

Table S1. Zero-kelvin energies (E(0K); including ZPE), enthalpies (H) and Gibbs free energies (G) of the minimum-enthalpy and minimum-free energy cluster structures shown in the figures. All values in hartree, computed using the CBS-QB3 method. Enthalpy and free energy values correspond to 298.15 K and 1 atm reference pressure. In the case where minimum-energy (after zero-point corrections) structure is different from either the minimum-enthalpy or the minimum-free energy structure, data for all three are given.

	E(0K)	H	G
free NH ₄ ⁺	-56.783214	-56.779417	-56.800525
free NH ₃	-56.460186	-56.456375	-56.47822
free H ₂ O	-76.33749	-76.333711	-76.355137
<u>H⁺(NH₃)_m(H₂O)_n</u>			
m=1, n=1	-133.15029	-133.14369	-133.177752
m=1, n=2	-209.512244	-209.502357	-209.545533
m=1, n=3	-285.870812	-285.857214	-285.910296
m=2	-113.282758	-113.276765	-113.308942
m=2, n=1	-189.64155	-189.632105	-189.674692
m=2, n=2	-265.998654	-265.985332	-266.038406
m=2, n=3	-342.353712	-342.336235	-342.400546
m=3	-169.770023	-169.760923	-169.802598
m=3, n=1	-246.125978	-246.112911	-246.166043
m=3, n=2	-322.479983	-322.462762	-322.526691
m=3, n=3	-398.830823	-398.811344	-398.879491 (best H)
m=3, n=3,	-398.831729	-398.811027	-398.886755 (best G)
m=4	-226.252782	-226.239971	-226.293453
m=4, n=1	-302.606000	-302.589005	-302.652817
m=4, n=2	-378.956940	-378.937589	-379.00600 (best H)
m=4, n=2	-378.957396	-378.937037	-379.01118 (best G)
m=4, n=3	-455.310444	-455.288679	-455.364742 (best E ₀)
m=4, n=3	-455.309076	-455.289508	-455.355636 (best H)
m=4, n=3	-455.308344	-455.284613	-455.369206 (best G)

m=5	-282.731687	-282.714993	-282.778018
m=5, n=1	-359.08309	-359.062964	-359.137025
m=5, n=2	-435.433602	-435.410145	-435.494939 (best G)
m=5, n=2	-435.433374	-435.411362	-435.488300 (best H)
m=5, n=3	-511.783948	-511.757152	-511.851167 (best G)
m=5, n=3	-511.785766	-511.762871	-511.838073 (best H)
m=6	-339.201850	-339.181527	-339.255661
m=6, n=1	-415.552755	-415.529058	-415.613228 (best G)
m=6, n=1	-415.553656	-415.530744	-415.611273 (best H)
m=6, n=2	-491.907302	-491.881679	-491.968861
m=7	-395.671453	-395.647495	-395.732559
m=7, n=1	-472.022892	-471.996949	-472.082465 (best H)
m=7, n=1	-472.023139	-471.996711	-472.086830 (best G)

Table S2. Optimized cartesian co-ordinates (in Ångström) of the minimum-enthalpy and minimum-free energy cluster structures shown in the figures, at the CBS-QB3 level (corresponds to B3LYP/6-311G(2d,d,p) geometries). In the case where minimum-energy (after zero-point corrections) structure is different from either the minimum-enthalpy or the minimum-free energy structure, all three are given.

free NH₃

N	0.017284	0.029936	1.032221
H	0.461520	-0.827803	1.346343
H	-0.008206	-0.014214	0.017758
H	-0.947658	-0.014214	1.346343

free NH₄[±]

N	0.000000	0.000000	0.999988
H	0.000000	0.000000	-0.026772
H	-0.484019	0.838346	1.342242
H	0.968039	0.000000	1.342241
H	-0.484019	-0.838346	1.342241

free H₂O

O	-0.008048	0.000000	-0.006176
H	0.001983	0.000000	0.955748
H	0.923695	0.000000	-0.245450

m=1,n=1

N	2.366500	1.326860	-0.671740
H	2.772840	1.545290	-1.615930
H	2.599500	2.096550	0.003940
H	1.341260	1.247180	-0.755090
H	2.756030	0.417980	-0.317570
O	-0.364550	1.031640	-0.965050
H	-0.281510	0.343370	-1.614580
H	-0.641400	0.588750	-0.171520

m=1,n=2

N	-0.172989	1.921885	-0.297451
H	-0.977206	1.399723	-0.720908
H	-0.344368	2.936877	-0.366079
H	-0.091401	1.651942	0.708559
H	0.713730	1.694466	-0.806698
O	-0.101047	1.192519	2.373702
H	-0.638524	1.661627	3.018025
H	0.449213	0.552629	2.895981
O	-0.564494	4.774155	-0.505736
H	-1.090277	5.264506	-1.145620
H	-0.240223	5.431349	0.118300

m=1,n=3

N	-0.086991	1.972582	-0.320007
H	-0.341798	2.973934	-0.378992
H	0.152605	1.724141	0.677064
H	0.728795	1.792823	-0.930899
H	-0.885959	1.398181	-0.640577
O	-2.285859	0.396764	-1.216937
H	-2.385046	-0.559922	-1.177642
H	-3.079879	0.722971	-1.652653
O	2.149826	1.491646	-2.019854
H	3.064653	1.759990	-1.886933
H	2.133926	1.031751	-2.865443
O	-0.790347	4.728125	-0.503853
H	-1.410409	5.222311	0.041936
H	-0.456150	5.356634	-1.151960

m=2

N	0.066174	-0.088086	-0.034961
H	-0.704405	-0.085787	-0.705723
H	0.609562	0.766772	-0.167899
H	-0.328741	-0.073740	0.907146
H	0.730285	-1.018404	-0.182659
N	1.610689	-2.251369	-0.378176
H	2.019369	-2.292487	-1.311304
H	2.389609	-2.280230	0.279000
H	1.094282	-3.121223	-0.251240

m=2,n=1

N	0.003055	-0.000518	-0.021774
H	-0.825059	-0.038779	-0.667583
H	0.565246	0.865861	-0.213069
H	-0.330139	0.019724	0.954440
H	0.605395	-0.849193	-0.163741
N	1.697030	-2.375410	-0.399191
O	-0.953578	0.059078	2.751126
H	2.160168	-2.392124	-1.306548
H	2.436034	-2.426583	0.300384
H	1.175095	-3.247531	-0.328733
H	-1.192282	0.840529	3.267174
H	-1.095956	-0.697689	3.335058

m=2,n=2

N	-0.271979	1.910211	-0.248437
H	-1.095849	1.388607	-0.684923
H	-0.392239	2.937453	-0.360757
H	-0.192176	1.671631	0.760738
H	0.588038	1.629403	-0.717897
N	-2.449443	0.508635	-1.412617
O	-0.026629	1.231424	2.468902
H	-3.315475	1.042895	-1.383928
H	-2.293725	0.272436	-2.390516
H	-2.640654	-0.370052	-0.935507
H	-0.684954	1.331148	3.164483
H	0.758944	0.878919	2.900327
O	-0.596184	4.680498	-0.572297
H	-0.589544	5.171173	-1.400886
H	-0.569328	5.344028	0.125106

m=2,n=3

N	-0.087116	1.974682	-0.320182
H	-0.342225	2.975917	-0.379420
H	0.146080	1.740136	0.660464
H	-0.896481	1.381008	-0.645405
H	0.738655	1.797428	-0.918280
O	2.198446	1.495853	-1.954177
H	2.757406	2.165107	-2.362135
H	2.585615	0.649207	-2.198907
H	-2.295378	0.187634	-2.216378
N	-2.306759	0.346119	-1.211314
H	-2.313565	-0.574434	-0.777782
H	-3.208397	0.767540	-0.999494
H	1.448814	1.171228	2.727276
O	0.567131	1.342455	2.380747
H	-0.026844	1.272395	3.134995
O	-0.773113	4.736274	-0.477426

H	-1.155739	5.211944	-1.221706
H	-0.642465	5.394757	0.212571

m=3

N	0.003055	-0.000518	-0.021774
H	-0.825059	-0.038779	-0.667583
H	0.565246	0.865861	-0.213069
H	-0.330139	0.019724	0.954440
H	0.605395	-0.849193	-0.163741
N	1.697030	-2.375410	-0.399191
N	-2.331680	-0.107735	-1.799037
H	2.160168	-2.392124	-1.306548
H	2.436034	-2.426583	0.300384
H	1.175095	-3.247531	-0.328733
H	-2.954836	0.684982	-1.652914
H	-2.093748	-0.106905	-2.789638
H	-2.891609	-0.943781	-1.639133

m=3,n=1

N	-0.053922	-0.082037	-0.010505
H	-0.890884	-0.116428	-0.663916
H	0.484041	0.759531	-0.213760
H	-0.375299	-0.035856	0.975659
H	0.573632	-0.927822	-0.149504
N	1.686145	-2.330211	-0.375591
N	-2.310717	-0.117022	-1.776635
O	-0.909305	0.095490	2.679579
H	2.169680	-2.313611	-1.271166
H	2.411956	-2.359288	0.337578
H	1.207159	-3.227033	-0.328627
H	-3.024556	0.545916	-1.481353
H	-2.067246	0.135823	-2.732106
H	-2.771102	-1.023064	-1.831686
H	-0.740609	0.827204	3.282505
H	-1.415836	-0.547667	3.186348

m=3,n=2

N	-0.172989	1.921885	-0.297451
H	-0.977206	1.399723	-0.720908
H	-0.344368	2.936877	-0.366079
H	-0.091401	1.651942	0.708559
H	0.713730	1.694466	-0.806698
N	2.318702	1.355157	-1.742310
N	-2.448434	0.439437	-1.397586
O	-0.101047	1.192519	2.373702
H	2.464008	2.022925	-2.495863
H	3.132471	1.427548	-1.136324

H	2.358363	0.431528	-2.166418
H	-3.259664	1.026811	-1.575241
H	-2.259902	-0.057883	-2.264537
H	-2.745611	-0.261635	-0.722919
H	-0.638524	1.661627	3.018025
H	0.449213	0.552629	2.895981
O	-0.564494	4.774155	-0.505736
H	-1.090277	5.264506	-1.145620
H	-0.240223	5.431349	0.118300

m=3,n=3, best H

N	-0.450276	1.958422	-0.257554
O	-0.721201	4.818990	-0.431693
O	-0.252903	0.814437	2.285465
N	-2.582601	0.750341	-1.847563
N	2.222339	0.977847	-0.780295
H	-1.202621	1.517812	-0.841203
H	-0.528975	2.985864	-0.306435
H	-0.534845	1.638939	0.725948
H	0.502830	1.651781	-0.581014
H	2.930925	1.680677	-0.974151
H	2.459747	0.549384	0.115079
H	2.325879	0.260868	-1.493578
H	-3.355324	1.396859	-1.988340
H	-2.291780	0.446213	-2.773611
H	-2.974300	-0.067532	-1.386541
H	-0.663597	0.877138	3.151894
H	0.639148	0.447966	2.415471
H	-0.478304	5.385602	-1.170813
H	-1.064718	5.410645	0.245331
O	2.389809	-0.178016	2.229586
H	3.070188	0.209820	2.792163
H	2.503630	-1.132025	2.312910

m=3,n=3, best G

N	-0.094886	1.998264	-0.350348
O	-0.815561	4.772394	-0.522522
O	0.528108	1.415488	2.266401
O	-2.347708	0.422441	-1.173299
N	2.194184	1.532822	-2.095684
H	-0.895795	1.421553	-0.653830
H	-0.358199	2.995443	-0.404482
H	0.151397	1.758439	0.638867
H	0.728466	1.821440	-0.977882
H	2.256412	2.218855	-2.844256
H	3.073219	1.583764	-1.586247
H	2.175045	0.620088	-2.544332
H	-2.724114	0.317992	-2.052872
H	-2.925487	-0.071832	-0.583148

H	0.342525	2.042978	2.970525
H	0.906610	0.611054	2.709305
H	-1.691626	5.126451	-0.705938
H	-0.270331	5.533506	-0.299393
N	1.589729	-0.803032	3.588615
H	1.011260	-1.075271	4.379403
H	1.681454	-1.627767	3.001135
H	2.515788	-0.605864	3.959372

m=4

N	0.000422	-0.000206	0.658427
H	0.977576	-0.228123	0.322588
H	-0.685574	-0.732309	0.322370
H	0.000316	-0.000454	1.677673
H	-0.290794	0.960000	0.322683
N	-0.799681	2.637175	-0.208011
N	2.684211	-0.626319	-0.208133
N	-1.884893	-2.010728	-0.208060
H	-0.880000	2.723182	-1.218955
H	-1.703751	2.909883	0.171931
H	-0.141899	3.356247	0.085795
H	2.977426	-1.556748	0.082972
H	2.798800	-0.596747	-1.219181
H	3.372931	0.018811	0.173863
H	-2.823136	-1.836916	0.146213
H	-1.971711	-2.073620	-1.220145
H	-1.630602	-2.942659	0.112633

m=4,n=1

N	0.015320	0.020445	0.054335
H	0.017269	0.037847	1.103653
H	1.002284	0.012531	-0.301139
H	-0.470831	-0.831672	-0.267920
H	-0.484707	0.865055	-0.316548
N	-1.385181	2.371011	-1.002712
N	0.015138	0.036196	2.985266
N	2.773927	-0.006041	-0.950528
O	-1.353021	-2.363687	-0.814043
H	-0.858588	3.233963	-0.888106
H	-1.571972	2.282125	-1.998948
H	-2.286766	2.527714	-0.558036
H	0.232046	-0.883676	3.362145
H	0.695072	0.676624	3.388511
H	-0.887257	0.296972	3.376188
H	2.815087	-0.121136	-1.960626
H	3.277733	0.852995	-0.742199
H	3.328027	-0.762547	-0.555719
H	-0.966510	-3.148885	-1.214836
H	-2.298657	-2.537867	-0.769024

m=4,n=2, best H

N	-0.063849	0.999340	-0.246557
O	-0.301758	3.624023	0.719106
O	1.534686	5.004849	-0.926665
N	1.856973	2.038788	-2.172856
N	1.041432	-0.985684	1.629393
N	-2.556483	-0.009645	-1.442496
H	-0.944142	0.633539	-0.678457
H	0.637322	1.236106	-0.990994
H	-0.260501	1.886272	0.251657
H	0.332603	0.293972	0.416447
H	1.398972	-1.817158	1.165076
H	1.812712	-0.609326	2.175527
H	0.348900	-1.308946	2.300754
H	-3.085265	0.739318	-1.883262
H	-2.409776	-0.716780	-2.158824
H	-3.176035	-0.426641	-0.751807
H	2.808261	1.685086	-2.114062
H	1.594047	1.992129	-3.153790
H	1.886045	3.025912	-1.915515
H	0.301953	4.219070	0.241928
H	-0.668447	4.120785	1.455179
H	2.329539	5.394214	-0.544104
H	1.184612	5.675901	-1.524176

m=4,n=2, best G

N	-0.228760	1.972900	-0.284810
H	-1.004550	1.425340	-0.734950
H	-0.409070	3.002060	-0.392490
H	-0.187960	1.738670	0.719130
H	0.688230	1.727500	-0.734400
N	2.349450	1.291020	-1.525770
N	-2.403210	0.428200	-1.512330
O	-0.121600	1.302500	2.569440
H	2.422060	1.610370	-2.490550
H	3.131540	1.710950	-1.025610
H	2.525990	0.287760	-1.542860
H	-3.299740	0.617500	-1.066840
H	-2.530720	0.616760	-2.505350
H	-2.249390	-0.575460	-1.428290
H	-0.618890	1.721700	3.284230
H	0.416390	0.617110	2.987470
O	-0.572780	4.706900	-0.603040
H	-1.343310	5.192780	-0.872640
H	-0.040810	5.333830	-0.127150
N	1.397500	-0.525910	3.759230
H	0.979180	-1.478660	3.437990
H	1.399160	-0.478570	4.847200

H 2.418060 -0.434720 3.390360

m=4,n=3, best E₀

N	-0.085572	1.759889	-0.645338
O	-0.875137	4.435561	-0.597319
O	-0.224007	4.955183	2.058356
N	1.614033	6.858987	2.806215
O	0.704840	2.331086	1.975570
N	-2.406980	0.003229	-1.024381
N	2.174994	0.960434	-2.340438
H	-0.373671	2.736917	-0.846478
H	0.711870	1.476206	-1.260671
H	0.217217	1.760630	0.348235
H	-0.901583	1.118202	-0.778848
H	-2.444238	-0.425676	-1.945882
H	-3.267542	0.535887	-0.921828
H	-2.457968	-0.757722	-0.351437
H	2.199042	-0.038057	-2.532680
H	3.056752	1.185519	-1.885972
H	2.189686	1.427191	-3.244004
H	0.406525	3.247351	2.143152
H	0.700515	1.875931	2.821847
H	-1.015140	5.114477	2.584339
H	0.438315	5.659315	2.327646
H	-0.656362	4.769148	0.295183
H	-0.928248	5.197275	-1.180196
H	1.718428	6.923752	3.815865
H	1.390023	7.794517	2.476243
H	2.533198	6.631352	2.434984

m=4,n=3, best H

N	0.302276	2.203499	-0.585375
H	0.322972	2.249988	0.446523
H	-0.629974	2.597252	-0.901201
H	1.113714	2.710012	-1.018596
H	0.306655	1.197876	-0.819583
N	-2.384674	2.929644	-1.159440
H	-2.779749	2.217442	-0.543477
H	-2.740304	3.831945	-0.855544
H	-2.755814	2.769213	-2.091927
N	2.530253	3.628581	-1.806850
H	2.799435	4.456821	-1.280778
H	2.297468	3.949784	-2.743823
H	3.371302	3.063757	-1.900076
O	-0.263353	-0.615081	-0.487898
H	-1.132812	-0.399051	-0.088200
H	-0.422025	-1.290871	-1.154738
O	-0.198074	1.635775	2.187904
H	0.339104	0.794429	2.353331

H	-0.170527	2.161985	2.993664
O	-2.347897	0.583148	0.859984
H	-3.052955	0.170366	1.369156
H	-1.740041	1.007768	1.505172
N	1.109938	-0.722122	2.263572
H	0.843066	-1.032458	1.327554
H	0.787220	-1.421475	2.926552
H	2.124853	-0.717656	2.312607

m=4,n=3, best G

H	-0.104361	0.004378	0.199194
N	0.893637	-0.058742	-0.110597
H	1.137954	0.781372	-0.655507
H	1.027144	-0.906942	-0.703273
H	1.511422	-0.113456	0.728844
N	-1.888971	0.125567	0.794675
H	-2.370180	-0.768493	0.736917
H	-2.449343	0.789635	0.266299
H	-1.936935	0.417125	1.767867
O	1.580919	2.306722	-1.624740
H	1.481281	3.225171	-1.355186
H	2.118308	2.328889	-2.422809
O	1.262635	-2.340543	-1.647358
H	0.862971	-2.642358	-2.502939
H	2.007247	-2.925600	-1.482982
O	2.498036	-0.123339	2.153523
H	2.639246	-0.823057	2.841596
H	3.200872	0.519219	2.284015
N	2.943309	-2.053672	4.135909
H	2.335570	-2.864332	4.052106
H	3.897611	-2.404202	4.125688
H	2.784172	-1.665887	5.062219
N	0.169459	-3.253827	-4.061680
H	-0.314175	-4.138835	-3.932951
H	-0.505332	-2.609766	-4.465941
H	0.880913	-3.410204	-4.771009

m=5

N	0.000388	0.000180	-0.000413
H	-0.615677	-0.418644	-0.736251
H	0.037860	-0.638643	0.828381
H	0.965559	0.129536	-0.385273
H	-0.386301	0.928403	0.291602
N	-1.092035	2.615049	0.822191
N	-1.736218	-1.182531	-2.072285
N	0.108065	-1.799206	2.335896
N	2.719928	0.366542	-1.085503
H	-2.035612	2.543867	1.195934
H	-0.533475	3.062030	1.545605

H	-1.141426	3.277900	0.051945
H	-1.454597	-2.126710	-2.325869
H	-2.707969	-1.246033	-1.777718
H	-1.736291	-0.645007	-2.936103
H	0.670700	-1.421200	3.094611
H	-0.811755	-1.983598	2.729655
H	0.507885	-2.707501	2.111760
H	3.120427	-0.500005	-1.437347
H	2.746156	1.025968	-1.859808
H	3.373620	0.719392	-0.390317

m=5,n=1

N	-1.388293	1.989505	1.309409
H	-1.738080	1.941046	2.295140
H	-1.910776	2.726596	0.781597
H	-0.372523	2.219215	1.318401
H	-1.528358	1.063614	0.841805
N	-1.764721	-0.630023	-0.027124
N	-2.315361	1.839477	4.113831
N	-2.860467	4.061384	-0.215562
O	1.379373	2.541492	1.361577
H	-2.742542	-0.862672	-0.192412
H	-1.305894	-0.652813	-0.936362
H	-1.373175	-1.400740	0.511720
H	-2.825525	2.665471	4.421769
H	-2.918055	1.041135	4.305784
H	-1.511044	1.749828	4.732539
H	-2.412512	4.236285	-1.113580
H	-3.824009	3.801512	-0.419478
H	-2.900269	4.958144	0.265724
H	1.895114	3.388181	1.486410
H	2.031047	1.841533	1.234090
N	2.849061	4.884703	1.709235
H	2.305150	5.637207	2.126659
H	3.212425	5.237523	0.825974
H	3.650814	4.731817	2.318165

m=5,n=2, best H

N	1.341856	0.609252	0.553547
H	1.248872	1.623745	0.742871
H	0.382138	0.275794	0.289745
H	1.678346	0.111375	1.409727
H	2.010133	0.458336	-0.237706
N	3.231873	0.222217	-1.668115
H	3.220652	1.020128	-2.299048
H	4.193745	0.122392	-1.352586
H	3.031673	-0.596442	-2.237656
N	2.301629	-0.786613	2.964818
H	1.738017	-0.571966	3.783992

H	2.291296	-1.799214	2.868271
H	3.257363	-0.532075	3.202761
N	-1.438017	0.071978	-0.127897
H	-1.851331	1.000085	-0.031629
H	-1.953165	-0.551481	0.488083
H	-1.625410	-0.242903	-1.076197
O	-2.170431	3.187711	0.328150
H	-2.809011	3.377747	1.025175
H	-2.492386	3.660799	-0.448022
H	-0.353813	3.405987	0.722196
O	0.603354	3.300281	0.860065
H	0.929722	4.124288	1.231034
N	-4.138487	3.637975	2.052198
H	-3.810764	3.942997	2.955317
H	-4.736360	4.345732	1.655094
H	-4.656637	2.779497	2.155149

m=5,n=2, best G

N	1.183827	1.156402	2.247415
H	0.342730	0.599516	2.519237
H	1.809319	1.290874	3.069170
H	1.689561	0.635352	1.500837
H	0.897085	2.099227	1.900507
N	0.472883	3.883389	1.389091
N	-1.142318	-0.527829	2.904476
O	2.437942	-0.423661	0.318297
H	0.939366	4.524689	2.026101
H	0.791744	4.123353	0.453867
H	-0.517468	4.111283	1.423624
H	-1.142237	-0.887966	3.855390
H	-2.050807	-0.094513	2.760175
H	-1.107499	-1.337434	2.289674
H	3.125022	-1.042054	0.582160
H	2.481362	-0.381802	-0.670786
O	2.903630	1.721840	4.372053
H	2.788660	1.723392	5.356271
H	3.852720	1.750311	4.221863
N	2.612856	-0.374818	-2.483051
H	1.771341	-0.019334	-2.929196
H	2.759834	-1.311196	-2.851225
H	3.385111	0.194906	-2.818499
N	2.662447	1.748744	7.168888
H	1.732433	2.008382	7.487041
H	3.305002	2.421722	7.578974
H	2.875145	0.848305	7.590137

m=5,n=3, best H

N	0.289194	2.183964	-0.563928
O	-0.197823	-0.584947	-0.502622

O	-2.374086	0.618315	0.871715
O	-0.211678	1.660999	2.216209
N	1.095626	-0.692029	2.214043
N	-2.404071	2.925408	-1.140655
N	2.545766	3.590276	-1.803558
H	0.309270	2.258634	0.465596
H	-0.632699	2.584716	-0.889703
H	1.104991	2.668674	-1.004484
H	0.276010	1.163959	-0.768999
H	-2.772530	2.207927	-0.513345
H	-2.766852	3.823084	-0.832303
H	-2.790583	2.755286	-2.064809
H	2.777501	4.447950	-1.308007
H	2.336216	3.861800	-2.761265
H	3.401545	3.041853	-1.842164
H	-1.083825	-0.420908	-0.131001
H	-0.287547	-1.298794	-1.184687
H	0.327518	0.817226	2.362948
H	-0.182465	2.172248	3.031088
H	-3.071195	0.207326	1.392502
H	-1.752151	1.028944	1.510881
H	0.808831	-0.941751	1.262654
H	0.774305	-1.422533	2.842703
H	2.110788	-0.697056	2.249705
N	-4.415426	-0.598972	2.050475
H	-4.383828	-0.539348	3.056213
H	-5.262841	-0.168519	1.714824
H	-4.396658	-1.567135	1.770525

m=5,n=3, best G

N	-0.098544	0.023460	0.220127
O	2.566419	-0.135381	-0.616597
O	-1.281759	2.377752	-0.720366
O	-1.535712	-2.208655	-0.663643
N	-4.258518	-2.893374	-0.504762
N	-0.422509	5.055153	-0.701876
N	4.501279	-2.161346	-0.373771
N	-0.149325	0.094142	3.166176
H	-0.649602	-0.791167	-0.119611
H	0.885933	-0.061073	-0.106101
H	-0.513939	0.903257	-0.148950
H	-0.116756	0.044805	1.263821
H	0.761362	0.317821	3.559139
H	-0.797687	0.793466	3.518866
H	-0.430816	-0.794458	3.572270
H	-1.184919	-2.769692	-1.360722
H	-2.498559	-2.429195	-0.599006
H	-1.967637	2.347352	-1.392961
H	-0.959104	3.313508	-0.706648

H	3.232934	-0.861366	-0.523155
H	2.892782	0.430226	-1.321796
H	-0.216637	5.411310	-1.631517
H	-1.138037	5.660529	-0.308036
H	0.416146	5.195376	-0.144716
H	-4.376486	-3.813406	-0.088637
H	-4.795697	-2.245107	0.064982
H	-4.710609	-2.923416	-1.414829
H	5.329419	-1.816607	0.104612
H	4.168423	-2.960736	0.158760
H	4.810756	-2.520377	-1.273109

m=6

N	-0.863520	1.585200	-0.739800
H	-1.894560	1.679300	-0.896380
H	-0.406150	1.249600	-1.619910
H	-0.464660	2.515600	-0.472100
H	-0.688700	0.896160	0.029000
N	-0.373010	-0.358370	1.425730
N	-3.768580	1.849290	-1.184880
N	0.427620	0.640620	-3.219390
N	0.260400	4.206720	0.016560
H	-0.759410	-1.276930	1.220730
H	0.618100	-0.501360	1.605610
H	-0.783070	-0.069380	2.310840
H	-3.989220	2.435410	-1.986670
H	-4.220420	0.953830	-1.355440
H	-4.250250	2.263130	-0.389990
H	1.430650	0.508520	-3.111800
H	0.056630	-0.251720	-3.537560
H	0.308600	1.289600	-3.993830
H	0.074970	4.926650	-0.678010
H	-0.117670	4.555490	0.894350
H	1.270640	4.179340	0.133930
N	3.010830	3.992740	0.374440
H	3.158520	3.045690	0.891340
H	3.451130	4.798430	0.960040
H	3.489070	3.951210	-0.603050

m=6,n=1, best H

N	-0.114810	-2.215120	0.691050
O	-0.378840	0.314900	1.228870
N	2.542600	-2.632730	-0.487110
N	-2.222880	-3.020250	-1.194700
N	-0.571970	-3.360130	3.093130
H	0.833370	-2.376220	0.267710
H	-0.247810	-2.563720	1.409010
H	-0.189110	-1.537260	0.836740
H	-0.862560	-2.506270	0.013220

H	-2.242580	-4.025160	-1.361420
H	-3.149510	-2.768250	-0.854080
H	-2.124780	-2.580940	-2.108710
H	3.273180	-2.197310	0.073910
H	2.799570	-3.614010	-0.581680
H	2.617220	-2.225700	-1.418130
H	-1.431450	-3.015660	3.518320
H	-0.665240	-4.373240	3.039240
H	0.172610	-3.177020	3.764040
H	-0.328760	0.034910	2.160260
H	-0.597500	1.248370	1.115800
N	-0.305350	-0.549980	3.632910
H	-1.240770	-0.234610	4.092730
H	0.521100	-0.339460	4.310090
H	-0.343720	-1.618890	3.428270
N	-0.998810	2.753760	0.704960
H	-2.077110	2.896610	0.757640
H	-0.603920	3.285930	-0.159210
H	-0.536630	3.140740	1.611910

m=6,n=1, best G

N	0.175137	1.133980	-1.735554
H	0.226865	0.128959	-1.460400
H	0.470702	1.244037	-2.729631
H	-0.804874	1.466641	-1.626796
H	0.814095	1.703659	-1.115927
N	1.945463	2.708849	-0.082045
N	0.293075	-1.713761	-0.918050
N	1.028895	1.494140	-4.557659
O	-2.461930	2.012271	-1.381383
H	2.909840	2.394748	-0.164550
H	1.945343	3.681428	-0.381456
H	1.727026	2.715111	0.925627
H	0.407830	-2.368531	-1.687576
H	1.051674	-1.900200	-0.266971
H	-0.566102	-1.977036	-0.441766
H	0.584702	2.311730	-4.968366
H	2.031808	1.638492	-4.645389
H	0.798737	0.709133	-5.161806
H	-3.306587	1.819967	-1.861203
H	-2.660046	2.743333	-0.789733
N	-4.902898	1.520969	-2.686165
H	-4.856839	0.763761	-3.362934
H	-5.240059	2.338489	-3.187787
H	-5.627035	1.268627	-2.018543
N	1.439643	2.846765	2.970101
H	1.355942	3.819728	3.252886
H	2.239582	2.472357	3.473621
H	0.620209	2.369316	3.335625

m=6,n=2

N	1.419547	0.462131	0.522666
H	1.240039	1.497519	0.540234
H	0.509187	0.014627	0.253440
H	1.724082	0.121064	1.457515
H	2.148923	0.249818	-0.190756
N	3.490612	-0.069240	-1.534778
H	3.543668	0.735264	-2.154645
H	4.425312	-0.204840	-1.158201
H	3.297009	-0.875878	-2.122750
N	2.290626	-0.552539	3.187046
H	1.621914	-0.329477	3.919950
H	2.397066	-1.563896	3.193597
H	3.183068	-0.167498	3.485996
N	-1.255531	-0.367141	-0.242562
H	-1.675518	0.565608	-0.292371
H	-1.804544	-0.915961	0.413293
H	-1.374025	-0.803600	-1.152608
O	-2.075520	2.590389	-0.228571
H	-2.676022	2.806792	0.491876
H	-2.480372	2.992663	-1.043143
H	-0.296061	3.050373	0.120270
O	0.660687	3.075468	0.301715
H	0.850238	3.906712	0.790424
N	1.276549	5.516446	1.658276
H	0.923045	5.604315	2.606949
H	2.286199	5.621752	1.711234
H	0.930005	6.319183	1.140029
N	-3.192842	3.718862	-2.527557
H	-2.506207	3.728938	-3.277412
H	-3.998011	3.204575	-2.875189
H	-3.494456	4.681153	-2.398254

m=7

N	-0.004682	0.711854	0.052390
N	1.490958	-1.714782	-0.481324
N	-2.681178	0.437833	-1.031480
N	-0.142170	1.222665	2.987842
N	1.266406	3.043871	-1.306270
N	-4.527080	-1.874493	-0.105225
N	4.572532	-1.805434	-0.137195
H	0.449545	1.524284	-0.416055
H	-0.048876	0.886495	1.078624
H	-0.982126	0.594488	-0.327060
H	0.555897	-0.161946	-0.134493
H	2.512178	-1.674601	-0.347603
H	1.155392	-2.476514	0.103962
H	1.339202	-2.017091	-1.441052

H	0.699332	3.886123	-1.248075
H	2.175889	3.283717	-0.919619
H	1.414321	2.866629	-2.296760
H	-0.539019	0.433653	3.492033
H	0.769370	1.398393	3.403088
H	-0.720684	2.027646	3.215099
H	-3.232618	1.276191	-0.862263
H	-2.644555	0.331627	-2.042902
H	-3.240510	-0.352665	-0.678044
H	-4.113268	-2.802675	-0.085284
H	-5.295149	-1.917538	-0.769982
H	-4.948354	-1.727001	0.808097
H	4.860275	-2.756538	-0.352367
H	5.095406	-1.200331	-0.764700
H	4.911537	-1.609552	0.800891

m=7,n=1, best H

N	-0.778602	-1.388216	0.137592
O	-0.889175	1.358282	0.093085
N	1.812611	2.206843	-0.272496
N	-2.693336	3.315302	-0.944947
N	-1.341782	-0.259401	2.704452
N	2.021717	-2.156219	-0.286496
N	-2.701374	-3.233735	-1.159723
N	4.448598	0.075269	-0.202765
H	-0.978681	-1.317226	1.161333
H	-1.454751	-2.023900	-0.336669
H	-0.877967	-0.399031	-0.180912
H	0.207734	-1.702550	-0.019054
H	2.345437	-2.804887	0.426643
H	2.175467	-2.613803	-1.181470
H	2.644793	-1.345715	-0.257247
H	-2.266546	-0.276978	3.124289
H	-0.675111	-0.197587	3.468142
H	-1.266023	0.596364	2.150421
H	-2.566112	-3.333289	-2.162727
H	-2.639494	-4.169814	-0.766797
H	-3.663652	-2.931740	-1.028599
H	-1.508175	2.022216	-0.289286
H	0.022533	1.712426	-0.028133
H	-3.661934	3.056249	-0.777398
H	-2.606523	3.486812	-1.942982
H	-2.549256	4.208209	-0.480927
H	4.778996	0.830116	-0.799209
H	4.970529	-0.749488	-0.490050
H	4.769840	0.295500	0.737022
H	2.113718	2.867867	0.438169
H	2.451796	1.412940	-0.239160
H	1.947001	2.660995	-1.171603

m=7,n=1, best G

N	0.565877	0.664810	-0.016612
H	0.553408	0.558197	1.022084
H	-0.375635	0.319703	-0.294734
H	0.689830	1.664672	-0.280706
H	1.331229	0.079513	-0.446444
N	2.677949	-0.908201	-1.208175
H	2.910222	-0.576686	-2.141648
H	2.408817	-1.883002	-1.319353
H	3.556680	-0.907367	-0.668829
N	-0.352712	0.048146	2.632027
H	-0.647140	0.743472	3.311260
H	-1.172956	-0.226255	2.086763
H	-0.042767	-0.762943	3.158909
O	-2.020702	-0.372758	0.056606
H	-2.246269	-1.291525	-0.215931
H	-2.841974	0.154673	-0.071966
N	-2.713893	-3.048136	-0.711321
H	-3.556800	-3.353883	-0.232294
H	-2.895634	-3.138445	-1.707328
H	-1.992224	-3.727106	-0.484521
N	-4.443433	1.125561	-0.283504
H	-4.399449	2.056110	0.123206
H	-5.218462	0.649921	0.170979
H	-4.706659	1.245913	-1.257893
N	0.980484	3.514541	-0.760942
H	0.580944	4.158269	-0.082337
H	1.971472	3.736751	-0.817320
H	0.579292	3.760221	-1.662695
N	5.365000	-0.996797	0.326840
H	6.105129	-1.280018	-0.309957
H	5.662230	-0.117218	0.740511
H	5.357426	-1.680388	1.079194