Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

[Electronic Supplementary Information]

Efficient structural elucidation of microhydrated biomolecules through interrogation of hydrogen bond networks

Yeonjoon Kim, Jaewook Kim, Kyung Yup Baek,* and Woo Youn Kim,*

Department of Chemistry, KAIST, 291 Daehak-ro, Yuseong-gu, Daejeon 34141, Korea

*E-mail: drchem@kaist.ac.kr (K.Y.B), wooyoun@kaist.ac.kr (W.Y.K)

1. Results of HB network analysis for (amino acid)-water clusters (AW_n)

Table S1. Numbers of HBs in the neutral states of GW_{10} and their relative energies (in kcal/mol)[a]

Rank	The number of HBs	M06-2X/ 6-311+G**	SCS-MP2/TZVPP[b]
1[c]	20	0.0	0.0
2	20	1.0	1.3
3	19	1.2	1.0
4	21	1.6	2.0
5[d]	18	3.0	0.4
6	20	5.8	5.1

[a]These were evaluated at the optimized geometries at the DFT level. [b]Re-optimizations were carried out at the same level of theory with that of ref. S1. [c]This is the most stable structure found newly in this work. Note that the most stable structure in this work has two more HBs than that of the previous one (Rank 5). [d]The previous global minimum in ref. S1.

Table S2. Numbers of HBs in the zwitterionic states of GW_{10} and their relative energies (in kcal/mol)[a]

Rank	The number of HBs	M06-2X/6-311+G**	SCS-MP2/TZVPP[b]
1[c]	20	0.0	0.0
2[d]	19	0.9	0.6
3	20	1.5	1.8
4	20	1.9	0.9
5	20	8.6	9.1
6	20	10.9	7.8

[a]These were evaluated at the optimized geometries at the DFT level. [b]Re-optimizations were carried out at the same level of theory with that of ref. S1. [c]This is the most stable structure found newly in this work. Note that the most stable structure in this work has one more HB than that of the previous one (Rank 3). [d]The previous global minimum in ref. S1.

Table S3. Relative energies (in kcal/mol) between the neutral and zwitterionic states of TW_n [a]

n	$E_{ZW} - E_{NE}$ (ZPE[b])	The number of HBs	
		neutral	zwitterion
8	3.0 (2.8)	18	19
9	1.4 (1.0)	20	21
10	-0.2 (-0.5)	21	22
11	-2.9 (-1.8)	23	24
12	-3.8 (-2.7)	25	25

[a]These were evaluated at the DFT level with M06-2X/6-311+G**. [b]Zero-point energy correction.

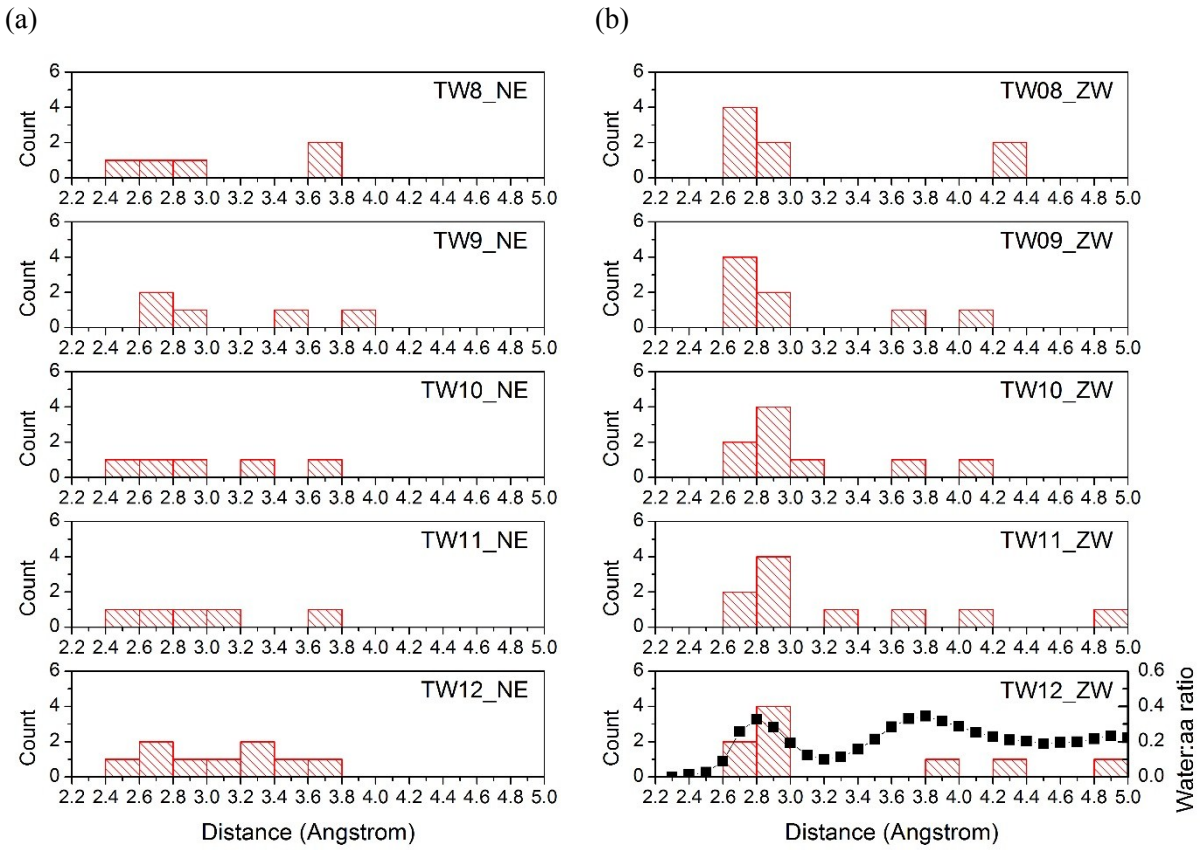

Figure S1. Distribution of distances between water molecules and an amino acid measured from DFT optimized structures. The water molecules along the path connecting the nitrogen atom and the hydrogen atom of carboxyl group by HBs were selected, and then the shortest distance between the oxygen atom of each water and non-hydrogen atoms of the amino acid was calculated. The red bar denotes our data, and the black square dotted line represents the experimental data quoted in the ref. S2.

2. Cartesian coordinates of GW_{10} and TW_n optimized at the DFT level

2.1 The six representative stable neutral structures of GW_{10} (Table S1)

Structure gw10n-01 : -1048.82533794 Hartree.

C	0.907815	-1.569570	-0.687020
H	1.350429	-0.571816	-0.750259
C	-0.598473	-1.432169	-0.765504
O	-1.002842	-0.592084	-1.700670
N	1.361914	-2.236106	0.521324
H	-2.005094	-0.436605	-1.645593
H	0.912591	-1.774724	1.309915
O	-1.352482	-2.047738	-0.039119
H	1.250744	-2.109085	-1.574280
H	1.041649	-3.198794	0.531114
O	-0.207626	2.021728	-0.894106

H	-0.376379	1.279049	-1.490311
H	-1.079201	2.421916	-0.728620
O	2.590700	2.069992	-0.611311
H	2.704118	1.933880	0.342872
H	1.661906	2.303382	-0.751447
O	3.804830	-0.035130	-1.808856
H	3.378321	0.795646	-1.512926
H	4.459235	0.210102	-2.465068
O	3.900044	-1.054454	0.771682
H	4.081938	-0.801198	-0.150111
H	3.138387	-1.668443	0.714523
O	2.889485	1.020306	1.992151
H	3.398268	1.310486	2.751809
H	3.354822	0.226098	1.601414
O	-3.839674	-1.500127	0.839921
H	-3.008784	-1.924665	0.550013
H	-4.407300	-2.179742	1.208941
O	-2.490174	0.805673	1.846745
H	-1.544917	0.576045	1.914903
H	-2.979589	-0.018939	1.711531
O	-3.470772	0.074049	-1.438756
H	-3.901314	-0.423261	-0.725084
H	-3.437388	0.998136	-1.135717
O	-2.850090	2.472335	-0.142278
H	-2.757213	1.938126	0.692377
H	-3.346618	3.265693	0.069750
O	0.214759	0.484095	1.442030
H	1.070218	0.681890	1.861059
H	0.162464	1.080825	0.675615

Structure gw10n-02 : -1048.82375183 Hartree.

C	0.082112	0.362291	-1.561061
H	0.628110	-0.106975	-2.384769
C	-1.295673	-0.273915	-1.463857
O	-1.343115	-1.582347	-1.438040
N	0.082738	1.804557	-1.713522
H	-0.424933	-1.990101	-1.362472
H	-0.437796	2.079660	-2.539483
O	-2.317555	0.388473	-1.413493
H	0.619546	0.100352	-0.642532
H	-0.383523	2.204706	-0.903271
O	2.662762	-0.651303	1.457331
H	2.416041	0.234193	1.770364
H	1.988453	-1.289849	1.742450
O	2.739130	2.015488	-0.878045
H	3.034558	1.128214	-1.132367
H	1.873335	2.128657	-1.327079

O	-3.885902	-0.745452	0.521477
H	-3.566643	-0.555872	-0.378559
H	-4.546289	-1.437358	0.445397
O	2.184071	2.104386	1.710156
H	2.457021	2.161746	0.756813
H	2.750411	2.700893	2.204159
O	3.214683	-0.824752	-1.099155
H	4.092812	-1.166557	-1.284724
H	3.122366	-0.776372	-0.111959
O	-0.467417	1.603570	1.183552
H	0.301105	2.013223	1.610632
H	-1.287679	2.084165	1.380150
O	0.699585	-2.616437	1.699565
H	0.631603	-3.304116	2.365035
H	-0.138775	-2.081865	1.732678
O	-3.117826	2.051000	0.808118
H	-3.658485	1.326220	1.145100
H	-2.918200	1.766598	-0.094952
O	-1.302184	-0.958638	1.701389
H	-0.998429	-0.039712	1.573035
H	-2.205031	-1.012714	1.350457
O	1.001970	-2.594228	-1.057046
H	1.793055	-2.056376	-1.233261
H	1.013966	-2.790985	-0.103156

Structure gw10n-03 : -1048.82342665 Hartree.

C	-1.390464	-1.081839	1.053152
H	-1.574180	-1.147086	2.129346
C	0.085315	-1.321907	0.825575
O	0.833967	-0.538538	1.578383
N	-2.288869	-1.968475	0.333452
H	1.827961	-0.686028	1.431968
H	-2.021733	-2.935514	0.485905
O	0.523501	-2.164220	0.068104
H	-1.592795	-0.046719	0.762567
H	-2.220328	-1.790112	-0.667977
O	3.020963	-2.239380	-1.024525
H	3.283984	-3.047194	-1.469714
H	2.109367	-2.366504	-0.689411
O	-3.361281	1.366875	-0.501171
H	-3.873703	0.862469	0.155731
H	-3.169368	0.740365	-1.218625
O	-2.209435	-0.487036	-2.264117
H	-2.242360	-0.604809	-3.215013
H	-1.326930	-0.104630	-2.044243
O	-1.276221	2.976233	-0.216209
H	-2.102523	2.430905	-0.227235

H	-1.526569	3.855686	-0.506164
O	3.407347	1.950175	0.383592
H	2.512407	2.211019	0.716602
H	4.001568	2.681918	0.562144
O	2.571128	0.445398	-1.856548
H	2.876807	-0.463567	-1.723339
H	3.046545	0.999386	-1.219473
O	-0.065759	0.661172	-1.243042
H	-0.256022	1.595489	-1.074100
H	0.876494	0.593128	-1.506106
O	-4.481270	-0.523329	1.188181
H	-5.365913	-0.891959	1.195604
H	-3.866467	-1.236388	0.897812
O	0.956173	2.313018	1.356696
H	0.715653	1.400153	1.569893
H	0.183278	2.675543	0.892511
O	3.372606	-0.693443	1.239125
H	3.601762	-1.272891	0.496401
H	3.622271	0.213731	0.990633

Structure gw10n-04 : -1048.82279892 Hartree.

C	-0.155623	0.385278	-1.495429
H	-0.378877	1.215756	-2.177915
C	1.328265	0.084864	-1.579082
O	2.146967	1.055472	-1.231836
N	-0.925264	-0.828683	-1.722023
H	1.669692	1.848139	-0.789846
H	-1.925525	-0.663133	-1.632440
O	1.748453	-0.993702	-1.944705
H	-0.366023	0.752581	-0.487226
H	-0.739211	-1.207679	-2.644594
O	1.035960	2.905901	0.068031
H	0.113078	3.144782	-0.165335
H	1.056797	2.610447	0.993115
O	-0.025984	-2.225478	0.464774
H	0.861824	-2.599287	0.374259
H	-0.302397	-1.884848	-0.425138
O	-0.855736	-0.066088	1.949722
H	-0.381929	-0.790194	1.496459
H	-0.169821	0.503442	2.331334
O	-2.771551	1.226622	0.396419
H	-3.308560	0.536133	-0.023384
H	-2.164858	0.768356	1.006802
O	-3.805288	-1.121285	-0.702319
H	-3.479341	-1.665760	0.048181
H	-4.688922	-1.428126	-0.913177
O	2.751112	-2.680798	-0.080480

H	3.335463	-3.429113	-0.219977
H	2.625411	-2.241053	-0.940466
O	-1.507255	3.268484	-0.743232
H	-2.070215	2.550929	-0.369587
H	-2.016605	4.078992	-0.686911
O	1.457245	1.465449	2.460546
H	2.116404	0.833638	2.089330
H	1.832248	1.808842	3.274901
O	3.165488	-0.147299	1.160109
H	3.215162	0.253456	0.281246
H	3.084498	-1.098504	0.992504
O	-2.627663	-2.281147	1.436929
H	-1.751180	-2.598638	1.163027
H	-2.420093	-1.568291	2.054402

Structure gw10n-05 : -1048.82057217 Hartree.

C	3.026651	-0.863935	1.114495
H	3.391454	-1.038522	2.135387
C	2.070124	0.309121	1.188754
O	0.894481	-0.016773	1.677120
N	4.071716	-0.567589	0.140389
H	0.233029	0.777623	1.679906
H	4.441468	0.363125	0.312631
O	2.392014	1.425643	0.849418
H	2.468473	-1.752236	0.810179
H	4.834071	-1.231126	0.207194
O	0.304966	-2.254908	-1.689395
H	0.619992	-2.988291	-2.223517
H	0.991183	-1.526082	-1.787392
O	-2.328856	-1.520524	-1.865877
H	-2.700821	-1.840276	-2.691214
H	-1.377954	-1.762173	-1.875349
O	-1.169055	2.971579	-0.889741
H	-1.508775	3.844655	-1.098585
H	-1.889190	2.322019	-1.088698
O	-3.038899	1.117691	-1.090867
H	-2.767197	0.243919	-1.416085
H	-3.353641	0.976130	-0.183895
O	2.094181	-0.416154	-1.919057
H	1.825624	0.525595	-1.957956
H	2.916160	-0.454362	-1.392477
O	-0.849447	1.795237	1.648356
H	-0.864815	2.346049	0.846089
H	-1.738440	1.402150	1.729755
O	1.440262	2.236808	-1.681558
H	0.516908	2.510654	-1.566467
H	1.829757	2.332859	-0.802717

O	-2.965131	-1.959460	0.889594
H	-2.067563	-2.287871	1.097057
H	-2.983350	-1.949371	-0.078630
O	-3.334087	0.519539	1.646773
H	-4.030842	0.622875	2.298273
H	-3.228057	-0.455470	1.472634
O	-0.281587	-2.567550	1.074848
H	0.112855	-1.761605	1.435714
H	-0.023717	-2.567279	0.139029

Structure gw10n-06 : -1048.81607113 Hartree.

C	-1.891806	-0.406975	1.404849
H	-2.253717	-0.144941	2.406695
C	-0.402432	-0.641195	1.518478
O	0.372341	0.296317	1.643615
N	-2.592939	-1.533369	0.795096
H	0.981746	-1.967423	1.450845
H	-2.627049	-2.327820	1.424631
O	-0.037843	-1.890730	1.488162
H	-2.032607	0.476087	0.777464
H	-3.538219	-1.227095	0.568316
O	2.990050	0.666546	0.613070
H	2.096635	0.575559	0.980330
H	2.909598	0.427586	-0.335986
O	2.578162	3.401669	0.546731
H	2.966870	2.508603	0.599641
H	3.203107	4.013397	0.937556
O	1.485333	-2.752929	-1.459643
H	0.538852	-2.503970	-1.402068
H	1.522913	-3.606530	-1.896904
O	-2.497886	2.220362	-1.085064
H	-1.926316	1.837419	-1.764922
H	-1.869127	2.686123	-0.512525
O	-0.057777	2.671516	0.280414
H	0.762387	3.196361	0.321121
H	0.019953	2.044728	1.016029
O	-4.418260	0.468937	-0.179225
H	-5.305499	0.808446	-0.305988
H	-3.813338	1.156877	-0.517735
O	2.559580	-0.145114	-1.960165
H	1.730742	0.307051	-2.191567
H	2.345552	-1.086917	-2.005473
O	2.464459	-2.115293	1.080223
H	2.392331	-2.404244	0.154913
H	2.952285	-1.275139	1.069294
O	-1.067287	-1.744728	-1.390487
H	-1.625700	-1.802926	-2.171142

H	-1.687905	-1.798903	-0.594601
O	-0.058612	0.877855	-1.883898
H	0.063658	1.465924	-1.115287
H	-0.389222	0.029090	-1.548138

2.2 The six representative stable zwitterionic structures of GW_{10} (Table S2)

Structure gw10z-01 : -1048.8283727 Hartree.

C	0.933167	-1.478298	-0.605936
H	1.314383	-0.503596	-0.908489
C	-0.599513	-1.548357	-0.699601
O	-1.153365	-2.224902	0.192333
N	1.322321	-1.706101	0.809497
H	-2.855561	-0.414880	-1.587991
H	0.888902	-0.928081	1.342323
O	-1.123998	-0.922303	-1.642552
H	1.393036	-2.239276	-1.236615
H	0.909493	-2.580241	1.135437
O	-0.311363	1.649997	-1.150707
H	-0.592333	0.811028	-1.568833
H	-1.134704	2.154448	-1.021157
O	2.475961	1.742021	-1.039249
H	2.630783	1.918923	-0.099970
H	1.538232	1.927826	-1.210184
O	3.950851	-0.411092	-1.727425
H	3.435431	0.418802	-1.667837
H	4.594936	-0.294313	-2.427847
O	3.893193	-0.909224	0.964590
H	4.156533	-0.781265	0.034486
H	2.361300	-1.635002	0.935520
O	2.747325	1.579057	1.808187
H	2.983006	2.222268	2.480439
H	3.755974	-0.020605	1.327298
O	-3.551996	-1.493795	1.025881
H	-2.707622	-1.894966	0.696701
H	-4.037036	-2.180231	1.487646
O	-2.390601	0.930295	1.908338
H	-0.696341	0.792698	1.786331
H	-2.877785	0.109307	1.724760
O	-3.686601	0.026500	-1.320271
H	-3.982776	-0.500755	-0.562812
H	-3.306812	1.553917	-0.879788
O	-2.912428	2.387722	-0.501576
H	-2.676004	1.564197	1.231780
H	-3.494465	3.113939	-0.734555
O	0.221096	0.768994	1.416802

H	1.790303	1.387947	1.906866
H	0.086365	1.114383	0.508402

Structure gw10z-02 : -1048.82691022 Hartree.

C	-0.954583	-1.044510	1.097413
H	-1.313770	-1.578434	1.977008
C	0.523673	-1.376726	0.843520
O	1.348790	-0.784106	1.562969
N	-1.743041	-1.479547	-0.082888
H	3.118210	-0.667547	1.209105
H	-1.267493	-2.308213	-0.459527
O	0.735139	-2.225625	-0.050647
H	-1.101345	0.024047	1.242928
H	-1.671898	-0.731285	-0.792514
O	3.004771	-1.940293	-1.364785
H	3.227229	-2.666577	-1.949929
H	2.199500	-2.204433	-0.852436
O	-3.508423	0.967141	0.302573
H	-4.083270	-0.448233	1.192876
H	-3.599840	0.917963	-0.662205
O	-3.226514	0.325424	-2.409193
H	-3.619812	0.486999	-3.268251
H	-2.287914	0.585636	-2.454103
O	-1.272116	2.651380	0.535050
H	-2.824513	1.630772	0.489966
H	-1.380759	3.603211	0.591723
O	3.333106	2.019680	0.060409
H	1.783973	2.158649	1.089867
H	4.052313	2.653341	0.028267
O	1.850181	0.598100	-1.892516
H	2.295384	-0.263390	-1.836924
H	2.371806	1.203393	-1.341793
O	-0.779900	0.771219	-1.481208
H	-0.875958	1.564327	-0.927551
H	0.186367	0.680213	-1.674838
O	-4.072333	-1.404145	1.396097
H	-4.962986	-1.666370	1.632099
H	-2.725055	-1.658407	0.171417
O	0.988970	1.938323	1.605134
H	1.084169	0.982765	1.784703
H	-0.419738	2.428429	1.008016
O	3.960987	-0.416458	0.781452
H	3.991154	-0.997525	0.006846
H	3.709743	1.149794	0.367206

Structure gw10z-03 : -1048.82603269 Hartree.

C	-0.700611	0.401037	-1.199504

H	-1.424560	1.128036	-1.567208
C	0.721033	0.959917	-1.255169
O	1.564524	0.290070	-1.863548
N	-0.793240	-0.849111	-1.989486
H	3.202363	-0.044843	-1.151955
H	-1.783559	-1.092544	-2.099445
O	0.879949	2.054457	-0.647947
H	-0.940703	0.163264	-0.161790
H	-0.321836	-0.726582	-2.885687
O	-3.232800	1.144414	0.707207
H	-2.741408	1.948304	0.455011
H	-2.745719	0.789778	1.468865
O	-2.037872	-2.307075	0.838607
H	-1.981393	-1.653010	1.552745
H	-2.695665	-1.964805	0.216471
O	0.993305	-0.104285	1.743918
H	1.614373	0.638409	1.669008
H	1.513548	-0.907828	1.578725
O	3.850484	-0.277851	-0.459662
H	3.161564	-1.534322	0.292063
H	3.838032	0.496958	0.123082
O	0.246175	-2.792231	-0.572986
H	-0.285427	-1.644816	-1.467412
H	-0.449153	-2.810494	0.111007
O	2.591818	-2.193623	0.782767
H	3.174432	-2.853950	1.163354
H	1.105464	-2.660969	-0.132419
O	-1.529578	-0.139488	2.562552
H	-1.584497	-0.099776	3.519879
H	-0.572270	-0.067345	2.328862
O	-1.489501	3.148835	-0.021013
H	-0.567021	2.850183	-0.200704
H	-1.490681	4.106762	-0.032912
O	-3.490036	-0.763583	-1.102321
H	-4.406610	-0.879723	-1.362180
H	-3.467172	0.006806	-0.473520
O	2.883119	1.905874	1.029088
H	3.209638	2.720770	1.414809
H	2.231703	2.145679	0.322481

Structure gw10z-04 : -1048.82528066 Hartree.

C	-0.765932	-1.677312	-1.353025
H	-0.056448	-2.380932	-1.783980
C	-0.418763	-0.223375	-1.732401
O	-1.324868	0.612899	-1.543795
N	-0.715008	-1.808771	0.140680
H	-1.362062	2.460689	-1.166096

H	-1.526274	-2.355939	0.472117
O	0.742900	0.005128	-2.132272
H	-1.780867	-1.915229	-1.667372
H	-0.742290	-0.872401	0.592667
O	-2.263282	2.085895	1.776192
H	-2.431775	2.475185	2.636701
H	-1.418667	1.593976	1.837063
O	-0.019085	0.648449	1.325774
H	0.735334	0.326229	1.868290
H	0.401664	1.189502	0.626778
O	1.330375	2.183205	-0.612115
H	2.844172	1.783986	0.117775
H	1.161721	1.600094	-1.380411
O	3.584108	1.240480	0.467578
H	4.366809	1.795735	0.471609
H	3.366354	-0.315019	-0.612814
O	-3.363496	0.019578	0.186234
H	-2.775086	0.268877	-0.552733
H	-3.246451	0.723566	0.841591
O	-3.289411	-2.600816	0.548632
H	-3.550803	-1.655621	0.477306
H	-4.075005	-3.132677	0.676152
O	1.911217	-2.688002	0.684617
H	0.175146	-2.248513	0.434619
H	2.309476	-3.560807	0.714466
O	2.248592	-0.383565	2.377448
H	2.276660	-1.278849	2.010655
H	2.900458	0.131632	1.876660
O	2.974031	-1.094666	-1.037576
H	2.399001	-2.151324	-0.010009
H	2.235308	-0.750910	-1.581046
O	-1.162205	3.263718	-0.655731
H	0.611912	2.847622	-0.619558
H	-1.656055	3.148246	0.167476

Structure gw10z-05 : -1048.81465980 Hartree.

C	-1.573400	-0.370553	1.425666
H	-1.930407	-0.126864	2.426030
C	-0.072106	-0.679877	1.459043
O	0.652203	0.290032	1.749286
N	-2.331540	-1.534426	0.898723
H	0.085687	1.887844	1.115155
H	-2.069079	-2.380723	1.404097
O	0.260953	-1.855904	1.202669
H	-1.769043	0.475426	0.767659
H	-2.070552	-1.660135	-0.113314
O	3.080680	0.712477	0.555245

H	2.262363	0.544622	1.064855
H	3.562804	-0.123322	0.654128
O	2.422336	3.342355	0.110755
H	2.899789	2.503662	0.239560
H	2.996022	4.038355	0.434601
O	1.124377	-2.610105	-1.338670
H	2.025199	-1.014367	-1.836652
H	0.338921	-2.645288	-1.895197
O	-2.690513	2.077163	-0.769457
H	-3.854031	0.919518	-0.091527
H	-1.999236	2.517770	-0.245755
O	-0.191674	2.530084	0.433279
H	0.606029	3.071576	0.285677
H	-0.183555	1.391875	-0.987635
O	-4.367280	0.179193	0.293489
H	-5.283914	0.460000	0.305962
H	-3.336748	-1.322810	0.927502
O	2.193370	-0.078409	-2.037601
H	0.635081	0.557239	-2.013622
H	2.609655	0.276981	-1.234274
O	3.136907	-2.069556	0.779940
H	3.062478	-2.612247	-0.011569
H	2.235211	-2.050532	1.140020
O	-1.563488	-1.452967	-1.693417
H	-2.219546	-1.424443	-2.394846
H	0.764490	-2.413137	-0.457019
O	-0.291630	0.802355	-1.758891
H	-2.226507	1.813136	-1.573905
H	-1.077218	-0.574314	-1.722247

Structure gw10z-06 : -1048.81101156 Hartree.

C	3.012401	-0.680548	1.099873
H	3.594576	-0.787613	2.015340
C	2.101371	0.568335	1.210045
O	1.021162	0.398489	1.806718
N	3.911476	-0.444470	-0.060207
H	-0.303724	1.590195	1.626988
H	4.149246	0.556281	-0.030666
O	2.558817	1.597784	0.685714
H	2.426385	-1.582969	0.929709
H	4.743943	-1.026865	-0.070660
O	0.298654	-2.497652	-1.121099
H	0.528147	-3.424659	-1.226871
H	1.493667	-1.295001	-1.776080
O	-2.354860	-1.908297	-1.665477
H	-2.708300	-2.400587	-2.409696

H	-1.401253	-2.118766	-1.610005
O	-1.311260	2.669597	-1.372734
H	-1.664535	3.467673	-1.771394
H	-2.020727	1.981875	-1.425617
O	-3.176707	0.782600	-1.261857
H	-2.885510	-0.117670	-1.474080
H	-3.457687	0.759854	-0.331731
O	2.204078	-0.655217	-1.969671
H	1.785402	0.242201	-2.030109
H	3.288691	-0.584067	-0.957639
O	-1.125179	2.084447	1.433821
H	-1.026299	2.449838	0.542314
H	-2.513918	1.262438	1.582356
O	1.317903	1.838463	-1.788907
H	0.390798	2.130340	-1.773139
H	1.678814	2.059138	-0.914745
O	-2.747474	-1.959498	1.202107
H	-1.004970	-2.085968	1.481728
H	-2.874324	-2.036645	0.247009
O	-3.370296	0.751835	1.528305
H	-3.979256	1.151689	2.152342
H	-3.053876	-1.066409	1.434095
O	-0.029786	-2.078370	1.374118
H	0.272625	-1.192795	1.664577
H	0.198700	-2.340394	-0.120386

2.3 The most stable neutral and zwitterionic structures of TW_8 (Table S3)

Structure tw08n : -1241.49919289 Hartree.

C	0.495054	-2.433747	-0.461469
C	0.031772	-1.609932	-1.486944
C	-1.308207	-1.248024	-1.568481
C	-2.208521	-1.698303	-0.606894
C	-1.779067	-2.587827	0.377716
C	-0.440641	-2.944168	0.442830
H	0.730526	-1.226378	-2.221388
H	-1.654891	-0.593751	-2.359458
O	-3.505037	-1.283491	-0.578654
H	-2.495760	-2.958954	1.101073
H	-0.111974	-3.614670	1.230486
H	-3.574713	-0.440398	-1.065140
C	1.967443	-2.717719	-0.298163
C	2.698089	-1.695484	0.593046
C	2.743757	-0.288132	0.007612
H	2.466253	-2.734176	-1.268330

H	2.106519	-3.704377	0.154759
H	3.752880	-2.007399	0.648725
N	2.072246	-1.593585	1.911944
H	2.093346	-2.490343	2.385430
H	2.577956	-0.922380	2.482002
O	2.707970	0.686702	0.740350
O	2.867870	-0.236254	-1.289131
H	2.704190	0.720496	-1.619532
O	-2.991852	2.522440	0.829473
H	-2.157031	2.951963	1.065165
H	-3.068515	1.746188	1.421596
O	-0.407050	1.681202	-1.175158
H	-1.306322	1.555288	-1.514352
H	-0.481028	2.285591	-0.413690
O	2.137730	2.070866	-2.059746
H	2.372173	2.785703	-1.449211
H	1.170947	1.965098	-1.942466
O	-0.248413	0.178117	1.420155
H	-0.259873	0.201386	0.449612
H	0.424683	-0.490099	1.657214
O	2.494369	3.378765	0.445523
H	2.701637	2.440911	0.629617
H	3.196834	3.905948	0.832838
O	-3.242240	1.335576	-1.496775
H	-3.216699	1.852118	-0.644025
H	-3.832049	1.809293	-2.088541
O	-0.196950	2.940404	1.272721
H	-0.033183	2.044984	1.620263
H	0.672964	3.349549	1.152251
O	-2.993743	0.059475	2.027148
H	-3.423399	-0.506108	1.373298
H	-2.040485	-0.100787	1.915418

Structure tw08z : -1241.49448801 Hartree.

C	1.355067	1.353048	1.398955
C	2.255251	1.812204	0.436085
C	1.828821	2.562774	-0.654120
C	0.476283	2.857496	-0.797247
C	-0.419899	2.484443	0.205654
C	0.013912	1.731374	1.285257
H	3.307932	1.555671	0.520683
H	2.519184	2.886330	-1.423607
O	0.057232	3.494557	-1.923701
H	-1.464570	2.762666	0.119422
H	-0.705286	1.421573	2.037134
H	-0.791286	3.099808	-2.176440
C	1.779416	0.344107	2.439104

C	1.359090	-1.074127	2.010715
C	-0.182060	-1.221061	2.018866
H	1.303656	0.531853	3.402518
H	2.863737	0.377865	2.582069
H	1.791313	-1.821894	2.677760
N	1.835971	-1.342764	0.627330
H	2.832461	-1.164352	0.486533
H	1.330934	-0.732947	-0.047382
O	-0.704153	-1.560192	0.924555
O	-0.741804	-0.943561	3.083291
H	-2.319324	-0.170541	2.958264
O	3.213601	-1.195714	-1.835886
H	2.413529	-0.676682	-2.049731
H	3.895494	-0.932687	-2.456884
O	-2.766882	-0.044343	0.035183
H	-3.426632	-0.825963	-1.420167
H	-2.035217	-0.612651	0.366647
O	-1.703185	1.279660	-2.161840
H	-2.192398	0.755603	-2.807308
H	-2.067263	0.983884	-1.304394
O	1.619945	-3.479673	-1.112673
H	1.641495	-2.304084	0.282524
H	2.228917	-3.000164	-1.691149
O	-3.354249	-1.190935	-2.325626
H	-1.829269	-2.293361	-2.010968
H	-4.225636	-1.504955	-2.575558
O	-0.955894	-2.502164	-1.640931
H	-1.025496	-2.385482	-0.677036
H	0.754477	-3.454111	-1.546998
O	0.681981	-0.303236	-1.775624
H	0.073281	-1.064114	-1.875136
H	0.119150	0.477929	-1.901363
O	-3.067648	0.412865	2.706733
H	-3.174966	0.268172	0.862870
H	-3.696863	0.382339	3.428927

2.4 The most stable neutral and zwitterionic structures of TW_9 (Table S3)

Structure tw09n : -1317.94084881 Hartree.

C	-0.909284	-2.412807	-0.027839
C	-0.240920	-1.871948	1.070796
C	1.145255	-1.741512	1.085924
C	1.889110	-2.168554	-0.013701
C	1.237800	-2.720927	-1.116927
C	-0.143120	-2.837824	-1.115517
H	-0.811367	-1.548279	1.935169
H	1.652884	-1.323345	1.948441

O	3.239953	-2.047897	-0.084740
H	1.831250	-3.060121	-1.958099
H	-0.635645	-3.278190	-1.976941
H	3.603006	-1.683835	0.750931
C	-2.413088	-2.533281	-0.057382
C	-3.131460	-1.296777	-0.625171
C	-2.991696	-0.064532	0.256026
H	-2.804077	-2.718039	0.944104
H	-2.696448	-3.389853	-0.676964
H	-4.210040	-1.517840	-0.627429
N	-2.623478	-0.949223	-1.951742
H	-2.779114	-1.713648	-2.600311
H	-3.113450	-0.132646	-2.304753
O	-2.846167	1.042712	-0.221610
O	-3.096938	-0.313748	1.539394
H	-2.874609	0.510710	2.069312
O	-0.074064	0.449647	-1.429857
H	-0.319226	1.347169	-1.710160
H	-0.823656	-0.132999	-1.662854
O	-2.071611	1.680685	2.851312
H	-1.163299	1.453198	2.584487
H	-2.189051	2.576920	2.512288
O	2.957498	1.422834	0.960063
H	2.889846	0.984525	0.091667
H	2.028596	1.476957	1.256122
O	0.213864	1.373314	1.247821
H	0.092066	0.765729	0.494696
H	-0.231918	2.192512	0.952523
O	2.543021	3.110894	-1.419840
H	2.795395	3.062969	-0.488018
H	2.796992	2.239130	-1.762369
O	2.660682	0.329432	-1.626463
H	1.699233	0.150814	-1.653537
H	3.101972	-0.521828	-1.509244
O	4.068969	-0.728267	2.134349
H	4.929331	-0.661827	2.551967
H	3.790222	0.175144	1.872098
O	-0.092018	3.289574	-1.897402
H	0.879240	3.311594	-1.723008
H	-0.223660	3.755222	-2.726606
O	-1.531191	3.369058	0.503625
H	-2.155991	2.689743	0.201372
H	-1.125682	3.697749	-0.313166

Structure tw09z : -1317.93863215 Hartree.

C	-1.830601	-0.754585	-1.506152
C	-2.849913	-1.055351	-0.599204

C	-3.423219	-0.074567	0.199037
C	-2.980454	1.245705	0.105606
C	-2.004542	1.572132	-0.841516
C	-1.436173	0.579020	-1.627347
H	-3.198933	-2.080382	-0.504057
H	-4.202930	-0.311326	0.913091
O	-3.521343	2.167639	0.928546
H	-1.695879	2.605251	-0.953209
H	-0.668107	0.840568	-2.345173
H	-2.905561	2.921159	0.998497
C	-1.106624	-1.847279	-2.256360
C	0.204004	-2.239908	-1.560702
C	1.303160	-1.150592	-1.649232
H	-0.841707	-1.527455	-3.264547
H	-1.747316	-2.730698	-2.340206
H	0.609892	-3.152947	-2.003407
N	-0.050021	-2.502804	-0.118085
H	-0.847873	-3.117462	0.054783
H	-0.268367	-1.605636	0.372675
O	2.030182	-1.022257	-0.634979
O	1.368358	-0.520208	-2.715523
H	1.672544	1.101825	-2.451554
O	-1.600820	-2.552953	2.282213
H	-1.499197	-1.589017	2.176878
H	-2.380353	-2.693380	2.823232
O	3.902717	1.041070	-0.606032
H	3.710644	1.621758	0.924028
H	3.391620	0.212683	-0.699827
O	0.780198	2.204013	0.578569
H	1.605515	2.200172	1.092683
H	1.051139	2.148343	-0.356102
O	1.210204	-3.253175	2.213252
H	0.755486	-2.885665	0.406203
H	0.338122	-3.138014	2.615563
O	3.336892	1.871477	1.810749
H	2.742589	0.142911	2.281759
H	3.966949	2.448117	2.247003
O	2.243731	-0.668998	2.096852
H	2.325857	-0.815580	1.136654
H	1.743815	-2.504392	2.517879
O	-0.394000	-0.252655	1.540152
H	0.509153	-0.285825	1.916966
H	-0.423425	0.601652	1.079456
O	1.757657	2.025922	-2.101912
H	3.460118	1.633182	-1.231294
H	1.566478	2.623395	-2.828236
O	-1.359142	3.878338	1.097069

H	-0.547805	3.348995	0.962963
H	-1.163230	4.514251	1.787467

2.5 The most stable neutral and zwitterionic structures of TW_{10} (Table S3)

Structure tw10n : -1394.38397359 Hartree.

C	1.323222	-2.241488	-0.877481
C	0.557412	-1.222176	-1.447077
C	-0.835852	-1.248688	-1.389652
C	-1.487537	-2.319092	-0.770054
C	-0.732189	-3.363605	-0.232328
C	0.651713	-3.314938	-0.286805
H	1.036808	-0.371777	-1.919243
H	-1.409680	-0.433398	-1.815666
O	-2.829830	-2.381556	-0.623835
H	-1.250071	-4.192255	0.235981
H	1.224886	-4.127672	0.148866
H	-3.261359	-1.547783	-0.936492
C	2.829232	-2.172323	-0.838460
C	3.381487	-1.310436	0.311483
C	3.134733	0.181012	0.122979
H	3.225635	-1.771668	-1.772434
H	3.234784	-3.181726	-0.720492
H	4.478246	-1.405442	0.283974
N	2.822037	-1.703095	1.606202
H	3.024998	-2.679341	1.794786
H	3.245043	-1.146777	2.343183
O	2.872208	0.894877	1.079235
O	3.297637	0.596228	-1.098073
H	3.035006	1.590771	-1.206256
O	-4.259411	0.611504	1.651451
H	-5.011591	0.604712	2.247067
H	-3.652399	-0.113099	1.940449
O	-2.756600	2.756262	0.665512
H	-3.319738	2.117686	1.133104
H	-1.855345	2.608975	1.000716
O	-0.027013	1.973983	-1.589274
H	-0.905616	2.149086	-1.959859
H	-0.155646	1.932039	-0.624852
O	2.461896	2.948350	-1.433435
H	2.426296	3.469271	-0.617074
H	1.527573	2.760357	-1.669906
O	0.101432	-0.635608	1.700628
H	-0.096224	-0.765005	0.762030
H	0.978750	-1.062372	1.799642
O	-2.807938	2.336255	-1.931259
H	-3.258339	3.009953	-2.445603

H	-2.839409	2.618360	-0.979664
O	2.329368	3.515991	1.325688
H	2.723399	2.621491	1.354421
H	2.766702	4.056312	1.986831
O	-4.028431	-0.070769	-1.094833
H	-4.282741	0.241095	-0.211540
H	-3.657284	0.699756	-1.554557
O	-0.114987	2.085595	1.216864
H	0.109203	1.207094	1.578189
H	0.618636	2.685298	1.421323
O	-2.611565	-1.423989	2.138481
H	-2.745666	-1.990264	1.365077
H	-1.656593	-1.248588	2.181750

Structure tw10z : -1394.38436564 Hartree.

C	1.576523	0.724055	1.599065
C	2.614776	1.071745	0.729661
C	2.508638	2.165676	-0.119508
C	1.347945	2.940896	-0.117025
C	0.326814	2.638833	0.789672
C	0.444137	1.539247	1.630176
H	3.513926	0.462982	0.704414
H	3.303928	2.422970	-0.809036
O	1.252242	3.968265	-0.987877
H	-0.554067	3.269743	0.828192
H	-0.358374	1.305726	2.319459
H	0.307528	4.161227	-1.132290
C	1.648127	-0.539810	2.423234
C	0.903516	-1.709649	1.767306
C	-0.634234	-1.546829	1.727153
H	1.195730	-0.394944	3.404996
H	2.693542	-0.827295	2.567140
H	1.111244	-2.632333	2.316625
N	1.389025	-1.905255	0.372940
H	2.413034	-2.043108	0.330250
H	1.145842	-1.072549	-0.210495
O	-1.211546	-2.027818	0.718731
O	-1.157082	-0.992464	2.704759
H	-2.388427	0.059619	2.334702
O	2.882856	-0.901493	-2.243583
H	2.281987	-0.160606	-2.070525
H	2.281942	-1.628935	-2.469387
O	-3.952703	-1.523997	0.500310
H	-4.082276	-1.027348	-1.065746
H	-3.053123	-1.863607	0.676951
O	-2.174815	1.287428	-0.729514
H	-2.791152	0.753397	-1.256451

H	-2.428124	1.140591	0.199767
O	0.955574	-3.039118	-2.262376
H	0.921996	-2.690950	-0.088235
H	1.056200	-3.864334	-2.742178
O	-3.904682	-0.647200	-1.967185
H	-2.327346	-1.583966	-2.273518
H	-4.733805	-0.622233	-2.448451
O	-1.449857	-1.891583	-1.992003
H	-1.489090	-1.982585	-1.019831
H	0.032784	-2.746401	-2.403529
O	0.402068	0.075647	-1.408028
H	-0.311210	-0.452794	-1.807141
H	-0.069074	0.804623	-0.975991
O	-3.030900	0.692543	1.922257
H	-4.007523	-0.748512	1.078499
H	-3.289844	1.320790	2.599850
O	-1.491869	3.901530	-1.354289
H	-1.793767	2.987265	-1.183438
H	-1.966863	4.205621	-2.129779
O	4.168719	-1.805698	-0.070831
H	3.935095	-1.423104	-0.944291
H	5.004613	-2.265484	-0.162493

2.6 The most stable neutral and zwitterionic structures of TW_{11} (Table S3)

Structure tw11n : -1470.82378303 Hartree.

C	0.875783	-2.279725	-1.096804
C	0.485567	-1.025270	-1.570791
C	-0.857572	-0.656483	-1.613129
C	-1.842257	-1.557495	-1.197651
C	-1.466380	-2.818542	-0.729462
C	-0.123454	-3.164317	-0.684556
H	1.225601	-0.307237	-1.905750
H	-1.135751	0.325342	-1.979816
O	-3.163970	-1.260485	-1.236144
H	-2.234231	-3.506951	-0.397488
H	0.153066	-4.147581	-0.316433
H	-3.312483	-0.284105	-1.364388
C	2.329694	-2.670738	-0.995366
C	3.046234	-2.125349	0.251933
C	3.260201	-0.617487	0.219564
H	2.883536	-2.328115	-1.870647
H	2.407488	-3.761950	-0.970824
H	4.066220	-2.540330	0.242079
N	2.325410	-2.455548	1.482495
H	2.231752	-3.461639	1.576262
H	2.844394	-2.111860	2.285220

O	3.180381	0.044539	1.243194
O	3.590119	-0.154063	-0.949188
H	3.632482	0.879084	-0.964535
O	-3.677874	1.696787	1.508560
H	-4.421137	1.933409	2.067611
H	-3.291523	0.863022	1.889467
O	-1.638212	3.444187	0.730029
H	-2.370605	2.941079	1.123696
H	-0.829244	2.993250	1.030067
O	0.867231	2.195489	-1.584060
H	0.086692	2.639685	-1.947236
H	0.662935	2.036243	-0.645041
O	3.499213	2.358927	-1.088588
H	3.526675	2.794677	-0.223279
H	2.589985	2.492643	-1.431996
O	0.013417	-0.725431	1.634688
H	-0.339162	-0.826296	0.739861
H	0.753863	-1.370299	1.664273
O	-4.175243	-2.430221	1.038766
H	-4.030176	-2.037807	0.158919
H	-5.119778	-2.566750	1.131346
O	-1.726923	3.309983	-1.892429
H	-1.962404	4.127539	-2.336814
H	-1.701475	3.499273	-0.917294
O	3.333481	2.686902	1.695679
H	3.489504	1.722154	1.677788
H	3.808593	3.054920	2.443268
O	-3.622179	1.305136	-1.276124
H	-3.735539	1.532323	-0.337132
H	-3.030337	1.977099	-1.652892
O	0.641324	1.937541	1.191835
H	0.562563	1.010502	1.490714
H	1.481063	2.286858	1.526565
O	-2.687432	-0.551555	2.465635
H	-3.149406	-1.319617	2.087073
H	-1.734582	-0.719179	2.392631

Structure tw11z : -1470.82839906 Hartree.

C	-1.289317	-0.214489	-2.069369
C	-2.558137	-0.091017	-1.499766
C	-2.975161	1.102113	-0.926932
C	-2.117122	2.198369	-0.909185
C	-0.873399	2.112913	-1.536325
C	-0.465229	0.912706	-2.105124
H	-3.219234	-0.951551	-1.473824
H	-3.948567	1.187843	-0.457876
O	-2.518474	3.320122	-0.252201

H	-0.224659	2.981721	-1.556779
H	0.513378	0.842846	-2.566237
H	-1.718948	3.761706	0.093368
C	-0.801284	-1.566450	-2.531357
C	0.055667	-2.263291	-1.467191
C	1.468345	-1.656466	-1.286164
H	-0.182093	-1.484020	-3.424965
H	-1.658750	-2.203194	-2.765728
H	0.199916	-3.312853	-1.738960
N	-0.633847	-2.244310	-0.145435
H	-1.580860	-2.663540	-0.177082
H	-0.726785	-1.263630	0.195366
O	1.975547	-1.783653	-0.143608
O	1.983592	-1.143260	-2.290697
H	2.862436	0.253777	-2.208176
O	-2.854463	-1.219101	2.070910
H	-2.896577	-0.251771	2.163905
H	-2.011497	-1.499577	2.456836
O	4.424554	-0.442458	0.079139
H	4.172318	0.427694	1.455450
H	3.673025	-1.050730	-0.065893
O	1.883275	1.966176	0.294634
H	2.535307	1.770104	0.989205
H	2.343507	1.816700	-0.550917
O	-0.378235	-2.517844	2.730116
H	-0.080276	-2.717171	0.575140
H	-0.457131	-3.198668	3.402455
O	3.753850	0.948096	2.192081
H	2.488597	-0.342013	2.684796
H	4.454299	1.355641	2.705464
O	1.792327	-0.979451	2.454447
H	2.013174	-1.312401	1.563403
H	0.443173	-2.026505	2.924842
O	-0.224391	0.302878	1.054349
H	0.387600	-0.033096	1.734987
H	0.355082	0.864983	0.506595
O	3.295390	1.116368	-1.982492
H	4.389598	0.151084	-0.685281
H	3.547563	1.538443	-2.806464
O	-0.200106	3.706754	1.142676
H	0.579941	3.219342	0.827193
H	-0.482935	3.256700	1.946259
O	-3.351456	-2.892490	0.056022
H	-3.387577	-2.261397	0.809368
H	-3.959886	-3.607353	0.250468
O	-2.360332	1.590219	2.205910
H	-1.612674	1.253370	1.677835

H	-2.808341	2.222508	1.631485

2.7 The most stable neutral and zwitterionic structures of TW_{12} (Table S3)

Structure tw12n : -1547.26314236 Hartree.

C	0.981927	-0.559339	-2.392662
C	2.236975	-0.168196	-1.919719
C	2.946125	-0.963800	-1.028610
C	2.399580	-2.166968	-0.588698
C	1.171860	-2.594580	-1.085997
C	0.475011	-1.792915	-1.982954
H	2.649692	0.791131	-2.215727
H	3.915291	-0.653519	-0.653716
O	3.095555	-2.892941	0.339158
H	0.761140	-3.545143	-0.763959
H	-0.483146	-2.132027	-2.361502
H	2.459831	-3.447095	0.818417
C	0.169023	0.368594	-3.262152
C	-0.791698	1.261386	-2.450614
C	-1.883700	0.462606	-1.752025
H	-0.417924	-0.194483	-3.989005
H	0.839011	1.032147	-3.815774
H	-1.324697	1.903646	-3.169265
N	-0.069036	2.015910	-1.437100
H	0.722413	2.519233	-1.834489
H	-0.672737	2.675059	-0.949068
O	-2.402139	-0.496941	-2.481972
O	-2.250459	0.732459	-0.621485
H	-3.726044	0.346928	0.266921
O	-0.951494	1.563541	2.605452
H	-0.510276	1.061974	1.876840
H	-1.238619	3.015346	1.560611
O	1.756392	3.308896	0.968871
H	1.832005	2.699591	1.718504
H	0.820166	3.560398	0.929725
O	-3.419254	-2.156143	-0.792740
H	-0.706312	-1.214966	0.606818
H	-2.938033	-1.119566	-1.889832
O	1.821354	1.558916	3.266578
H	2.416288	1.803287	3.979309
H	-0.213597	1.728363	3.209864
O	-4.464251	-0.049881	0.773405
H	-4.077177	-1.725314	-0.227588
H	-5.207085	0.554508	0.714227
O	-1.226622	-1.971275	0.950214
H	1.771742	-1.727444	2.430849
H	-2.636668	-2.260922	-0.215693

O	0.854982	-3.314722	1.991190
H	0.035947	-2.929214	1.590776
H	0.564634	-3.937442	2.661974
O	-2.649067	-0.667739	2.845439
H	-3.456842	-0.432978	2.365524
H	-1.734056	-1.573612	1.698372
O	0.343142	0.291634	0.653004
H	1.257755	0.030722	0.825269
H	-2.167810	0.168584	2.964889
O	2.691861	3.098805	-1.598286
H	0.332128	0.916741	-0.127840
H	2.474652	3.141080	-0.645192
O	2.369678	-0.963162	2.349331
H	2.060311	0.645030	3.013582
H	3.113721	-1.315865	1.845581
O	-1.065280	3.718016	0.902553
H	-1.553891	4.493212	1.185537
H	3.255656	3.854804	-1.770369

Structure tw12z : -1547.26922899 Hartree.

C	0.239737	2.079830	1.559809
C	0.138682	2.764092	0.344977
C	-1.062247	2.818836	-0.350686
C	-2.191870	2.186571	0.165862
C	-2.120805	1.531841	1.394543
C	-0.912276	1.491182	2.082401
H	1.016744	3.248475	-0.073476
H	-1.139622	3.339947	-1.297902
O	-3.332215	2.216902	-0.582677
H	-3.006220	1.053044	1.799739
H	-0.853972	0.975987	3.034363
H	-4.006390	1.623621	-0.197768
C	1.578613	1.930916	2.245359
C	2.357347	0.684759	1.804954
C	1.715976	-0.666619	2.219701
H	1.447379	1.844101	3.324526
H	2.191393	2.815767	2.047336
H	3.361505	0.714510	2.237035
N	2.520496	0.648960	0.324155
H	2.984207	1.486473	-0.055208
H	3.012945	-0.207690	0.030086
O	1.011328	-0.670836	3.236915
O	1.991183	-1.621590	1.449219
H	1.191606	-3.046114	1.485093
O	0.972123	-2.209891	-2.171670
H	0.613177	-1.607780	-1.480956
H	2.671222	-1.869805	-1.773158

O	2.213182	0.968518	-2.622950
H	1.398656	0.687177	-3.070560
H	2.770281	0.180965	-2.530615
O	-1.152313	-1.686190	1.858134
H	-0.368268	-0.837130	0.382560
H	-0.610529	-1.276180	2.558666
O	-0.104730	-0.144822	-3.804663
H	-0.344432	-0.023480	-4.726206
H	0.701247	-1.776161	-2.994374
O	0.552127	-3.811980	1.434656
H	-0.800436	-2.592387	1.812736
H	0.877384	-4.496468	2.022083
O	-2.919175	-1.691978	-0.234836
H	-2.578528	-0.536156	-1.581586
H	-2.477353	-1.507061	0.615011
O	-4.895389	0.120437	0.194724
H	-4.424587	-0.710290	0.000784
H	-5.830526	-0.081588	0.254303
O	-1.117089	-3.692077	-0.832363
H	-0.571339	-3.927667	-0.063728
H	-2.458586	-2.505047	-0.534605
O	0.000546	-0.415997	-0.420478
H	-0.726080	0.082017	-0.826399
H	-0.467287	-3.412724	-1.493441
O	3.215388	2.977833	-1.158535
H	1.586771	0.561089	-0.117878
H	2.857129	2.460579	-1.906043
O	-2.234644	0.156897	-2.180353
H	-0.928070	-0.017538	-3.283729
H	-2.727675	0.962665	-1.965051
O	3.476128	-1.331983	-1.611284
H	4.223264	-1.933374	-1.627995
H	3.900982	3.551123	-1.504942

References

1. R. Pérez de Tudela and D. Marx, *J. Phys. Chem. Lett.,* 2016, **7**, 5137-5142.
2. L. Biedermannová and B. Schneider, *Acta Crystallogr. Sect. D Biol. Crystallogr.,* 2015, **71**, 2192-2202.