Supplementary Material

Temperature Dependent Structural Variations of $OH^-(H_2O)_n$ *n=4-7:* Effects on Vibrational and Photoelectron Spectra

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Comparison of different quantum chemistry methods

In Fig S1, we present the structure and relative energies of the different topological isomers calculated for $OH^-(H_2O)_n$ n=4-7 using B3LYP/6-31+G(d). Generally speaking the obtained structures are similar with those obtained using the bigger basis set 6-311+G(d,p) given in Fig 1 of the manuscript. However, one can clearly notice that the energies of the open Tree and Linear speacies are much higher than those calculated by the bigger basis set. Thereby for the deprotonated species, the smaller basis set can be said to oversetimate the binding of compact multiring and double ring structures.

Furthermore, in Fig S2 we compare the relative energies of B3LYP/6-311+G(d,p) versus those obtained by MP2 and CCSD both with 6-311+G(d,p) basis set. For n=4-6 we notice that the B3LYP results tend to over stabilize the most stable compact structure. Therefore the MP2 and CCSD energies lie on the upper right side of the red 1:1 line. However, as can be seen from the scattering, the general trend is clearly reproduced by the B3LYP method, thus giving us confidence that the temperature dependence on the dominant topology will not vary with quantum chemistry methods. Of course due to the difference in absolute energy differences, the phase transition temperature may vary with the method used for the calcualtion. This can be seen from the population analysis performed using two different basis set with the B3LYP functional. As given in Fig S3, the temperature dependent rise and fall of the different topolozies are similar between the two basis set calculations, but the transition temperature vary greatly. Due to the overstabilization of the most stable compact structure with the smaller basis set, the population of this compact structure dominates to higher temperature for the small basis set.

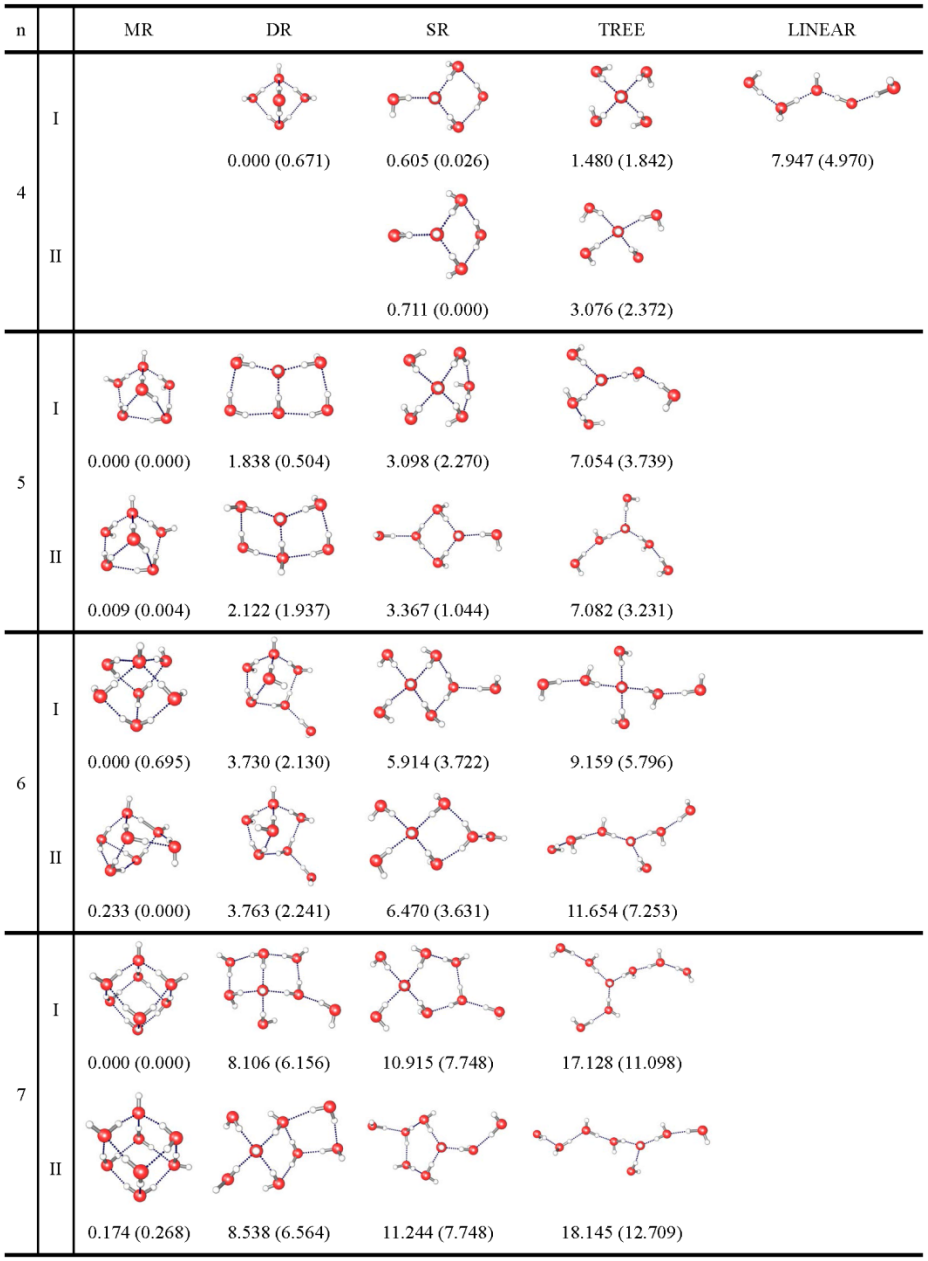

Figure S1. Low-energy isomers of $OH^-(H_2O)_{n=4-7}$, grouped according to their topologies, namely from left to right, MR (multi-ring), DR (double-ring), SR (single-ring), L (linear) and T (tree) and their relative electronic energies (E_0) optimized at B3LYP/6-31+G(d). The numbers enclosed in parentheses denote the relative energies with ZPE correction. All values are shown in the unit of kcal/mol.

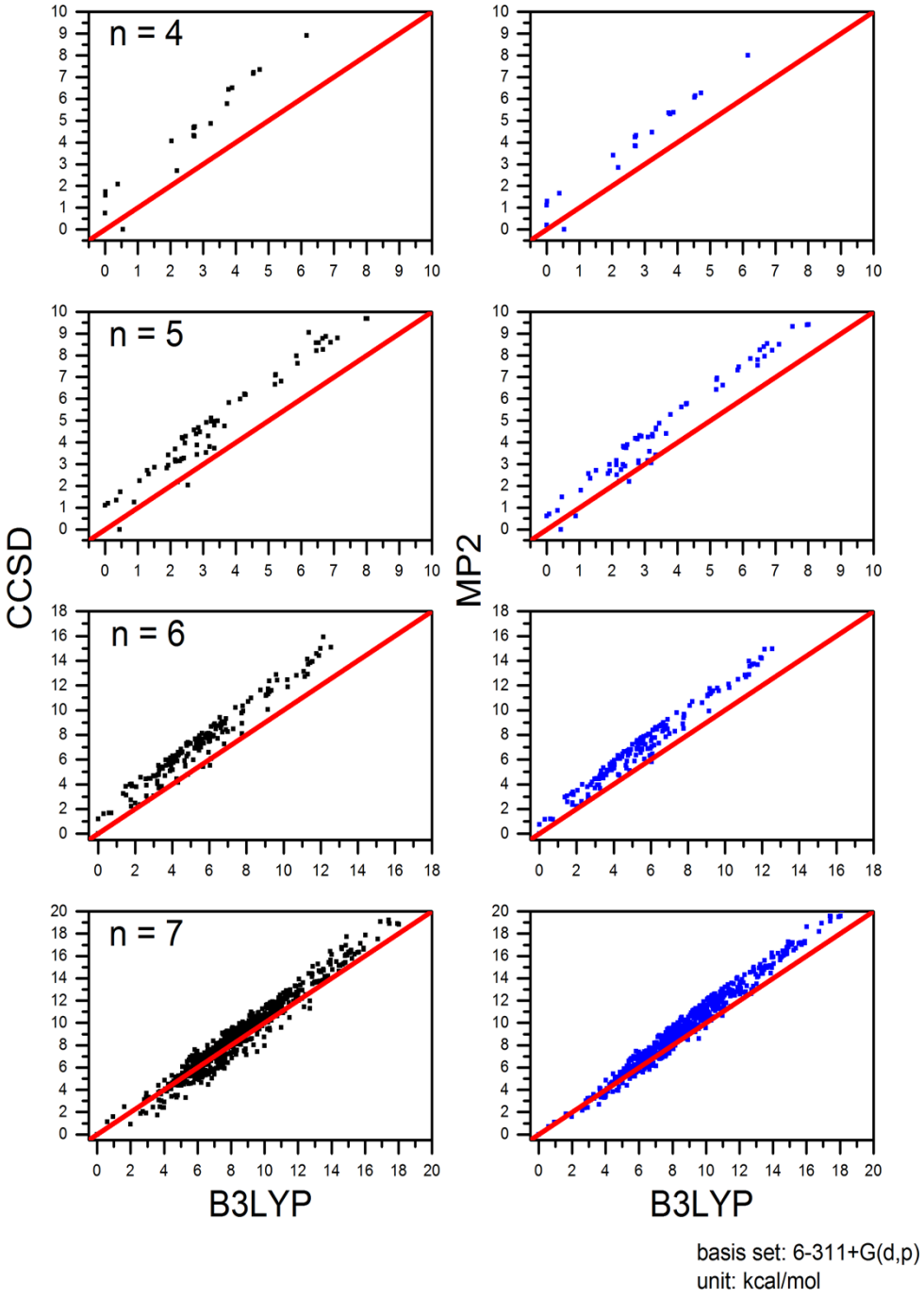

Figure S2: Comparison of the relative energies calculated by B3LYP versus MP2 and CCSD using the 6-311+G(d,p) basis set.

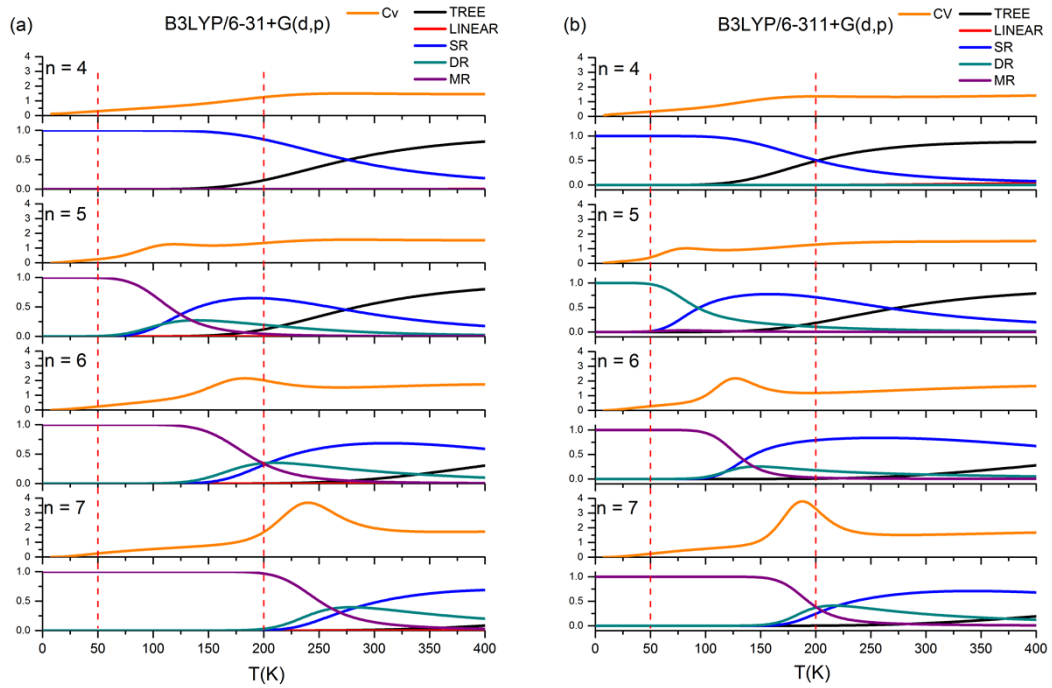

Figure S3. The HSA calculated with B3LYP using 6-311+G(d,p) versus 6-31+G(d). Contributions from Tree, Linear, Single Ring, Double Ring, and Multi Ring isomers are given by black, red, blue, green and violet lines.

Vibrational Spectra

The vibrational sepctra for the 4- and 5-coordinated isomers using the populationat 200 K are given in Fig S4. Due to the small number of isomers the general features are similar to the low temperature 50 K results given in Fig 4 of the manuscript. However, one can clearly see that due to increase in different isomers broad absorptions are seen in the IHB region for $OH^-(H_2O)_7$.

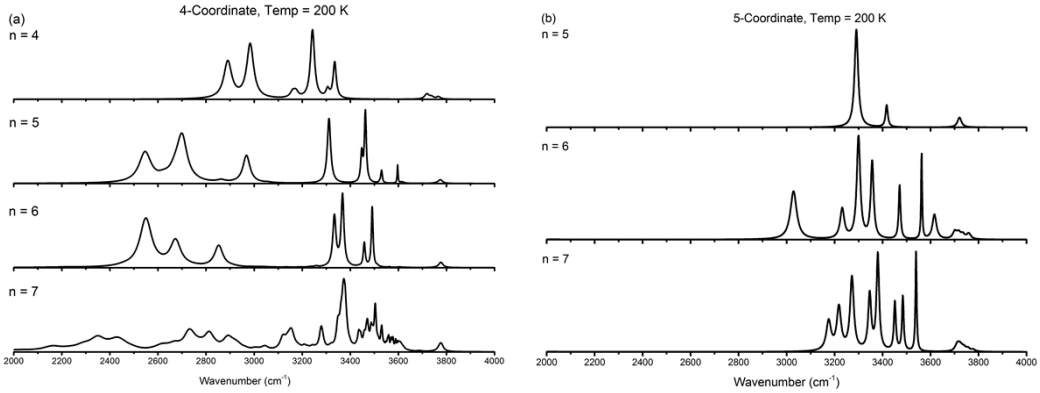

Figure S4. IR spectra of $OH^-(H_2O)_{n=4\text{-}7}$ for the (a) 4- and (b) 5-coordinated isomers calculated using the population at 200 K.

Raman Spectra

The Raman spectra calculate using the scaled harmonic frequencies and the Raman activity calculated using B3LYP/6-311+G(d,p) are given in Fig S5. One can clearly notice that in opposition to the IR absorption spectra, the free OH peaks as well as the hydroxide stretching peaks are obvious in the Raman spectra.

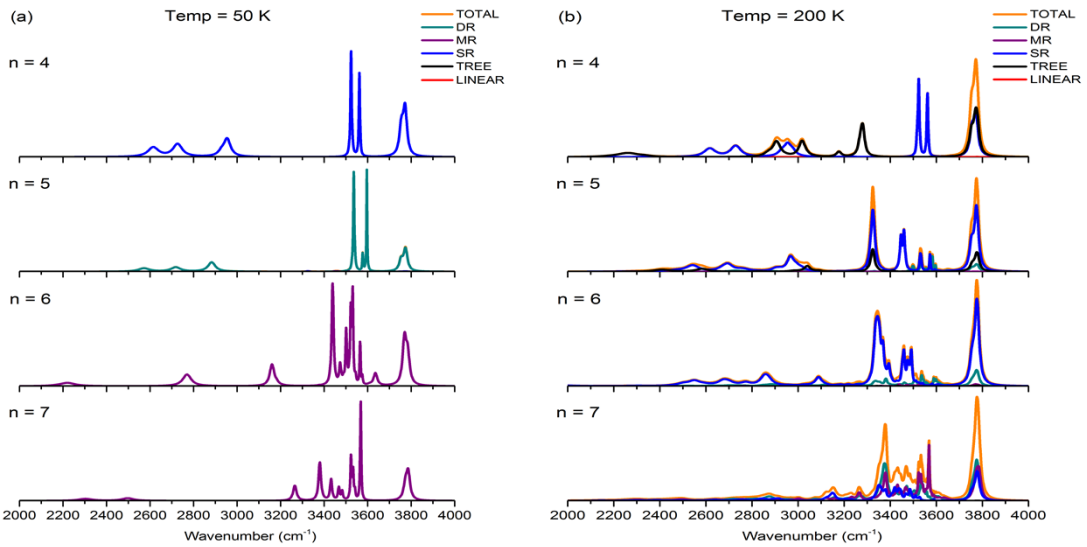

Figure S5. Raman spectra of $OH^-(H_2O)_{n=4\text{-}7}$ at two characteristic temperatures (50K and 200K).

Vertical detachment energy spectra

The vertical detachment energy spectra of $OH^-(H_2O)_n$ n=4-7 of the 4- and 5-coordianted isomers using the population at 50 K are given in Fig S6. Due to the symmetry 1st and 2nd exciations show up at nearly equal energy while the 3rd excitaiton is observed at slightly higher energies. Interestingly, while the first two excitations show n depenedence the 3rd excitation stay nearly constant with increase of second solvation shell waters.

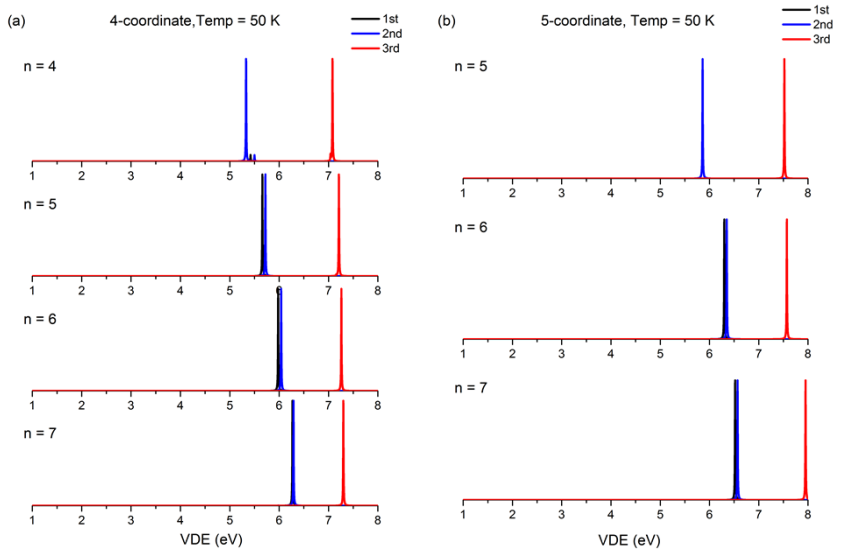

Figure S6. The 1st, 2nd, and 3rd vertical electron detachment spectra of $OH^-(H_2O)_{n=4-7}$ at 50 K calculated using EOM-CCSD methods for the 4 and 5-coordinated species.

Geometry parameter of lowest energy of different topology isomers.

N=4,

DR-I

O	-0.171012 -0.953559 1.785390
O	0.731060 1.723237 1.075226
O	-0.117976 0.839488 -1.197965
O	1.694748 -1.173364 -0.758999
O	-1.889070 -0.923968 -0.563171
H	-0.875492 -1.014848 1.112172
H	0.102069 -0.017832 1.731967
H	0.360013 1.485620 0.152504
H	1.676873 1.581674 0.972539
H	-1.271309 -0.168986 -0.873744
H	-0.247390 1.428774 -1.945072
H	1.126651 -0.431146 -1.083807
H	1.310503 -1.352314 0.111695
H	-1.574048 -1.684467 -1.060474

SR-I

O	-0.644897 -2.709228 -1.174856
O	-0.309279 0.026553 2.081894
O	0.915890 -0.899489 -0.013178
O	-0.888301 2.489766 0.609880
O	0.793301 1.263515 -1.448587
H	0.354015 0.961631 -2.248177
H	1.810691 -1.205182 0.160921
H	-0.340398 2.223949 -0.150800
H	0.904359 0.414019 -0.893063
H	-1.460575 -2.203416 -1.222813
H	0.219539 -0.354183 1.295267
H	-0.768752 1.742513 1.223714
H	-1.034950 -0.593010 2.195630
H	-0.001145 -2.070169 -0.735003

SR-II

O	0.054082 1.179442 0.250869

O	0.309970	-0.027007	-2.040883
O	2.292120	1.736285	1.555132
O	-1.286013	-0.738675	1.402532
O	-1.393386	-2.221500	-1.107554
H	-0.797002	0.046223	0.973842
H	1.414966	1.528242	1.099595
H	-0.668334	-1.060244	2.064856
H	-0.862084	-1.549381	-1.571380
H	-0.469159	1.983254	0.177572
H	2.914737	1.777182	0.824703
H	1.226995	-0.313810	-2.025797
H	0.196920	0.490376	-1.167052
H	-1.460030	-1.846507	-0.210265

TREE-I

O	1.383005	-0.229191	-2.399346
O	-1.358224	-0.632523	0.756151
O	2.902242	-0.365009	1.443835
O	-3.744413	0.614044	0.244342
O	0.792961	0.528305	0.081727
H	2.085576	0.000137	0.984809
H	-0.483077	-0.136834	0.470359
H	-1.160126	-0.994305	1.623661
H	0.687081	-0.877970	-2.535366
H	3.400497	-0.744087	0.714495
H	1.195831	0.107253	-1.469259
H	-3.505157	1.100146	-0.549324
H	-2.907233	0.146168	0.484434
H	0.706749	1.482546	0.165541

TREE-II

O	2.749887	0.809523	-0.088166
O	-1.433520	0.468968	-0.470306
O	-2.548250	-0.069214	-2.905128
O	0.612117	-0.648361	0.516875
O	0.654536	-0.443358	3.174871

H -0.584668 -0.012159 -0.089708
H 2.318653 1.538624 -0.542104
H 1.454829 0.081634 3.264056
H 0.586392 -0.568711 2.179935
H -2.192159 0.074068 -1.993760
H -1.830163 0.228043 -3.470051
H -1.986937 0.630764 0.297944
H 1.978659 0.205424 0.145791
H 0.678175 -1.561886 0.223681

LINEAR-I
O -0.061202 0.267042 -0.295609
O -1.861363 -1.468445 -0.053488
O 3.844635 1.636260 1.348819
O 2.438627 0.122223 -0.432985
O -4.396713 -0.568185 -0.514049
H 1.384365 0.179493 -0.353772
H -1.110005 -0.735545 -0.171819
H -1.655757 -1.892154 0.783473
H -3.500755 -0.941401 -0.314333
H 3.171215 1.764549 2.022178
H -0.357605 1.136882 -0.014538
H 3.380695 1.085127 0.668216
H 2.616505 0.220497 -1.371584
H -4.197462 0.191218 -1.068149

N=5,
MR-I
O 0.780108 -1.388798 1.863068
O -1.741096 1.006547 0.121579
O 0.781381 1.067414 1.037659
O -0.519152 -0.379845 -2.076614
O -1.455618 -2.050990 0.209541
O 1.999077 0.760298 -1.211951
H -1.023155 0.241045 -1.513900

H 1.581351 -1.739239 1.463561
H -1.984478 0.112696 0.404946
H -1.106619 -1.731637 -0.640609
H 0.406609 -0.125435 -1.897350
H 2.021478 1.625136 -1.630291
H 0.794086 -0.398766 1.611094
H -0.835392 1.137899 0.523371
H 1.582843 0.931030 -0.290937
H 1.078428 1.722861 1.674226
H -0.711920 -1.921767 0.832286

MR-II
O 0.024670 0.615176 2.215820
O -1.262157 -1.664618 0.997219
O 0.080857 -1.721745 -1.628936
O 2.243229 0.013460 -0.942309
O -1.773749 0.451903 -1.168043
O 0.404884 1.637830 -0.115106
H -0.706787 1.097381 2.610793
H -1.991912 -0.112102 -0.411218
H -0.747426 -0.982748 1.471335
H 0.202775 1.097137 1.328189
H -0.573301 -1.009712 -1.762106
H 1.562437 0.719397 -0.654383
H 2.643326 -0.269436 -0.115069
H 0.912793 -1.227645 -1.482898
H -1.011208 1.001836 -0.831977
H -0.727375 -1.883680 0.212912
H 0.578586 2.577997 -0.209432

DR-I
O 1.461653 -0.853068 -0.365817
O -1.281490 1.500112 -1.796288
O 1.775905 -0.998068 2.573953
O -1.056853 -0.290628 2.540958
O 1.509607 1.124744 -2.567632

O -1.077453 -0.457569 -0.071017
H -1.248459 0.734788 -1.129439
H -1.382126 2.286399 -1.253249
H 0.831835 -0.809593 2.723437
H 0.446430 -0.744644 -0.268468
H 1.674327 0.501469 -1.839389
H 0.563527 1.329249 -2.456966
H -1.176329 0.645715 2.720552
H -1.110754 -0.362957 1.529344
H 1.852847 -0.921622 1.607424
H 1.585790 -1.731848 -0.735074
H -1.650614 -1.181511 -0.340228

DR-II
O -0.188510 0.691617 -0.902865
O -1.842186 -2.827677 -0.412866
O -0.738197 -0.609830 1.287307
O -0.369911 -1.385138 -2.465422
O 1.699898 2.144157 0.151189
O 0.712433 1.530635 2.817683
H 0.533389 -1.647473 -2.660381
H 2.527627 1.752887 -0.139588
H 1.126978 1.845440 1.993346
H 0.062382 0.884781 2.495729
H -0.894798 1.294299 -1.156032
H -1.708504 -2.136489 0.256264
H -0.282373 -0.542671 -1.899074
H -0.566662 -0.077535 0.433672
H 0.974343 1.598438 -0.311381
H -1.394924 -2.456478 -1.195588
H 0.048836 -1.152311 1.396828

SR-I
O -2.452623 2.245130 2.201318
O -1.335448 -1.328568 0.075296
O 0.704631 -0.778027 -1.803750

O 1.391484 1.294581 0.004539
O -0.475357 0.557691 1.634284
O 2.467869 -2.647783 -2.806813
H -1.726816 1.576041 2.002948
H -2.054037 3.085182 1.959975
H 0.683510 1.018004 0.693777
H -1.012391 -0.619658 0.737442
H 1.822526 -1.963856 -2.510713
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H 1.064619 -0.034513 -1.277618
H 1.122797 2.171713 -0.281248
H -2.235942 -1.065715 -0.133722
H -0.119034 0.215748 2.459733
H 2.792386 -3.013427 -1.979550

SR-II
O -0.510876 1.989260 0.062534
O 0.091558 -0.652115 -4.288516
O -2.024641 -0.634261 3.111382
O 0.654158 0.129713 -1.720914
O 0.154583 0.486867 2.054952
O 1.424230 -1.248845 0.624801
H 0.967898 -0.567284 1.240273
H -2.420442 -1.006255 2.318782
H 0.197178 -0.423608 -3.335555
H 0.982749 -0.455950 -1.007886
H -0.237261 1.449124 0.890183
H 0.869520 -0.257103 -4.690946
H 1.000662 -2.085341 0.835107
H 0.202371 0.849977 -1.234611
H -1.188166 -0.192696 2.770941
H 0.703247 0.928545 2.709466
H -1.468519 2.046408 0.117445

TREE-I
O -0.155135 1.014987 -1.822273

O -2.773799 -1.298670 3.416063
O 0.506946 3.373233 -3.060687
O 2.727479 -1.540070 -0.299056
O 0.711417 0.079620 0.391724
O -0.906697 -1.620138 1.430132
H -1.063783 0.704501 -1.847374
H 2.674395 -1.459267 -1.255254
H 0.215114 0.674188 -0.918151
H -3.476006 -0.903089 2.893058
H 1.400081 3.154666 -3.339375
H 0.217703 2.566365 -2.572349
H 2.005579 -0.921798 0.018581
H -0.378988 -2.423070 1.410353
H -2.042493 -1.412214 2.763905
H -0.283386 -0.897881 1.042398
H 0.963530 0.772167 1.009427

TREE-II
O -0.085931 -0.933807 0.197982
O -3.341160 0.825470 -2.577433
O 1.610123 0.555241 1.411762
O -0.726149 0.141249 -2.042496
O 1.332754 -3.121105 -0.411911
O 1.147074 2.501659 3.290075
H 2.369201 -0.027011 1.501468
H 1.219063 -3.134134 -1.366161
H -2.403837 0.549950 -2.439000
H -0.121908 0.887881 -2.078086
H 0.864613 3.207284 2.702273
H 1.303742 1.745135 2.676830
H 0.893438 -0.023705 0.948111
H -0.510151 -0.315278 -1.143314
H 0.794341 -2.323656 -0.131891
H -0.842877 -1.143022 0.753002
H -3.673794 0.938760 -1.683050

N=6,

MR-I

O	1.436527	0.325089	0.888830
O	-0.188621	-1.558676	1.925090
O	-0.936161	-0.546192	-1.913466
O	-2.269505	-0.054851	0.604058
O	-0.551473	2.192958	1.054177
O	1.455188	-1.714079	-0.729885
O	0.878920	1.744692	-1.522214
H	2.240686	0.505138	1.384776
H	1.552464	-0.916331	-0.106292
H	-1.509925	-0.397915	-1.134809
H	-1.727148	-0.667455	1.136901
H	-1.853355	0.811740	0.787028
H	0.076235	-2.267357	1.328010
H	0.228087	1.099546	-1.853070
H	-0.203707	-1.087595	-1.566611
H	-0.371385	2.513280	0.158016
H	1.236580	1.296189	-0.725705
H	2.157395	-1.617363	-1.378636
H	0.441276	-0.823872	1.676030
H	0.191711	1.544865	1.167712

MR-II

O	-1.535462	0.152244	1.262216
O	2.110341	1.130434	0.161571
O	-0.494096	2.143150	-0.541014
O	-1.063753	0.303740	-2.662447
O	1.009724	-0.149029	2.559573
O	1.411814	-1.672789	-0.047965
O	-1.207724	-1.389711	-0.699809
H	1.301083	1.592455	-0.134396
H	1.491278	0.446376	1.957002
H	-0.924479	1.616696	0.158580
H	-2.443577	0.149638	1.574213
H	-1.479342	-0.543784	0.479982

H 1.985089 0.210507 -0.141105
H -1.179739 -0.414038 -1.952019
H -0.233293 0.077540 -3.090946
H -0.717749 1.652690 -1.357376
H 0.081262 -0.046303 2.279539
H -1.731546 -2.190947 -0.779694
H 1.353463 -1.550384 0.911872
H 0.461545 -1.655845 -0.342206

DR-I
O 0.703842 0.822302 -4.239856
O 0.835448 1.740423 1.880710
O 0.232472 -0.288969 -1.769304
O -1.284460 0.234790 2.047162
O -0.093067 -2.091953 1.859171
O -2.202031 0.171493 -0.367966
O 1.906944 -0.543677 0.515517
H -0.014041 1.201773 2.021518
H -1.910674 0.211301 0.610439
H 0.552154 0.521113 -3.314000
H -0.585702 -1.220896 2.015801
H -2.527090 1.052890 -0.569481
H 0.888941 -0.367787 -1.045250
H 0.776272 -0.002937 -4.726552
H -0.599843 -2.522388 1.164107
H -0.628478 -0.154922 -1.322508
H -1.889854 0.347564 2.784759
H 1.718123 0.286964 0.995778
H 1.367104 -1.201233 0.997805
H 0.604968 2.376708 1.197911

DR-II
O -1.968213 -0.788898 1.722810
O 1.711369 -0.353647 -0.895563
O 3.783049 -2.123141 -0.391079
O -1.912480 1.250670 -1.557611

O	-0.954744	-1.367841	-0.911583
O	1.131490	1.668708	1.020204
O	-1.477427	1.649063	0.983344
H	-2.922786	-0.892426	1.682464
H	-1.807528	0.195801	1.518269
H	-1.156371	1.664052	-1.984951
H	-1.903880	2.390029	1.421979
H	3.099222	-1.448099	-0.609129
H	1.578711	0.390595	-0.272364
H	3.290646	-2.779818	0.108812
H	-1.801944	1.483321	-0.576173
H	-1.235789	-1.346341	0.024112
H	1.348113	1.259379	1.862716
H	0.116666	1.718830	1.020128
H	0.834540	-0.788170	-0.941482
H	-1.364791	-0.558068	-1.277163

SR-I

O	0.569090	-1.576366	0.793358
O	-0.164866	1.840786	-0.552504
O	4.452781	1.120700	0.797217
O	-3.112885	0.607707	-1.410428
O	2.214379	0.254663	-0.590988
O	-1.559125	0.073879	0.788347
O	-2.332119	-2.364015	-0.209384
H	-2.666175	0.430744	-0.545045
H	-0.703266	1.204123	0.025169
H	-0.177098	-0.923789	0.908241
H	-1.904611	0.336801	1.646464
H	3.690392	0.838700	0.240827
H	4.205331	0.821873	1.676480
H	-2.720035	-2.040304	-1.029861
H	-2.446143	1.124930	-1.874780
H	1.770052	-0.500513	-0.152918
H	-0.127652	2.663797	-0.058118
H	0.132883	-2.294265	0.318471

H 1.489100 0.901746 -0.688263
H -2.118382 -1.520418 0.260844

SR-II
O 1.135085 2.120776 -2.670018
O -1.952429 2.521060 -2.005093
O -1.748210 -0.199965 0.503107
O 0.301839 -1.824535 1.632333
O 1.920768 0.063962 0.297946
O 0.483318 -4.474025 2.370032
O -0.094940 1.734910 -0.208361
H -1.281908 2.263454 -1.311547
H 1.004689 -1.295493 1.204427
H 0.310214 2.267081 -3.146248
H -1.135889 0.573207 0.283776
H -1.944408 -0.594432 -0.351751
H 0.602860 -4.318144 3.310572
H 0.815497 2.022372 -1.742589
H 2.318417 -0.076791 -0.566373
H 0.409747 -3.564769 2.002087
H 1.181509 0.722161 0.123458
H -0.013585 2.452331 0.428302
H -0.516033 -1.366260 1.356141
H -2.768632 2.112012 -1.705702

TREE-I
O -0.611145 -2.080014 1.144499
O 0.180510 2.430421 -0.265469
O 4.661173 -0.164944 1.816187
O -4.287715 -0.138970 -2.578461
O 2.057335 0.569228 1.238468
O 0.298592 -0.242909 -0.609459
O -2.377734 -0.308531 -0.584479
H -2.413306 -0.983228 0.105892
H 0.219117 1.464558 -0.510159
H 0.697067 -0.567115 -1.422844

H -0.195464 -1.483765 0.461893
H 3.772362 0.149015 1.535324
H 4.462128 -0.914836 2.382976
H -3.594835 -0.293483 -1.897666
H -4.344664 0.819150 -2.622838
H 1.785529 1.494029 1.175543
H -0.735771 2.558070 -0.003408
H -0.228438 -1.773543 1.971634
H 1.490119 0.145908 0.532107
H -1.392220 -0.225512 -0.731937

TREE-II
O 4.653355 2.529514 -0.219407
O -2.480538 -1.480402 -1.645957
O 0.694118 -0.079917 -0.425645
O -1.782885 0.167842 0.366950
O -0.231976 -0.904916 2.334809
O -3.098512 -2.046388 1.358939
O 2.400714 1.600284 -1.612242
H -2.172592 1.045354 0.414710
H -2.286759 -0.784568 -0.957164
H 4.433112 2.307437 0.689380
H 0.961553 -0.526231 0.389491
H 2.557124 1.139887 -2.440905
H -3.154661 -2.452945 0.485309
H 3.873066 2.228358 -0.730200
H -0.751153 -1.710012 2.445385
H -2.734084 -1.159078 1.125098
H -0.815294 -0.373631 1.734844
H -0.275257 0.135127 -0.226100
H 1.747893 1.026299 -1.127018
H -1.604914 -1.711691 -1.969688

N=7,
MR-I

O 1.077254 -1.172193 1.953544
O 1.265578 0.302644 -1.634758
O -1.691813 -0.419935 2.026192
O 1.733434 1.354727 0.872099
O -1.115244 1.173873 -1.700023
O -1.066070 2.191393 1.012594
O 0.785739 -2.044350 -0.799341
O -2.000940 -1.366803 -0.700793
H -0.124238 0.871730 -1.765195
H 1.049167 -1.638225 1.099231
H 1.054571 -1.127366 -1.204759
H -0.770234 -0.726260 2.151574
H -1.185643 1.985543 0.068436
H 1.890628 0.477490 -2.342572
H -1.945920 -0.812895 1.169257
H -1.120117 -1.780318 -0.768936
H -1.367159 1.377510 1.466095
H -1.867387 -0.497490 -1.122976
H 1.671975 1.034828 -0.061363
H 0.878310 1.801058 1.016396
H 1.260167 -2.716422 -1.294471
H 1.416966 -0.284079 1.706794
H -1.330312 1.610322 -2.527777

MR-II
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O -0.594459 -1.878004 -1.547592
O -1.763583 0.704697 -1.522651
O 1.686017 -0.610628 1.413100
O -1.823180 0.733846 1.341673
O 0.469944 1.738551 1.359806
O 2.092125 -0.766304 -1.187495
O 0.783236 1.933982 -1.305055
H 2.975941 -1.096726 -1.366998
H 0.713270 1.986890 -0.311083
H 1.344009 1.157340 -1.451967

H -2.439347 1.195596 1.915249
H -1.326013 -1.103714 1.435197
H -1.966101 0.742552 -0.568361
H -0.844776 -2.087618 0.357720
H 0.908109 -1.188957 1.538975
H 0.341861 -1.617837 -1.575198
H 2.006425 -0.729109 -0.184566
H -0.890830 1.225308 1.423035
H -0.935109 1.226612 -1.589052
H 1.304160 0.316894 1.489838
H 0.698983 2.440991 1.973362
H -1.075254 -1.029056 -1.655493

DR-I
O -1.808741 -0.697083 -0.937513
O -1.762009 -2.823686 0.876546
O 1.096497 1.433327 1.020918
O -0.341901 1.458191 -1.766258
O -1.319590 0.158519 1.561287
O 2.477927 3.264144 2.594153
O 0.118349 -2.341364 -1.544688
O 1.961677 -0.147026 -1.240008
H -2.657739 -0.662064 -1.387789
H 0.285053 0.970138 1.325976
H 1.510157 -1.011022 -1.268436
H -1.294274 -0.722806 1.955484
H -0.671572 -1.717029 -1.416154
H -1.944568 -2.100305 0.232008
H -1.606425 -0.042521 0.629045
H 1.308336 0.441355 -1.666151
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H -0.934776 0.701843 -1.507588
H 1.540934 0.813066 0.411260
H 2.031914 2.534720 2.111648
H 0.064898 -2.643430 -2.455133
H -0.969899 -3.220612 0.495338

H 2.218515 4.044953 2.097815

DR-II

O 2.330358 -2.045710 -1.427946
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O -1.338270 3.430154 1.317308
O -1.700648 -1.158346 1.120325
O -0.184513 1.040087 2.012307
O 0.521049 3.530183 -1.015888
O -0.260247 -1.406725 -1.148459
O 1.170224 0.715309 -0.466172
H 1.348777 -1.860535 -1.394828
H -0.769974 -1.317951 -1.959511
H -0.061326 3.655927 -0.248838
H 2.513559 -2.236931 -2.351304
H -0.771251 0.266556 1.880088
H -1.546450 -2.056775 1.436749
H 2.041186 0.315563 -0.576821
H 0.795431 2.600463 -0.942567
H -0.379214 -2.996092 -0.441051
H -0.952007 2.587828 1.661581
H 0.563120 -3.993761 0.234353
H -1.251728 -1.175770 0.230421
H 0.448657 0.960111 1.272181
H -2.173472 3.159861 0.924771
H 0.551757 -0.014474 -0.778484

SR-I

O 0.233708 0.985205 1.819072
O 0.327222 -1.962087 -1.821667
O -1.157881 3.311984 1.841415
O -0.399442 -1.397487 0.846450
O 1.698898 -4.042716 -3.008421
O -1.543794 0.117600 3.703575
O 0.413127 0.728015 -2.806322
O 0.342693 2.200196 -0.545791

H -1.355474 -1.300352 0.802369
H 0.389919 1.666655 0.302967
H -0.082860 -0.509419 1.201241
H 0.312664 1.284424 -1.992893
H -1.418861 -0.833512 3.637300
H -0.615234 2.483317 1.933925
H -0.881759 0.477480 3.056110
H -1.988265 3.091362 2.272828
H 0.926576 -4.507928 -3.340492
H 1.095334 1.020816 2.246557
H 1.309121 -3.274002 -2.534900
H 0.330985 -1.068508 -2.213821
H -0.290255 2.891747 -0.315310
H 1.301602 0.922002 -3.118076
H 0.156056 -1.820645 -0.867906

SR-II
O 0.544668 -0.839564 1.367115
O 4.855337 -1.558821 -0.859719
O -2.921002 2.469199 0.517837
O 2.081942 -1.582543 -0.886247
O -1.511480 0.784633 -1.567595
O -1.617318 0.761506 3.520591
O 0.729649 0.013590 -2.851042
O -1.942171 -0.029804 0.925894
H 0.930816 -0.016043 1.680050
H -1.816133 1.688123 -1.416271
H -0.977717 0.112562 3.827734
H 1.666686 -1.040075 -1.582799
H -1.792341 0.481801 2.583541
H -2.656505 1.533686 0.726412
H 0.361941 -0.534482 -3.549845
H -0.412265 -0.598624 1.166570
H 1.550506 -1.408172 -0.082289
H -0.063404 0.364240 -2.371101
H -1.640320 0.364776 -0.664572

H	-2.594594	-0.737399	0.934491
H	3.875273	-1.642560	-0.845545
H	4.995264	-0.614207	-0.966685
H	-2.629520	2.965720	1.287887

TREE-I

O	-1.737958	-0.330796	2.427127
O	-3.922073	-0.063497	-4.298928
O	2.231233	1.224462	0.453662
O	-1.187579	0.025803	-0.484718
O	0.691688	-0.751474	1.214915
O	1.038042	0.666873	3.540695
O	-2.209419	-1.407654	-2.521160
O	4.799486	0.919831	-0.581551
H	-0.400352	-0.338362	0.020763
H	1.639856	1.707690	-0.131360
H	3.920308	1.057345	-0.165195
H	1.074173	-1.630505	1.140284
H	-1.418531	0.278164	3.103739
H	-2.548168	-2.197897	-2.091968
H	-0.889525	-0.656647	2.039258
H	1.695023	0.410169	0.729151
H	-3.321107	-0.562668	-3.707968
H	-1.808699	0.199959	0.237180
H	4.678422	0.124970	-1.107784
H	1.561337	1.392080	3.184066
H	-1.805254	-0.873759	-1.787092
H	-3.841408	0.844444	-3.994461
H	0.975974	0.052678	2.767725

TREE-II

O	0.556862	0.224097	-0.280386
O	5.207500	-0.796680	-0.359807
O	-2.052164	2.286740	2.816695
O	-1.509547	0.559714	-4.539345
O	2.525582	-1.494598	-0.229887

O	-3.324680	-0.473036	2.580209
O	-1.041553	-0.719520	-2.120763
O	-0.547648	0.138809	1.983785
H	5.168644	-0.092342	-1.012210
H	-1.822963	-0.973328	-1.621580
H	-2.401097	-0.546572	2.283507
H	0.866075	1.110467	-0.489442
H	-1.414154	1.585407	2.547727
H	-3.370366	0.461054	2.825076
H	-1.319246	0.056188	-3.716577
H	4.267853	-1.066574	-0.255032
H	-0.406315	-0.333090	-1.431683
H	2.239906	-2.158004	-0.864060
H	0.116987	-0.247292	2.561683
H	-0.094475	0.192341	1.039498
H	1.786712	-0.800365	-0.236332
H	-2.134092	2.846166	2.039414
H	-1.536099	1.473488	-4.243669