Electronic Supplementary Information

Hydration of 3-hydroxy-4,4-dimethylglutaric Acid with Dimethylamine Complex and Its Atmospheric Implications

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Figure Captions

Figure S1. The local minima for (HDMGA)$(W)_n$ (n = 1-2) optimized at the M06-2X/6-311++G(3df, 3pd) level.

Figure S2. The local minima for (HDMGA)$(W)_3$ optimized at the M06-2X/6-311++G(3df, 3pd) level.

Figure S3. The local minima for (HDMGA)(DMA)$(W)_n$ (n = 0-1) optimized at the M06-2X/6-311++G(3df, 3pd) level.

Figure S4. The local minima for (HDMGA)(DMA)$(W)_2$ optimized at the M06-2X/6-311++G(3df, 3pd) level.

Figure S5. The local minima for (HDMGA)(DMA)$(W)_3$ optimized at the M06-2X/6-311++G(3df, 3pd) level.

Figure S1

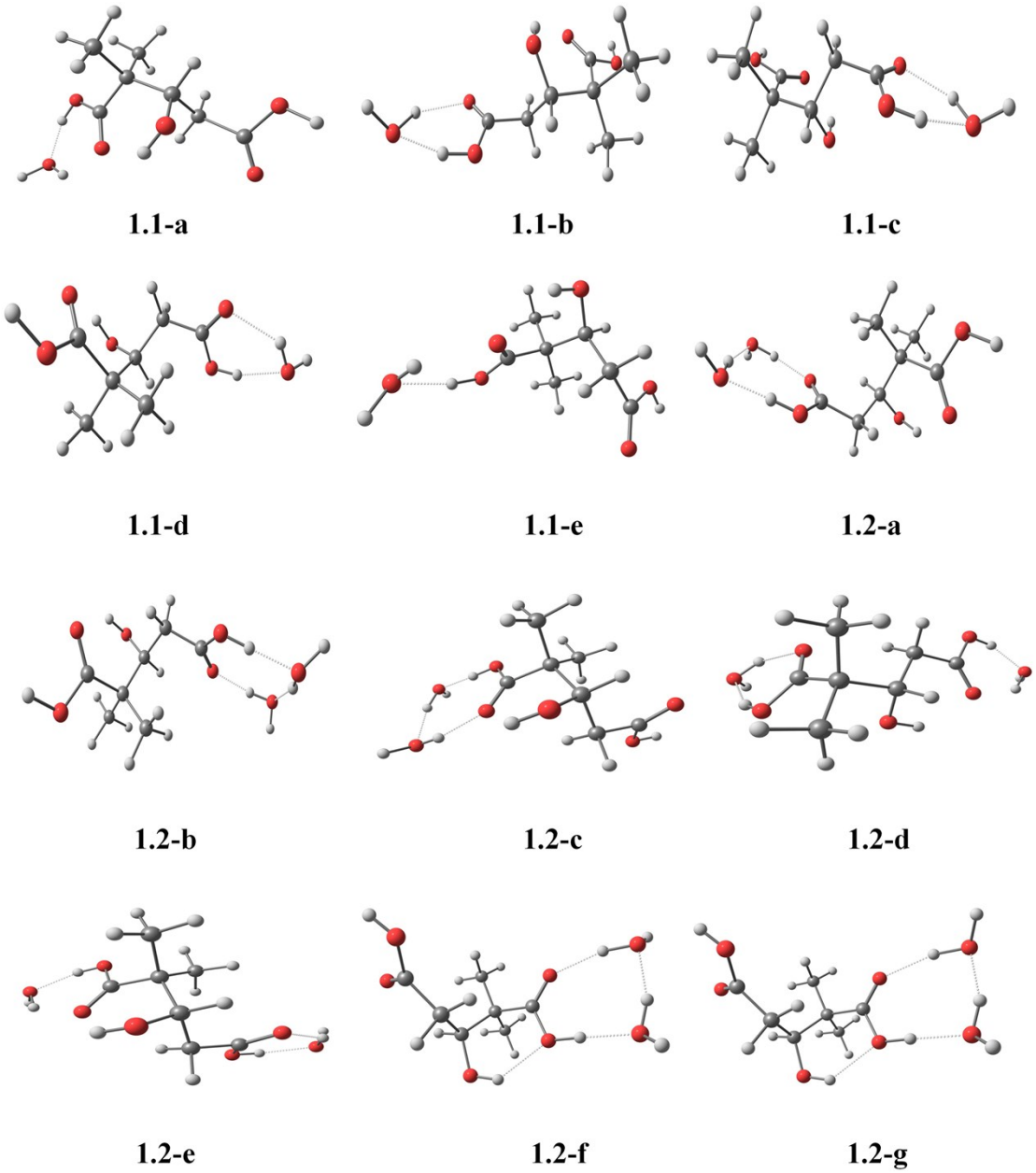


Figure S2

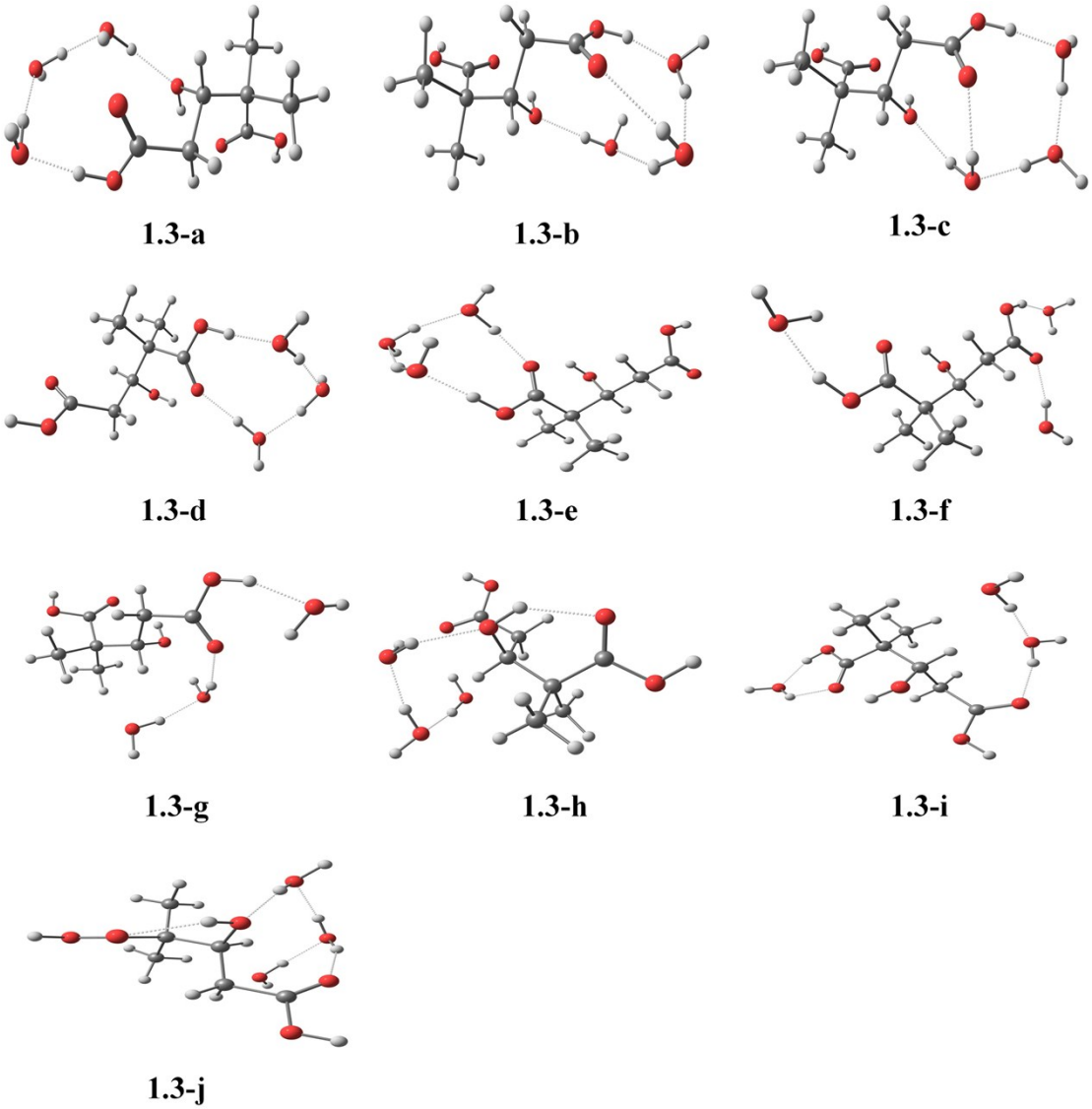
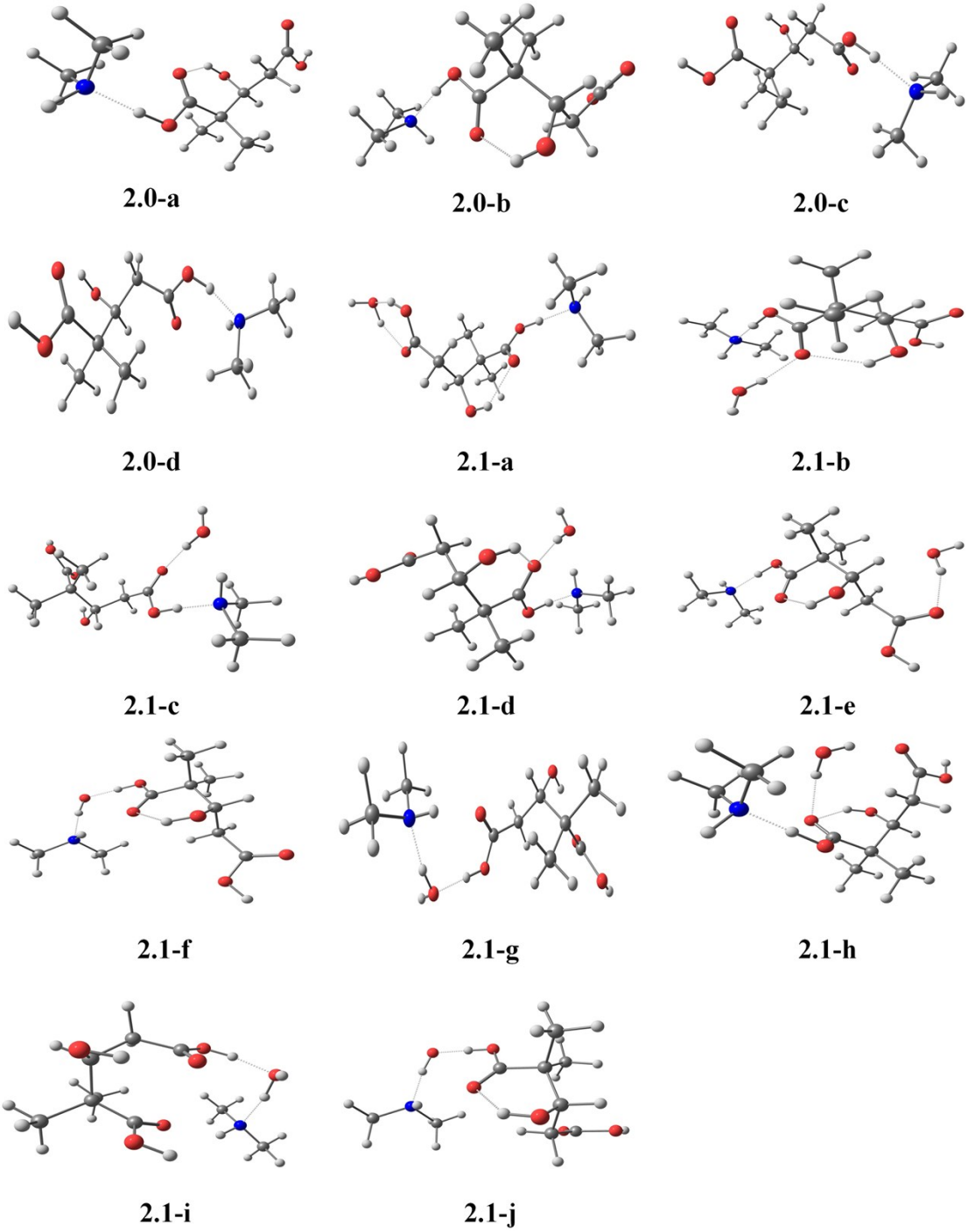


Figure S3



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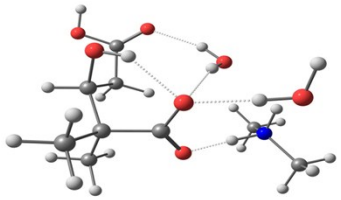
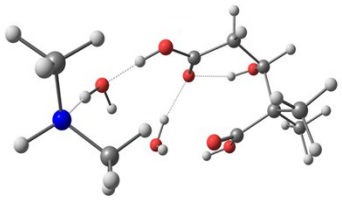


2.2-a



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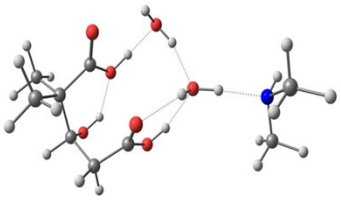

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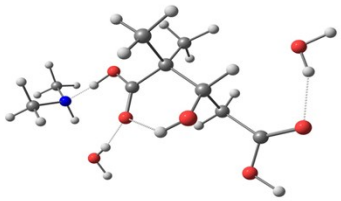

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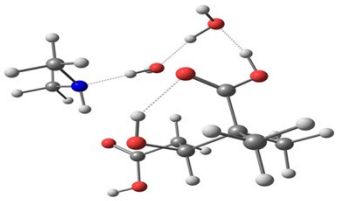

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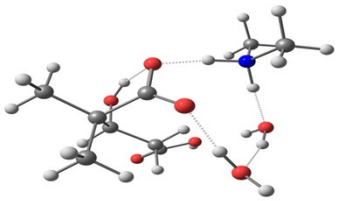

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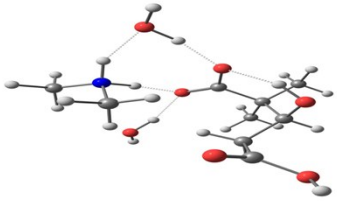

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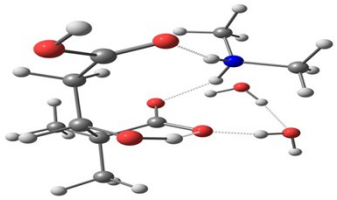

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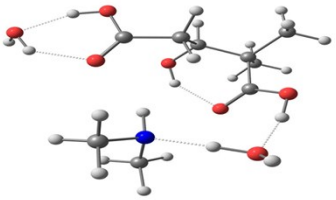

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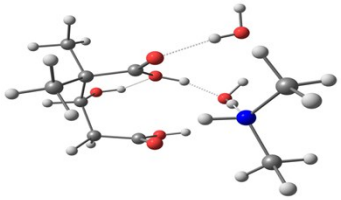
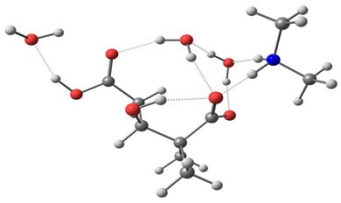


2.2-j

Figure S5



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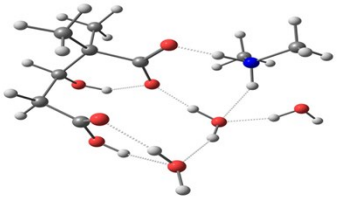

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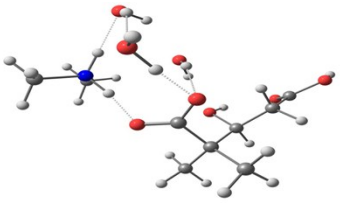

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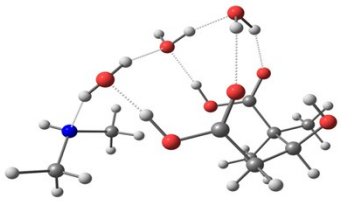

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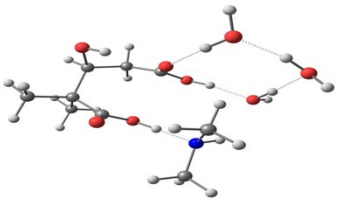

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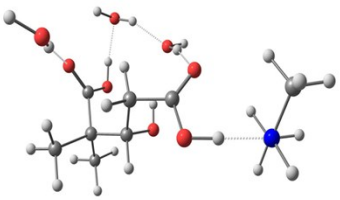

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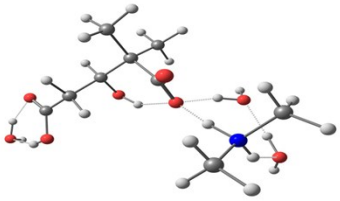

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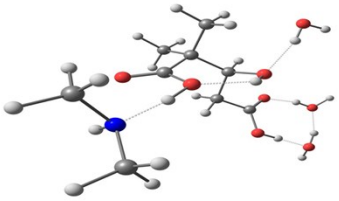

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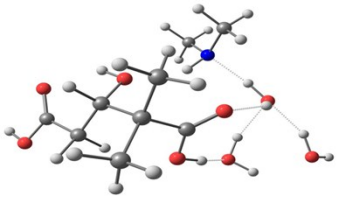

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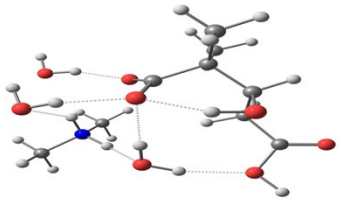

2.3-j

Table Captions

Table S1. The ZPE-corrected binding energies(ΔE_0), intermolecular enthalpies (ΔH), Gibbs free energy changes (ΔG) and Boltzmann averaged Gibbs free energies of (HDMGA) $(H_2O)_n$ (n = 0-3) (in kcal mol^{-1}) based on M06-2X/6-311++G(3df, 3pd) calculations.

Table S2. The ZPE-corrected binding energies(ΔE_0), intermolecular enthalpies (ΔH), Gibbs free energy changes (ΔG) and Boltzmann averaged Gibbs free energies of (HDMGA) (DMA)$(H_2O)_n$ (n = 0-3) (in kcal mol^{-1}) based on M06-2X/6-311++G(3df, 3pd) calculations.

Table S3. Optimized Cartesian coordinates of (HDMGA)$(W)_1$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S4. Optimized Cartesian coordinates of (HDMGA)$(W)_2$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S5. Optimized Cartesian coordinates of (HDMGA)$(W)_3$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S6. Optimized Cartesian coordinates of (HDMGA)(DMA) at the M06-2X/6-311++G(3df, 3pd) level.

Table S7. Optimized Cartesian coordinates of (HDMGA)(DMA)$(W)_1$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S8. Optimized Cartesian coordinates of (HDMGA)(DMA)$(W)_2$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S9. Optimized Cartesian coordinates of (HDMGA)(DMA)$(W)_3$ at the M06-2X/6-311++G(3df, 3pd) level.

Table S1.

n	isomer	ΔE_0	ΔH	ΔG	Boltzmann averaged Gibbs free energy
n=1	1.1-a	-8.31	-8.74	0.02	0.54
	1.1-b	-8.16	-8.73	0.29	
	1.1-c	-7.97	-8.47	0.34	
	1.1-d	-7.90	-8.59	0.95	
	1.1-e	-7.68	-8.28	1.11	
n=2	1.2-a	-31.37	-19.28	-1.35	-0.26
	1.2-b	-17.65	-19.00	-0.46	
	1.2-c	-17.59	-18.88	-0.45	
	1.2-d	-17.57	-18.72	-0.29	
	1.2-e	-17.29	-18.48	0.04	
	1.2-f	-16.75	-17.99	0.24	
	1.2-g	-16.33	-17.50	0.49	
n=3	1.3-a	-27.10	-29.13	-1.10	1.87
	1.3-b	-26.93	-29.10	0.01	
	1.3-c	-26.22	-28.37	0.19	
	1.3-d	-24.08	-25.80	1.06	
	1.3-e	-24.00	-25.92	1.78	
	1.3-f	-23.54	-25.05	2.39	
	1.3-g	-23.41	-25.01	2.79	
	1.3-h	-23.35	-25.18	3.27	
	1.3-i	-21.75	-23.18	3.99	
	1.3-j	-22.15	-23.90	4.28	

Table S2.

n	isomer	ΔE_0	ΔH	ΔG	Boltzmann averaged Gibbs free energy
n=0	2.0-a	-13.18	-12.90	-3.65	-2.13
	2.0-b	-12.59	-12.43	-2.51	
	2.0-c	-12.38	-12.32	-1.52	
	2.0-d	-11.78	-11.72	-0.85	
n=1	2.1-a	-21.94	-22.46	-3.24	-1.13
	2.1-b	-21.16	-21.47	-2.46	
	2.1-c	-20.69	-21.02	-1.59	
	2.1-d	-20.89	-21.30	-1.47	
	2.1-e	-19.79	-20.00	-0.80	
	2.1-f	-19.17	-19.57	-0.77	
	2.1-g	-19.28	-19.68	-0.65	
	2.1-h	-21.14	-21.92	-0.53	
	2.1-i	-20.49	-21.26	-0.51	
	2.1-j	-18.52	-19.15	0.75	
n=2	2.2-a	-32.66	-34.06	-2.91	-0.43
	2.2-b	-30.95	-32.61	-1.63	
	2.2-c	-28.36	-29.97	-0.57	
	2.2-d	-28.20	-28.91	-0.36	
	2.2-e	-29.12	-30.36	-0.32	
	2.2-f	-29.78	-31.28	-0.10	
	2.2-g	-29.60	-30.86	0.06	
	2.2-h	-29.48	-30.91	0.40	
	2.2-i	-28.62	-29.95	0.50	
	2.2-j	-30.03	-31.60	0.64	
n=3	2.3-a	-41.69	-44.12	-2.23	-0.80
	2.3-b	-40.87	-44.12	-2.19	
	2.3-c	-40.83	-43.01	-2.11	
	2.3-d	-40.78	-43.35	-1.37	
	2.3-e	-39.46	-41.44	-0.97	
	2.3-f	-38.23	-39.97	-0.41	
	2.3-g	-36.49	-38.05	-0.09	
	2.3-h	-35.46	-36.84	0.12	
	2.3-i	-35.23	-36.92	0.65	
	2.3-j	-37.67	-39.73	0.65	

Table S3

(HDMGA)$(W)_1$

O	0.948662	0.050876	1.581912
O	-2.695303	0.310448	-0.599862
O	-1.342327	-1.068512	0.503440
O	3.665583	0.199404	-0.141247
O	3.077696	-1.952635	-0.176404
C	-0.552167	1.158623	-0.019886
C	0.867658	0.649710	0.311073
C	-0.569716	1.873463	-1.374326
C	-0.998023	2.136656	1.080037
C	1.440327	-0.286487	-0.761322
C	-1.548629	0.011960	-0.014805
C	2.786861	-0.803049	-0.331019
H	1.508037	1.532233	0.364181
H	0.238169	2.605486	-1.405012
H	-1.513916	2.392911	-1.516330
H	-0.442060	1.181410	-2.204919
H	-0.332003	2.999702	1.077115
H	-0.947699	1.669639	2.060709
H	-2.012960	2.482390	0.892294
H	0.792957	-1.145849	-0.920026
H	1.568916	0.250800	-1.700833
H	0.358282	-0.712534	1.575766
H	-3.302983	-0.460286	-0.521215
H	4.491496	-0.198986	0.160772
O	-3.835203	-2.095978	-0.160756
H	-2.990768	-2.228872	0.294231
H	-4.526199	-2.362110	0.448088

Table S4

(HDMGA)$(W)_2$

O	-1.889942	1.354307	1.683758
O	-3.085576	-1.372747	-1.297906
O	-2.939406	-1.095025	0.898929
O	1.936392	-1.339042	0.780330
O	1.898741	0.833029	0.269480
C	-1.651566	0.375092	-0.547010
C	-0.958405	0.886402	0.736024
C	-0.621379	-0.103273	-1.576375
C	-2.489554	1.512064	-1.153148
C	0.000387	-0.129293	1.366776
C	-2.603076	-0.759100	-0.208019
C	1.369665	-0.155313	0.736614
H	-0.368302	1.756006	0.444522
H	0.110355	0.685480	-1.746554
H	-1.110898	-0.339358	-2.518009
H	-0.092137	-0.996596	-1.241960
H	-1.822802	2.326027	-1.437527
H	-3.207585	1.895129	-0.431703
H	-3.014900	1.168583	-2.042139
H	0.158536	0.183803	2.401105
H	-0.411924	-1.135773	1.394628
H	-2.441759	0.605438	1.936039
H	-3.701022	-2.053896	-0.996601
H	2.862708	-1.315698	0.407634
O	4.342062	1.259647	-0.909964
H	4.835509	1.966211	-0.490819
H	3.455068	1.264173	-0.505707
O	4.399649	-1.320568	-0.165194
H	4.602985	-1.913996	-0.890110
H	4.574370	-0.411817	-0.487439

Table S5

(HDMGA)$(W)_3$

O	-0.225882	1.041302	0.471269
O	-4.208991	-0.367576	0.885518
O	-2.265136	-0.100733	1.925702
O	1.842014	-1.622266	0.710333
O	1.784475	-0.824545	-1.371686
C	-2.355365	0.266018	-0.469192
C	-0.816729	0.162938	-0.470464
C	-2.959099	-0.637162	-1.548604
C	-2.761426	1.725548	-0.738248
C	-0.285365	-1.258891	-0.271515
C	-2.899731	-0.092526	0.901483
C	1.221904	-1.220765	-0.369681
H	-0.475150	0.513629	-1.446655
H	-2.448511	-0.455464	-2.494764
H	-4.015680	-0.417163	-1.678876
H	-2.865001	-1.693251	-1.302790
H	-2.409771	2.012661	-1.729136
H	-2.316904	2.397839	-0.008515
H	-3.844635	1.828914	-0.712689
H	-0.592821	-1.658175	0.692771
H	-0.645188	-1.907761	-1.068491
H	-0.538643	0.778533	1.346786
H	-4.483834	-0.534189	1.797067
H	2.836899	-1.505297	0.578837
O	2.293948	1.890725	-0.569085
H	2.302578	1.100441	-1.125124
H	1.473078	1.789161	-0.066160
O	4.658876	1.436113	0.695784
H	4.759497	1.853652	1.551754
H	3.802554	1.738930	0.329360
O	4.343667	-1.209185	0.184232
H	4.563427	-0.291189	0.450398
H	4.249197	-1.172909	-0.772974

Table S6

(HDMGA)(DMA)

O	1.576261	0.141676	1.589685
O	-1.895854	1.012881	-0.718439
O	-0.927149	-0.468228	0.624154
O	4.233318	-0.511518	-0.083504
O	3.160479	-2.464693	0.008247
C	0.370312	1.428974	-0.124013
C	1.631993	0.633229	0.272519
C	0.524844	2.017791	-1.528305
C	0.167545	2.570001	0.886371
C	1.955011	-0.505421	-0.705531
C	-0.872172	0.549745	-0.041446
C	3.143204	-1.290653	-0.221530
H	2.465392	1.338405	0.257141
H	1.483720	2.532922	-1.602700
H	-0.269192	2.732915	-1.727569
H	0.482199	1.251981	-2.301078
H	1.021806	3.246295	0.839817
H	0.092761	2.183884	1.900129
H	-0.732805	3.132500	0.644491
H	1.118235	-1.195027	-0.791459
H	2.197125	-0.101262	-1.688736
H	0.784747	-0.409919	1.644702
H	-2.714877	0.404997	-0.578474
H	4.941217	-1.071881	0.257888
C	-3.523134	-1.909455	-0.810447
N	-3.947858	-0.598337	-0.317654
C	-4.185333	-0.609690	1.126349
H	-3.389636	-1.869462	-1.889394
H	-4.243313	-2.695846	-0.567493
H	-2.567231	-2.150513	-0.348787
H	-4.790447	-0.309059	-0.799810
H	-4.539979	0.367284	1.447506
H	-3.239429	-0.818280	1.623072
H	-4.915341	-1.369638	1.419377

Table S7

(HDMGA)(DMA)$(W)_1$

O	-0.240979	2.110148	-1.660352
O	1.899907	-0.013259	1.288221
O	1.635382	0.252672	-0.899752
O	-2.805014	-1.754278	-0.544703
O	-3.570061	0.298374	-0.118006
C	-0.045317	1.163252	0.590663
C	-0.915300	1.371097	-0.668265
C	-0.818819	0.394043	1.666130
C	0.365993	2.535546	1.145813
C	-1.467486	0.063718	-1.252174
C	1.237612	0.416166	0.239973
C	-2.715018	-0.429530	-0.570322
H	-1.768736	1.980536	-0.367236
H	-1.772695	0.887119	1.851643
H	-0.247008	0.367690	2.590312
H	-1.016319	-0.637675	1.371708
H	-0.529517	3.083053	1.440637
H	0.890234	3.119566	0.392701
H	1.003100	2.414759	2.019961
H	-1.755686	0.274417	-2.284198
H	-0.721573	-0.727909	-1.277942
H	0.562860	1.617858	-1.867562
H	2.767740	-0.474103	0.991221
H	-3.656206	-2.003084	-0.124424
C	4.850869	-0.251789	-0.349613
N	4.101035	-1.220267	0.450505
C	3.628187	-2.345311	-0.356346
H	5.695211	-0.711898	-0.871120
H	5.220164	0.545606	0.291613
H	4.172349	0.177479	-1.084598
H	4.682218	-1.562753	1.206068
H	2.923142	-1.962040	-1.092078
H	3.112317	-3.061183	0.279991
H	4.444353	-2.852829	-0.878602
O	-5.211245	-1.736751	0.755934
H	-5.012992	-0.798001	0.609784
H	-6.088442	-1.893135	0.402705

Table S8

(HDMGA)(DMA)$(W)_2$

O	2.156398	0.286872	1.378395
O	-1.144113	1.157005	-0.878540
O	-0.495969	0.799064	1.216753
O	3.833047	-1.718736	-0.295124
O	1.909502	-2.713844	0.213752
C	1.094777	1.792109	-0.261111
C	2.120587	0.665769	0.024322
C	1.206302	2.238690	-1.714672
C	1.372203	2.974861	0.671252
C	1.856234	-0.567581	-0.872574
C	-0.302130	1.223592	0.043101
C	2.497595	-1.778150	-0.264084
H	3.114809	1.053520	-0.210047
H	2.227373	2.560691	-1.926365
H	0.534890	3.074352	-1.902251
H	0.933036	1.445338	-2.406066
H	2.381431	3.351302	0.499257
H	1.283817	2.686868	1.714782
H	0.667779	3.782364	0.471751
H	0.789871	-0.770406	-0.964689
H	2.273279	-0.404220	-1.865403
H	1.245772	0.337330	1.708320
H	-2.255280	0.168549	-0.601246
H	4.170804	-2.493611	0.171914
C	-4.338452	0.195866	-0.497280
N	-3.068239	-0.550456	-0.514001
C	-2.952255	-1.518275	-1.617522
H	-4.343181	0.839993	0.375595
H	-5.173742	-0.498898	-0.448350
H	-4.403808	0.788454	-1.406231
H	-2.923956	-1.004075	0.393323
H	-1.997080	-2.022417	-1.519789
H	-3.003711	-0.977581	-2.559225
H	-3.764686	-2.239276	-1.562030
O	-2.898699	-0.018884	2.212919
H	-2.043548	0.381569	1.952597
H	-2.723237	-0.493642	3.026675
O	-0.879398	-1.983436	0.653175
H	-0.664091	-1.111488	1.013522
H	-0.024177	-2.427135	0.562728

Table S9

(HDMGA)(DMA)$(W)_3$

O	-1.401424	0.732126	-1.490172
O	1.224261	0.328750	-0.997603
O	1.908517	1.120600	0.960899
O	-3.878606	0.084168	0.372786
O	-2.498473	-1.664683	0.327951
C	0.010611	2.184177	-0.081832
C	-1.332113	1.439573	-0.274119
C	-0.033839	3.016305	1.195345
C	0.255367	3.097137	-1.288496
C	-1.625232	0.495051	0.913006
C	1.147509	1.146774	-0.009670
C	-2.694820	-0.478601	0.516325
H	-2.125668	2.189609	-0.312721
H	-0.894886	3.686511	1.174150
H	0.870447	3.615325	1.281069
H	-0.089217	2.393053	2.084948
H	-0.545757	3.833804	-1.361668
H	0.288968	2.531312	-2.215446
H	1.198768	3.630029	-1.168863
H	-0.737536	-0.068301	1.198691
H	-1.970213	1.070716	1.770351
H	-0.509724	0.396596	-1.669039
H	2.477543	-0.582309	-0.673838
H	-4.514599	-0.588265	0.039867
C	4.510699	-0.384660	-0.285987
N	3.280306	-1.193891	-0.310622
C	3.375741	-2.438587	-1.092077
H	5.315249	-0.954282	0.172874
H	4.304133	0.513444	0.289059
H	4.782382	-0.120520	-1.305181
H	2.980600	-1.404436	0.666006
H	2.422411	-2.956184	-1.026775
H	4.168802	-3.063379	-0.688061
H	3.596806	-2.192967	-2.127958
O	0.295190	-2.157043	0.054907
H	-0.669307	-2.198358	0.154378
H	0.449348	-1.331950	-0.429916
O	-5.103195	-2.164628	-0.524470
H	-5.292054	-2.298641	-1.455214
H	-4.193046	-2.466166	-0.383592
O	2.056147	-1.457240	2.149940
H	1.286625	-1.820277	1.680765

H	1.934907	-0.496557	2.091582