766577	-2.129420
H	-2.260353	0.161535	2.289162
H	2.112215	2.000027	0.629766
H	2.726970	-1.490420	-0.608522

boat

O	-1.564602	-2.077412	-0.256213
O	-2.628558	0.400639	-0.332300
O	-0.999384	2.363525	0.550510
O	2.628545	-0.400675	-0.332328
O	0.999384	-2.363474	0.550692
O	1.564617	2.077392	-0.256330
H	-2.045874	1.107636	-0.006470
H	-0.070693	2.277616	0.278993
H	1.947685	1.184464	-0.291579
H	0.070694	-2.277582	0.279163
H	-1.947687	-1.184491	-0.291479
H	0.991820	-2.521152	1.486435
H	-0.991823	2.521308	1.486235
H	2.967117	-0.704995	-1.165327
H	-2.967161	0.704894	-1.165310
H	2.045869	-1.107643	-0.006423
H	2.265212	2.662602	0.001683
H	-2.265177	-2.662627	0.001841

book

O	0.111865	1.539732	0.863192
H	0.948370	1.510228	0.359444
H	0.255739	2.115605	1.604514

O	-0.019426	-1.384032	0.913599
H	-0.039954	-0.449300	1.121331
H	-0.847511	-1.548250	0.445405
O	-2.336427	1.357384	-0.421898
H	-1.480037	1.522799	-0.007826
H	-2.344310	1.851108	-1.232587
O	-2.453854	-1.399201	-0.441743
H	-2.526893	-0.436992	-0.496516
H	-3.236903	-1.700583	0.002242
O	2.403493	1.213232	-0.464869
H	2.475355	0.240846	-0.494013
H	2.522127	1.517823	-1.356069
O	2.285691	-1.458948	-0.445403
H	1.433742	-1.558767	0.020363
H	2.909540	-2.009855	0.010699

cage

O	0.861654	-1.703255	-0.485943
H	1.673206	-1.197016	-0.318777
H	1.124056	-2.568032	-0.776678
O	-0.731584	0.443095	-1.612582
H	-0.275348	-0.393593	-1.509860
H	-1.605780	0.298209	-1.231184
O	0.615327	1.727353	0.275262
H	0.093247	1.378894	-0.480007
H	0.536060	2.673341	0.258363
O	-0.723293	-0.510870	1.637389
H	-0.233641	-1.106310	1.066682
H	-0.299428	0.338002	1.507221
O	2.807224	0.095564	0.075666
H	2.171606	0.817538	0.179485
H	3.296383	0.049989	0.888246
O	-2.902902	0.016858	0.057501
H	-2.269920	-0.240126	0.743916
H	-3.621849	-0.600859	0.094250

prism

O	-1.474387	-0.269582	1.430266
H	-0.567861	-0.634799	1.536449
H	-1.975204	-0.520675	2.196527
O	-1.709882	-0.437763	-1.309728
H	-1.837084	-0.541527	-0.358394
H	-2.456613	-0.837251	-1.739133
O	-0.665342	2.006132	-0.103509
H	-1.017682	1.508723	0.637066
H	-1.057240	1.573475	-0.860313

O	1.017474	-1.142343	1.423612
H	1.048061	-1.504744	0.527460
H	1.549194	-0.351097	1.337977
O	1.043426	-1.358346	-1.341487
H	0.132366	-1.124640	-1.527449
H	1.504115	-0.522135	-1.269127
O	1.920754	1.145425	-0.116119
H	1.050889	1.577062	-0.125003
H	2.570712	1.829430	-0.220331

ring

O	0.000000	2.677074	0.149799
H	-0.111534	3.195363	0.937031
H	-0.830423	2.185569	0.029104
O	-2.318414	-1.338537	0.149799
H	-1.477547	-1.811952	0.029104
H	-2.711499	-1.694273	0.937031
O	2.318414	1.338537	-0.149799
H	2.711499	1.694273	-0.937031
H	1.477547	1.811952	-0.029104
O	0.000000	-2.677074	-0.149799
H	0.830423	-2.185569	-0.029104
H	0.111534	-3.195363	-0.937031
O	2.318414	-1.338537	0.149799
H	2.823032	-1.501090	0.937031
H	2.307970	-0.373618	0.029104
O	-2.318414	1.338537	-0.149799
H	-2.823032	1.501090	-0.937031
H	-2.307970	0.373618	-0.029104

Table S17. Cartesian Coordinates (Å) for PBEh/MG3S Optimized Geometries

bag

O	-0.895193	1.669899	-0.394134
O	-0.211117	-1.931902	0.419685
O	1.731444	1.600471	-0.177328
O	2.265828	-0.988601	0.073790
O	-1.349149	0.180824	1.950629
O	-1.371422	-0.698039	-1.836744
H	1.381856	-1.411460	0.212479
H	1.985152	0.644561	-0.132268
H	0.097601	1.695152	-0.324988
H	-0.611851	-1.355358	1.089937
H	-0.666110	-1.682164	-0.401697
H	-1.295261	0.194139	-1.457384
H	-1.335905	0.816169	1.216152
H	-1.168042	2.544679	-0.671265
H	-2.285521	-0.801502	-2.099848
H	-2.243277	0.180116	2.291218
H	2.087563	1.992908	0.620308
H	2.690660	-1.478442	-0.629824

boat

O	-1.617957	-1.999158	-0.338981
O	-2.623291	0.49547	-0.280374
O	-0.888835	2.367695	0.577732
O	2.623281	-0.495495	-0.280388
O	0.888839	-2.36765	0.577902
O	1.617964	1.999133	-0.339125
H	-1.991203	1.178782	0.037283
H	0.035328	2.242261	0.267947
H	1.984974	1.086663	-0.325053
H	-0.035325	-2.24224	0.268108
H	-1.984975	-1.08669	-0.324953
H	0.838441	-2.476635	1.527069
H	-0.838434	2.476773	1.526888
H	2.966471	-0.828219	-1.109568
H	-2.966504	0.828135	-1.109568
H	1.9912	-1.178782	0.037335
H	2.329174	2.576931	-0.064899
H	-2.329162	-2.576949	-0.064726

book

O	0.113614	1.531180	0.868423
H	0.959009	1.501298	0.356123
H	0.258634	2.124489	1.605643

O	-0.018983	-1.387506	0.938974
H	-0.034616	-0.443042	1.144321
H	-0.852057	-1.541329	0.455047
O	-2.326112	1.360619	-0.423795
H	-1.460771	1.524917	-0.004904
H	-2.316207	1.839438	-1.252408
O	-2.426308	-1.394255	-0.452895
H	-2.500282	-0.421672	-0.502176
H	-3.212667	-1.693678	0.003338
O	2.396140	1.209077	-0.462118
H	2.451797	0.223720	-0.499881
H	2.482714	1.513782	-1.365309
O	2.252779	-1.454731	-0.464712
H	1.401792	-1.551495	0.028123
H	2.893608	-1.991498	0.001069

cage

O	0.854447	-1.685517	-0.515045
H	1.674235	-1.175801	-0.336436
H	1.123345	-2.549892	-0.825738
O	-0.726575	0.482438	-1.610997
H	-0.264509	-0.362729	-1.520538
H	-1.604527	0.324001	-1.217522
O	0.610789	1.708728	0.315446
H	0.085300	1.375241	-0.460596
H	0.540172	2.663338	0.312294
O	-0.729136	-0.547477	1.641540
H	-0.233203	-1.134815	1.053126
H	-0.303724	0.311599	1.517332
O	2.806266	0.095696	0.068572
H	2.157965	0.817152	0.192553
H	3.275310	0.017027	0.899598
O	-2.891395	0.021522	0.051122
H	-2.253327	-0.258915	0.738347
H	-3.592201	-0.629325	0.042477

prism

O	-1.454891	-0.266753	1.433769
H	-0.531590	-0.624265	1.541819
H	-1.952655	-0.523197	2.209712
O	-1.700538	-0.484774	-1.297225
H	-1.824346	-0.578040	-0.334540
H	-2.446877	-0.910796	-1.718719
O	-0.704115	2.004795	-0.126713
H	-1.041679	1.498603	0.626570
H	-1.093270	1.544130	-0.879104

O	1.041652	-1.110773	1.436595
H	1.072245	-1.475884	0.529847
H	1.557933	-0.300818	1.335767
O	1.061707	-1.368488	-1.321214
H	0.137338	-1.148738	-1.505288
H	1.507525	-0.513045	-1.265638
O	1.890982	1.171664	-0.141092
H	1.005173	1.594366	-0.152930
H	2.531832	1.872323	-0.260449

ring

O	0.000000	2.672882	0.131968
H	-0.104254	3.182782	0.934984
H	-0.838708	2.170135	0.023873
O	-2.314784	-1.336441	0.131968
H	-1.460038	-1.811410	0.023873
H	-2.704243	-1.681678	0.934984
O	2.314784	1.336441	-0.131968
H	2.704243	1.681678	-0.934984
H	1.460038	1.811410	-0.023873
O	0.000000	-2.672882	-0.131968
H	0.838708	-2.170135	-0.023873
H	0.104254	-3.182782	-0.934984
O	2.314784	-1.336441	0.131968
H	2.808497	-1.501104	0.934984
H	2.298746	-0.358725	0.023873
O	-2.314784	1.336441	-0.131968
H	-2.808497	1.501104	-0.934984
H	-2.298746	0.358725	-0.023873

Table S18. Harmonic Frequency Scaling Factors

MP2/aug'-cc-pVTZ	0.9814
BLYP/6-31+G(d,p)	1.0160
B3LYP/6-31+G(d,2p)	0.9856
M06-L/aug-cc-pVTZ	0.9878
PBE/aug-cc-pVTZ	1.0143
PBE1W/6-311+G(2d,2p)	1.0113
BLYP/MG3S	1.0149
B3LYP/MG3S	0.9850
M06-L/MG3S	0.9855
PBE/MG3S	1.0118
PBE1W/MG3S	1.0106
PBEh/MG3S	0.9775
PWB6K/MG3S	0.9528
MPWB1K/MG3S	0.9566
MPW1K/MG3S	0.9546
M05-2X/MG3S	0.9633
M06-2X/MG3S	0.9702

Table S19. Absolute Energies (in hartrees) for Optimized Hexamer Structures

	bag	boat	book	cage	prism	ring
MP2/aug'-cc-pVTZ	-458.040789670	-458.039087597	-458.042170846	-458.042650328	-458.042668980	-458.040683409
BLYP/6-31+G(d,p)	-458.574519998	-458.575093768	-458.576751984	-458.574319321	-458.573918367	-458.577410852
B3LYP/6-31+G(d,2p)	-458.693370074	-458.693960304	-458.695443090	-458.693504242	-458.693188919	-458.696009991
M06-L/aug-cc-pVTZ	-458.739663071	-458.735813308	-458.740209120	-458.743269955	-458.743999724	-458.737207185
PBE/aug-cc-pVTZ	-458.355346348	-458.356919375	-458.359010319	-458.357589957	-458.356974794	-458.358602200
PBE1W/6-311+G(2d,2p)	-458.852507348	-458.851564613	-458.854042731	-458.852889629	-458.852769666	-458.853233557
BLYP/MG3S	-458.739968412	-458.740204979	-458.741794051	-458.739874669	-458.739412643	-458.741950043
B3LYP/MG3S	-458.844714499	-458.844677534	-458.846549470	-458.845224936	-458.845095674	-458.846482479
M06-L/MG3S	-458.744112372	-458.740679266	-458.744886651	-458.747911334	-458.748742323	-458.742259812
PBE/MG3S	-458.337924770	-458.336845190	-458.339498528	-458.338510952	-458.338426895	-458.338575963
PBE1W/MG3S	-458.855354264	-458.854584535	-458.856897121	-458.855691068	-458.855580649	-458.856280647
PBEh/MG3S	-458.332433514	-458.331640321	-458.334105697	-458.333419372	-458.333597711	-458.333462718
PWB6K/MG3S	-458.981978297	-458.980835215	-458.983505534	-458.984442303	-458.985100811	-458.982553614
MPWB1K/MG3S	-458.591646211	-458.591094826	-458.593306329	-458.593891113	-458.594350226	-458.592833034
MPW1K/MG3S	-458.654669772	-458.654656940	-458.656474307	-458.655528965	-458.655611346	-458.656477774
M05-2x/MG3S	-458.751618409	-458.748859538	-458.752889913	-458.755055229	-458.756351576	-458.750622976
M06-2X/MG3S	-458.627253521	-458.623002759	-458.627296224	-458.630550928	-458.632054499	-458.624713400

Table S20. Absolute Single-Point Energies (in hartrees) at the MP2/aug'-cc-pVTZ Geometry

	bag	boat	book	cage	prism	ring
CCSD(T)	-458.120279970	-458.118259459	-458.121653836	-458.122450109	-458.122778097	-458.119857841
MP2/aug'-cc-PVTZ	-458.040789670	-458.039087597	-458.042170846	-458.042650328	-458.042668980	-458.040683409
BLYP/6-31+G(d,p)	-458.571345622	-458.572006942	-458.573588154	-458.571065481	-458.570673329	-458.574354185
B3LYP/6-31+G(d,2p)	-458.692963940	-458.693561384	-458.695072148	-458.693070737	-458.692766588	-458.695661845
M06-L/aug-cc-pVTZ	-458.739138005	-458.735574663	-458.740009520	-458.743039515	-458.743791170	-458.737037487
PBE/aug-cc-pVTZ	-458.355346348	-458.354726851	-458.356972421	-458.355699407	-458.355269571	-458.356490261
PBE1W/6-311+G(2d,2p)	-458.851114143	-458.850045929	-458.852613111	-458.851467813	-458.851501950	-458.851836908
BLYP/MG3S	-458.738181959	-458.738518147	-458.740051670	-458.737969148	-458.737572965	-458.740329345
B3LYP/MG3S	-458.844412686	-458.844443760	-458.846281539	-458.844865921	-458.844736495	-458.846288312
M06-L/MG3S	-458.743555125	-458.740374766	-458.744634610	-458.747643083	-458.748474215	-458.741972530
PBE/MG3S	-458.336237164	-458.334961445	-458.337765944	-458.336932133	-458.337014066	-458.336802668
PBE1W/MG3S	-458.854078303	-458.853262154	-458.855604133	-458.854365428	-458.854356075	-458.855042711
PBEH/MG3S	-458.332111325	-458.331256843	-458.333763594	-458.333126958	-458.333317516	-458.333113116
PWB6K/MG3S	-458.979578987	-458.978623338	-458.981205934	-458.982016612	-458.982710094	-458.980395142
MPWB1K/MG3S	-458.589744080	-458.589346222	-458.591501572	-458.591970048	-458.592460373	-458.591145892
MPW1K/MG3S	-458.653013058	-458.653046793	-458.654840260	-458.653866085	-458.653912806	-458.654918953
M05-2x/MG3S	-458.750975857	-458.748282068	-458.752291713	-458.754400285	-458.755741738	-458.750123685
M06-2X/MG3S	-458.625670135	-458.622692907	-458.626934796	-458.630020124	-458.631463484	-458.624428851