

Supplementary Material

for

Effect of Intramolecular Hydrogen Bonds on the Gas-phase Basicity of Guanidines

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S1. Calculation results for the investigated bases and their protonated forms

Table S1. Electronic energies, enthalpies and Gibbs energies for c1 and c2 hydrogen bonded conformations calculated for the DMG series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{zpv}	H_{corr}	G_{corr}	H	G	PA	GB _{sc} ^B
DMG:1	c2	-536.06118	0.29346	0.30911	0.25235	-535.75208	-535.80883	1083	1042
DMG:1H⁺	c2	-536.48542	0.30744	0.32338	0.26645	-536.16203	-536.21897		
DMG:2	c2	-516.61430	0.25227	0.26696	0.21147	-516.34735	-516.40283	1073	1030
DMG:2H⁺	c2	-517.03500	0.26661	0.28143	0.22648	-516.75357	-516.80852		
DMG:3	c2	-839.59973	0.24831	0.26367	0.20607	-839.33606	-839.39366	1068	1027
DMG:3H⁺	c2	-840.01842	0.26231	0.27790	0.22054	-839.74052	-839.79787		
DMG:4	c2	-897.99925	0.29029	0.30817	0.24595	-897.69109	-897.75330	1096	1057
DMG:4H⁺	c1	-898.42856	0.30398	0.32233	0.25934	-898.10623	-898.16922		
DMG:5	c2	-914.82666	0.25183	0.26788	0.20933	-914.55878	-914.61733	1080	1040
DMG:5H⁺	c1	-915.25007	0.26582	0.28223	0.22342	-914.96784	-915.02665		
DMG:6	c2	-990.08105	0.25747	0.27423	0.21359	-989.80682	-989.86746	1067	1027
DMG:6H⁺	c1	-990.49961	0.27146	0.28861	0.22773	-990.21100	-990.27188		
DMG:7	c1	-554.75292	0.25614	0.27196	0.21329	-554.48097	-554.53963	1082	1039
DMG:7H⁺	c1	-555.17719	0.27059	0.28649	0.22863	-554.89070	-554.94856		
DMG:8	c1	-649.45872	0.30280	0.32117	0.25621	-649.13755	-649.20251	1100	1057
DMG:8H⁺	c1	-649.88986	0.31725	0.33579	0.27141	-649.55407	-649.61845		
DMG:9	c1	-726.90435	0.33991	0.35877	0.29247	-726.54559	-726.61189	1105	1061
DMG:9H⁺	c1	-727.33755	0.35435	0.37328	0.30805	-726.96427	-727.02951		
DMG:10	c1	-666.47625	0.29888	0.31658	0.25293	-666.15967	-666.22332	1104	1060
DMG:10H⁺	c1	-666.90879	0.31322	0.33100	0.26840	-666.57779	-666.64039		
DMG:11	c2	-666.47506	0.29949	0.31687	0.25469	-666.15818	-666.22037	1113	1072
DMG:11H⁺	c2	-666.91076	0.31336	0.33103	0.26863	-666.57973	-666.64213		
DMG:12	c2	-649.22341	0.28894	0.30515	0.24574	-648.91826	-648.97767	1094	1053
DMG:12H⁺	c2	-649.65192	0.30284	0.31938	0.25972	-649.33254	-649.39220		
DMG:13	c2	-853.79485	0.29117	0.31004	0.24337	-853.48481	-853.55148	1069	1028
DMG:13H⁺	c2	-854.21384	0.30518	0.32434	0.25759	-853.88950	-853.95625		
DMG:14	c2	-741.49154	0.28719	0.30531	0.24104	-741.18624	-741.25051	1071	1030
DMG:14H⁺	c2	-741.91146	0.30121	0.31962	0.25528	-741.59184	-741.65618		
DMG:15	c2	-763.79036	0.32182	0.34061	0.27516	-763.44975	-763.51520	1103	1062
DMG:15H⁺	c2	-764.22225	0.33561	0.35476	0.28905	-763.86749	-763.93320		
DMG:16	c2	-783.23955	0.36239	0.38315	0.31277	-782.85640	-782.92678	1116	1073
DMG:16H⁺	c2	-783.67627	0.37626	0.39729	0.32716	-783.27898	-783.34911		
DMG:17	c2	-860.68713	0.39951	0.42077	0.34926	-860.26636	-860.33787	1119	1078
DMG:17H⁺	c2	-861.12511	0.41331	0.43488	0.36307	-860.69024	-860.76204		

^A PAs and GB_{sc} are given in kJ mol⁻¹ while other energies are given in Hartrees.

^B GB_{sc} values represent the estimation of the experimental GBs and were obtained by scaling the calculated GBs according to equation $GB_{sc} = (GB_{calc} - (-11.17))/1.019$.^[1]

¹ Z. Glasovac, F. Pavošević, V. Štrukil, M. Eckert-Maksić, M. Schlangen, R. Kretschmer, *Int. J. Mass Spectrom.* **2013**, 354–355, 113–122. doi:10.1016/j.ijms.2013.06.012

Table S2. Electronic energies, enthalpies and Gibbs energies for the „open chain“ (oc) conformations calculated for the DMG series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{ZPV}	H_{corr}	G_{corr}	H	G	PA
DMG:1	oc	-536.05783	0.29182	0.30834	0.24799	-535.74948	-535.80984	1054
DMG:1H⁺	oc	-536.47126	0.30571	0.32287	0.26096	-536.14839	-536.21030	
DMG:2	oc	-516.61225	0.25100	0.26624	0.20859	-516.34601	-516.40365	1050
DMG:2H⁺	oc	-517.02435	0.26492	0.28076	0.22204	-516.74359	-516.80231	
DMG:3	oc	-839.59919	0.24723	0.26318	0.20327	-839.33601	-839.39593	1047
DMG:3H⁺	oc	-840.00994	0.26111	0.27764	0.21651	-839.73230	-839.79342	
DMG:4	oc	-897.99291	0.28898	0.30771	0.24180	-897.68520	-897.75112	1050
DMG:4H⁺	oc	-898.40483	0.30276	0.32209	0.25492	-898.08275	-898.14992	
DMG:5	oc	-914.82159	0.25080	0.26757	0.20597	-914.55403	-914.61562	1042
DMG:5H⁺	oc	-915.23061	0.26468	0.28199	0.21925	-914.94862	-915.01136	
DMG:6	oc	-990.07764	0.25652	0.27393	0.21072	-989.80371	-989.86692	1036
DMG:6H⁺	oc	-990.48418	0.27052	0.28841	0.22411	-990.19576	-990.26006	
DMG:7	oc	-554.74974	0.25500	0.27133	0.21006	-554.47841	-554.53968	1051
DMG:7H⁺	oc	-555.16225	0.26896	0.28585	0.22341	-554.87641	-554.93884	
DMG:8	oc	-649.45343	0.30157	0.32048	0.25303	-649.13294	-649.20040	1061
DMG:8H⁺	oc	-649.86973	0.31571	0.33515	0.26715	-649.53458	-649.60257	
DMG:9	oc	-726.89870	0.33870	0.35813	0.28908	-726.54057	-726.60962	1064
DMG:9H⁺	oc	-727.31614	0.35268	0.37268	0.30271	-726.94347	-727.01343	
DMG:10	oc	-666.47204	0.29818	0.31624	0.25076	-666.15580	-666.22128	1060
DMG:10H⁺	oc	-666.88771	0.31180	0.33065	0.26174	-666.55705	-666.62596	
DMG:11	oc	-666.47146	0.29809	0.31623	0.25033	-666.15524	-666.22113	1071
DMG:11H⁺	oc	-666.89159	0.31205	0.33075	0.26403	-666.56083	-666.62756	
DMG:12	oc	-649.22071	0.28767	0.30466	0.24132	-648.91605	-648.97939	1060
DMG:12H⁺	oc	-649.63656	0.30150	0.31908	0.25459	-649.31748	-649.38197	
DMG:13	oc	-853.79401	0.29003	0.30960	0.23934	-853.48440	-853.55466	1042
DMG:13H⁺	oc	-854.20286	0.30394	0.32404	0.25313	-853.87882	-853.94973	
DMG:14	oc	-741.49050	0.28604	0.30486	0.23702	-741.18563	-741.25347	1043
DMG:14H⁺	oc	-741.89985	0.29991	0.31929	0.25055	-741.58056	-741.64930	
DMG:15	oc	-763.78724	0.32061	0.34015	0.27093	-763.44709	-763.51631	1066
DMG:15H⁺	oc	-764.20518	0.33451	0.35461	0.28459	-763.85057	-763.92059	
DMG:16	oc	-783.23538	0.36121	0.38267	0.30875	-782.85271	-782.92663	1073
DMG:16H⁺	oc	-783.65601	0.37499	0.39714	0.32207	-783.25887	-783.33394	
DMG:17	oc	-860.68268	0.39821	0.42026	0.34473	-860.26242	-860.33795	1075
DMG:17H⁺	oc	-861.10417	0.41201	0.43470	0.35813	-860.66948	-860.74604	
DMG:18	oc	-402.05704	0.21779	0.23052	0.17983	-401.82651	-401.87721	1053
DMG:18H⁺	oc	-402.47018	0.23166	0.24499	0.19310	-402.22519	-402.27709	

^A PAs are given in kJ mol⁻¹ while other energies are given in Hartrees.

Table S3. Electronic energies, enthalpies and Gibbs energies for c1 and c2 hydrogen bonded conformations calculated for the DIG series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{ZPV}	H_{corr}	G_{corr}	H	G	PA	GB_{sc}^B
DIG:1	c2	-693.37245	0.40641	0.42746	0.35743	-692.94499	-693.01502	1091	1047
DIG:1H⁺	c2	-693.80010	0.42088	0.44205	0.37291	-693.35805	-693.42719		
DIG:2	c2	-673.92662	0.36566	0.38543	0.31809	-673.54119	-673.60853	1082	1043
DIG:2H⁺	c2	-674.35073	0.37959	0.39980	0.33171	-673.95093	-674.01902		
DIG:3	c2	-996.91199	0.36150	0.38212	0.31178	-996.52986	-996.60021	1077	1036
DIG:3H⁺	c2	-997.33414	0.37551	0.39643	0.32623	-996.93772	-997.00792		
DIG:4	c2	-1055.30991	0.40364	0.42687	0.35146	-1054.88303	-1054.95845	1106	1064
DIG:4H⁺	c2	-1055.74308	0.41760	0.44109	0.36610	-1055.30199	-1055.37698		
DIG:5	c2	-1072.13714	0.36547	0.38675	0.31553	-1071.75039	-1071.82161	1091	1050
DIG:5H⁺	c1	-1072.56474	0.37942	0.40105	0.32985	-1072.16368	-1072.23489		
DIG:6	c2	-1147.39251	0.37104	0.39304	0.31996	-1146.99947	-1147.07255	1077	1038
DIG:6H⁺	c1	-1147.81487	0.38498	0.40739	0.33359	-1147.40748	-1147.48128		
DIG:7	c1	-712.06454	0.36987	0.39073	0.31999	-711.67381	-711.74455	1092	1050
DIG:7H⁺	c1	-712.49238	0.38394	0.40511	0.33465	-712.08727	-712.15773		
DIG:8	c1	-806.76999	0.41675	0.44010	0.36385	-806.32988	-806.40614	1108	1069
DIG:8H⁺	c1	-807.20419	0.43071	0.45452	0.37724	-806.74967	-806.82695		
DIG:9	c1	-884.21559	0.45392	0.47774	0.40017	-883.73785	-883.81542	1114	1072
DIG:9H⁺	c1	-884.65178	0.46793	0.49211	0.41445	-884.15967	-884.23733		
DIG:10	c1	-823.78672	0.41278	0.43554	0.35991	-823.35119	-823.42681	1112	1069
DIG:10H⁺	c2	-824.22209	0.42687	0.44982	0.37455	-823.77227	-823.84754		
DIG:11	c1	-823.78382	0.41263	0.43545	0.35973	-823.34837	-823.42409	1125	1081
DIG:11H⁺	c2	-824.22424	0.42673	0.44972	0.37469	-823.77452	-823.84955		
DIG:12	c2	-806.53377	0.40214	0.42375	0.35080	-806.11002	-806.18297	1101	1058
DIG:12H⁺	c2	-806.96541	0.41644	0.43822	0.36617	-806.52720	-806.59924		
DIG:13	c2	-1011.10554	0.42765	0.42859	0.34870	-1010.67695	-1010.75684	1078	1035
DIG:13H⁺	c2	-1011.52812	0.41864	0.44308	0.36380	-1011.08504	-1011.16432		
DIG:14	c2	-898.80218	0.40043	0.42389	0.34640	-898.37828	-898.45578	1080	1037
DIG:14H⁺	c2	-899.22562	0.41468	0.43838	0.36146	-898.78724	-898.86416		
DIG:15	c2	-921.10074	0.43491	0.45912	0.38016	-920.64162	-920.72058	1109	1065
DIG:15H⁺	c2	-921.53538	0.44925	0.47364	0.39555	-921.06174	-921.13983		
DIG:16	c2	-940.54965	0.47555	0.50174	0.41765	-940.04791	-940.13200	1121	1075
DIG:16H⁺	c2	-940.98892	0.48999	0.51625	0.43377	-940.47268	-940.55516		
DIG:17	c2	-1017.99718	0.51257	0.53927	0.45405	-1017.45791	-1017.54312	1124	1079
DIG:17H⁺	c2	-1018.43765	0.52713	0.55391	0.46997	-1017.88374	-1017.96768		

^APAAs and GB_{sc} are given in kJ mol⁻¹ while other energies are given in Hartrees.

^BGB_{sc} values represent the estimation of the experimental GBs and were obtained by scaling the calculated GBs according equation $GB_{sc} = (GB_{calc} - (-11.17))/1.019$.^[1]

Table S4. Electronic energies, enthalpies and Gibbs energies for the „open chain“ (oc) conformations calculated for the DIG series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{ZPV}	$H_{C_{corr}}$	G_{corr}	H	G	PA
DIG:1	oc	-693.36942	0.40520	0.42688	0.35397	-692.94254	-693.01545	1069
DIG:1H⁺	oc	-693.78870	0.41896	0.44134	0.36680	-693.34737	-693.42191	
DIG:2	oc	-673.92387	0.36454	0.38488	0.31526	-673.53900	-673.60862	1066
DIG:2H⁺	oc	-674.34189	0.37813	0.39920	0.32777	-673.94269	-674.01412	
DIG:3	oc	-996.91080	0.36072	0.38180	0.30960	-996.52900	-996.60120	1063
DIG:3H⁺	oc	-997.32750	0.37439	0.39612	0.32254	-996.93138	-997.00496	
DIG:4	oc	-1055.30457	0.40246	0.42631	0.34820	-1054.87826	-1054.95637	1065
DIG:4H⁺	oc	-1055.72238	0.41627	0.44066	0.36167	-1055.28172	-1055.36071	
DIG:5	oc	-1072.13307	0.36409	0.38606	0.31183	-1071.74701	-1071.82124	1058
DIG:5H⁺	oc	-1072.54830	0.37796	0.40049	0.32549	-1072.14781	-1072.22281	
DIG:6	oc	-1147.38928	0.37000	0.39252	0.31720	-1146.99676	-1147.07209	1052
DIG:6H⁺	oc	-1147.80208	0.38371	0.40686	0.32994	-1147.39521	-1147.47213	
DIG:7	oc	-712.06201	0.36839	0.38986	0.31636	-711.67215	-711.74565	1065
DIG:7H⁺	oc	-712.47979	0.38228	0.40435	0.32960	-712.07544	-712.15019	
DIG:8	oc	-806.76572	0.41475	0.43890	0.35838	-806.32682	-806.40734	1074
DIG:8H⁺	oc	-807.18704	0.42898	0.45364	0.37304	-806.73340	-806.81401	
DIG:9	oc	-884.21104	0.45216	0.47670	0.39593	-883.73434	-883.81511	1077
DIG:9H⁺	oc	-884.63339	0.46599	0.49117	0.40898	-884.14221	-884.22440	
DIG:10	oc	-823.78413	0.41185	0.43496	0.35788	-823.34917	-823.42625	1074
DIG:10H⁺	oc	-824.20501	0.42512	0.44915	0.36898	-823.75586	-823.83602	
DIG:11	oc	-823.78369	0.41161	0.43487	0.35698	-823.34882	-823.42671	1084
DIG:11H⁺	oc	-824.20867	0.42542	0.44928	0.37038	-823.75939	-823.83829	
DIG:12	oc	-806.53305	0.40120	0.42328	0.34812	-806.10976	-806.18493	1073
DIG:12H⁺	oc	-806.95385	0.41490	0.43761	0.36152	-806.51623	-806.59232	
DIG:13	oc	-1011.10617	0.40329	0.42807	0.34465	-1010.67810	-1010.76152	1056
DIG:13H⁺	oc	-1011.52037	0.41729	0.44258	0.35902	-1011.07779	-1011.16135	
DIG:14	oc	-898.80267	0.39942	0.42342	0.34313	-898.37925	-898.45954	1057
DIG:14H⁺	oc	-899.21739	0.41331	0.43788	0.35651	-898.77951	-898.86088	
DIG:15	oc	-921.09950	0.43406	0.45874	0.37736	-920.64075	-920.72213	1079
DIG:15H⁺	oc	-921.52238	0.44782	0.47313	0.39078	-921.04925	-921.13160	
DIG:16	oc	-940.54762	0.47453	0.50116	0.41484	-940.04646	-940.13279	1085
DIG:16H⁺	oc	-940.97304	0.48842	0.51570	0.42801	-940.45734	-940.54502	
DIG:17	oc	-1017.99511	0.51160	0.53882	0.45042	-1017.45629	-1017.54469	1087
DIG:17H⁺	oc	-1018.42119	0.52553	0.55326	0.46498	-1017.86793	-1017.95620	
DIG:18	oc	-559.36933	0.33136	0.34916	0.28658	-559.02017	-559.08276	1067
DIG:18H⁺	oc	-559.78751	0.34470	0.36335	0.29857	-559.42416	-559.48894	

^APAAs are given in kJ mol⁻¹ while other energies are given in Hartrees.

Table S5. Electronic energies, enthalpies and Gibbs energies for c1 and c2 hydrogen bonded conformations calculated for the TRIS series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{ZPV}	H_{corr}	G_{corr}	H	G	PA	GB_{sc}^B
TRIS:1	c2	-961.37307	0.55661	0.58478	0.49677	-960.78829	-960.87630	1143	1088
TRIS:1H ⁺	c2	-961.82159	0.57312	0.60033	0.51719	-961.22126	-961.30441		
TRIS:2	c2	-903.03590	0.43420	0.45852	0.37840	-902.57738	-902.65751	1117	1067
TRIS:2H ⁺	c2	-903.47465	0.45023	0.47401	0.39714	-903.00065	-903.07752		
TRIS:3	c2	-1871.99373	0.42233	0.44894	0.36130	-1871.54479	-1871.63243	1101	1051
TRIS:3H ⁺	c2	-1872.42512	0.43730	0.46350	0.37891	-1871.96161	-1872.04620		
TRIS:4	c2	-2047.18488	0.54824	0.58288	0.47972	-2046.60200	-2046.70516	1182	1131
TRIS:4H ⁺	c2	-2047.64717	0.56322	0.59746	0.49715	-2047.04972	-2047.15002		
TRIS:5	c2	-2097.66848	0.43326	0.46221	0.37003	-2097.20626	-2097.29845	1148	1094
TRIS:5H ⁺	c2	-2098.11798	0.44829	0.47669	0.38914	-2097.64128	-2097.72883		
TRIS:6	c2	-2323.43484	0.45048	0.48137	0.38399	-2322.95347	-2323.05085	1105	1054
TRIS:6H ⁺	c2	-2323.86765	0.46519	0.49564	0.40193	-2323.37201	-2323.46572		
TRIS:7	c1	-1301.56426	0.58629	0.62163	0.51285	-1300.94263	-1301.05141	1192	1134
TRIS:7H ⁺	c1	-1302.03159	0.60264	0.63734	0.53441	-1301.39424	-1301.49718		
TRIS:8	c1	-1533.90036	0.69754	0.73445	0.62072	-1533.16592	-1533.27964	1205	1143
TRIS:8H ⁺	c1	-1534.37253	0.71403	0.75011	0.64340	-1533.62242	-1533.72913		
TRIS:9	c1	-1017.44971	0.44644	0.47399	0.38463	-1016.97572	-1017.06508	1148	1095
TRIS:9H ⁺	c1	-1017.89976	0.46226	0.48928	0.40393	-1017.41048	-1017.49583		
TRIS:10	c2	-1300.86098	0.54361	0.57333	0.47762	-1300.28765	-1300.38335	1164	1106
TRIS:10H ⁺	c2	-1301.31752	0.55983	0.58882	0.49911	-1300.72871	-1300.81842		
TRIS:11	c2	-1702.90526	0.76420	0.80738	0.67984	-1702.09788	-1702.22542	1218	1161
TRIS:11H ⁺	c2	-1703.38231	0.78022	0.82288	0.70073	-1702.55944	-1702.68159		
TRIS:12	c2	-1935.24917	0.87527	0.91928	0.79099	-1934.32989	-1934.45818	1219	1170
TRIS:12H ⁺	c2	-1935.72718	0.89135	0.93551	0.80925	-1934.79167	-1934.91793		
TRIS:13	c2	-1914.57702	0.55088	0.58832	0.47180	-1913.98870	-1914.10522	1100	1044
TRIS:13H ⁺	c2	-1915.00868	0.56632	0.60320	0.49246	-1914.40548	-1914.51622		
TRIS:14	c2	-1577.66699	0.53889	0.57413	0.46474	-1577.09287	-1577.20225	1105	1049
TRIS:14H ⁺	c2	-1578.10077	0.55461	0.58926	0.48546	-1577.51151	-1577.61531		
TRIS:15	c2	-1644.56111	0.64242	0.67983	0.56675	-1643.88128	-1643.99436	1184	1127
TRIS:15H ⁺	c2	-1645.02532	0.65855	0.69529	0.58798	-1644.33003	-1644.43734		
TRIS:16	c2	-1352.61903	0.57573	0.60860	0.50504	-1352.01044	-1352.11399	1194	1145
TRIS:16H ⁺	c2	-1353.08624	0.59047	0.62329	0.52223	-1352.46295	-1352.56400		
TRIS:17	c2	-1352.61542	0.57492	0.60816	0.50352	-1352.00726	-1352.11191	1206	1145
TRIS:17H ⁺	c2	-1353.08809	0.59138	0.62376	0.52620	-1352.46433	-1352.56189		

^APAs and GB_{sc} are given in kJ mol⁻¹ while other energies are given in Hartrees.

^BGB_{sc} values represent the estimation of the experimental GBs and were obtained by scaling the calculated GBs according equation $GB_{sc} = (GB_{calc} - (-11.17))/1.019$.^[1]

Table S6. Electronic energies, enthalpies and Gibbs energies for the „open chain“ (oc) conformations calculated for the TRIS series of base/conjugated acid pairs^A

Molecule	conf.	E_{scf}	E_{ZPV}	H_{corr}	G_{corr}	H	G	PA
TRIS:1	oc	-961.36740	0.55397	0.58352	0.48962	-960.78388	-960.87779	1072
TRIS:1H ⁺	oc	-961.78791	0.56760	0.59821	0.50189	-961.18970	-961.28602	
TRIS:2	oc	-903.03093	0.43163	0.45738	0.37125	-902.57355	-902.65968	1065
TRIS:2H ⁺	oc	-903.44767	0.44531	0.47099	0.38826	-902.97668	-903.05941	
TRIS:3	oc	-1871.99057	0.42065	0.44837	0.35665	-1871.54220	-1871.63391	1055
TRIS:3H ⁺	oc	-1872.40429	0.43438	0.46272	0.37031	-1871.94157	-1872.03398	
TRIS:4	oc	-2047.17131	0.54584	0.58187	0.47266	-2046.58944	-2046.69866	1065
TRIS:4H ⁺	oc	-2047.58900	0.55973	0.59619	0.48599	-2046.99281	-2047.10301	
TRIS:5	oc	-2097.65687	0.43096	0.46130	0.36302	-2097.19558	-2097.29385	1045
TRIS:5H ⁺	oc	-2098.06704	0.44494	0.47566	0.37710	-2097.59138	-2097.68994	
TRIS:6	oc	-2323.42504	0.44838	0.48056	0.37801	-2322.94448	-2323.04703	1028
TRIS:6H ⁺	oc	-2323.82833	0.46210	0.49484	0.39068	-2323.33349	-2323.43765	
TRIS:7	oc	-1017.44439	0.44364	0.47269	0.37505	-1016.97171	-1017.06934	1063
TRIS:7H ⁺	oc	-1017.86146	0.45771	0.48725	0.39062	-1017.37421	-1017.47084	
TRIS:8	oc	-1301.55716	0.58345	0.62022	0.50394	-1300.93694	-1301.05323	1086
TRIS:8H ⁺	oc	-1301.98330	0.59750	0.63495	0.51868	-1301.34835	-1301.46462	
TRIS:9	oc	-1533.89307	0.69487	0.73315	0.61376	-1533.15992	-1533.27931	1094
TRIS:9H ⁺	oc	-1534.32217	0.70900	0.74783	0.62801	-1533.57435	-1533.69416	
TRIS:10	oc	-1352.60755	0.57305	0.60729	0.49803	-1352.00026	-1352.10952	1096
TRIS:10H ⁺	oc	-1353.03698	0.58623	0.62161	0.50863	-1352.41537	-1352.52835	
TRIS:11	oc	-1352.60937	0.57266	0.60712	0.49705	-1352.00225	-1352.11232	1114
TRIS:11H ⁺	oc	-1353.04627	0.58703	0.62198	0.51160	-1352.42429	-1352.53467	
TRIS:12	oc	-1300.85586	0.54143	0.57244	0.46992	-1300.28342	-1300.38594	1090
TRIS:12H ⁺	oc	-1301.28291	0.55514	0.58686	0.48350	-1300.69605	-1300.79942	
TRIS:13	oc	-1914.57302	0.54878	0.58744	0.46462	-1913.98558	-1914.10840	1044
TRIS:13H ⁺	oc	-1914.98268	0.56267	0.60188	0.47752	-1914.38080	-1914.50517	
TRIS:14	oc	-1577.66280	0.53667	0.57318	0.45679	-1577.08963	-1577.20601	1047
TRIS:14H ⁺	oc	-1578.07366	0.55062	0.58766	0.47013	-1577.48600	-1577.60353	
TRIS:15	oc	-1644.55572	0.64011	0.67885	0.55678	-1643.87687	-1643.99894	1102
TRIS:15H ⁺	oc	-1644.98786	0.65430	0.69351	0.57453	-1644.29435	-1644.41332	
TRIS:16	oc	-1702.90076	0.76195	0.80643	0.67181	-1702.09433	-1702.22895	1119
TRIS:16H ⁺	oc	-1703.33940	0.77630	0.82131	0.68957	-1702.51809	-1702.64983	
TRIS:17	oc	-1935.24300	0.87295	0.91822	0.78319	-1934.32478	-1934.45981	1121
TRIS:17H ⁺	oc	-1935.68348	0.88721	0.93392	0.79540	-1934.74956	-1934.88808	
TRIS:18	oc	-559.36499	0.33191	0.35008	0.28490	-559.01492	-559.08009	1070
TRIS:18H ⁺	oc	-559.78494	0.34577	0.36468	0.29785	-559.42026	-559.48709	

^A PAs are given in kJ mol^{-1} while other energies are given in Hartrees.

S2. Calculation of the pK_{HB} for 4-nitropyridine using Taft's correlation

Table S7. The substituent parameters^[2] of various substituents attached to the para- position in pyridine used for determination of pK_{HB} for 4-nitropyridine.

Substituent	s(P)	s(F)	s(R ⁺)	pK_{HB}	$pK_{HB}(\text{calc})$
H-	0.00	0.00	0.00	1.86	1.90
-CN	-0.46	0.60	0.00	0.92	0.92
CH ₃ O-	-0.17	0.25	-0.42	2.13	2.18
(CH ₃) ₂ N-	-0.44	0.10	-0.64	2.8	2.78
Cl	-0.43	0.45	-0.17	1.54	1.44
-NH ₂	-0.16	0.14	-0.52	2.56	2.52
-CH ₃	-0.35	0.00	-0.08	2.07	2.03
(CH ₃) ₃ C-	-0.75	0.00	-0.06	2.11	1.98
Ph-	-0.81	0.10	-0.22	1.96	2.08
H ₂ C=CH-	-0.50	0.06	-0.16	1.95	2.06
CH ₃ CH ₂ -	-0.49	0.00	-0.07	2.07	2.01
CH ₃ C(O)-	-0.55	0.26	0.00	1.41	1.47
-NO ₂	-0.26	0.65	0.00		0.85

$pK_{HB}(\text{calc})$ is calculated using equation (S1):

$$pK_{HB}(\text{calc}) = P \times \sigma(P) + F \times \sigma(F) + R^+ \times \sigma(R^+) + c \quad (\text{S1})$$

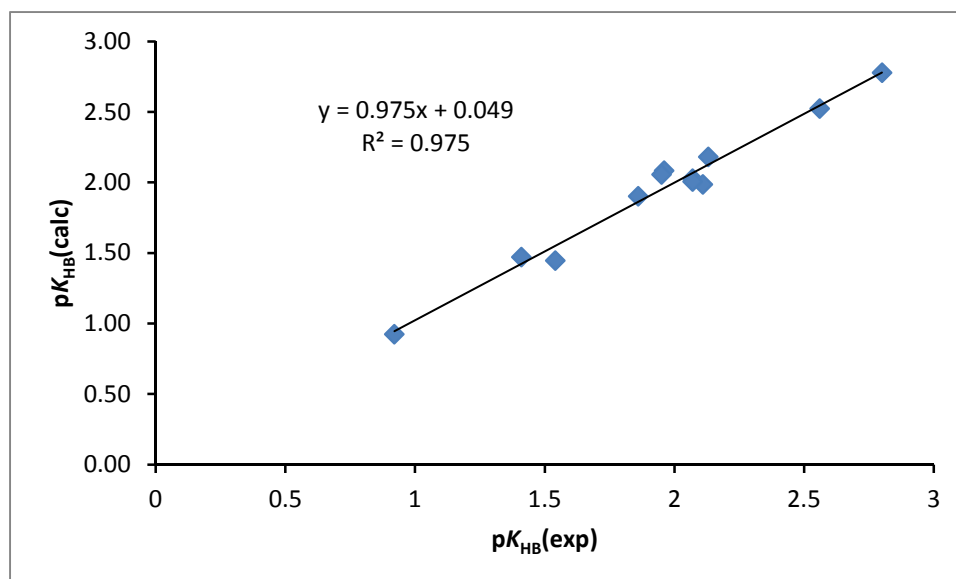


Figure S1. Correlation of the $pK_{HB}(\text{calc})$ calculated according eq. (S1) against experimental pK_{HB} ^[3] used for the evaluation of pK_{HB} (4-nitropyridine).

[2] C. Hansch, A. Leo, R. W. Taft, *Chem. Rev.* **1991**, *91*, 165–195. doi:10.1021/cr00002a004

[3] C. Laurence, J. F. Gal, Chapter 4 in: „*Lewis Basicity and Affinity scales. Data and Measurements*“ **2010** (J. Wiley and Sons, Ltd., Chichester, UK), and the references therein.

S3. Correlation of GB against pK_{HB}

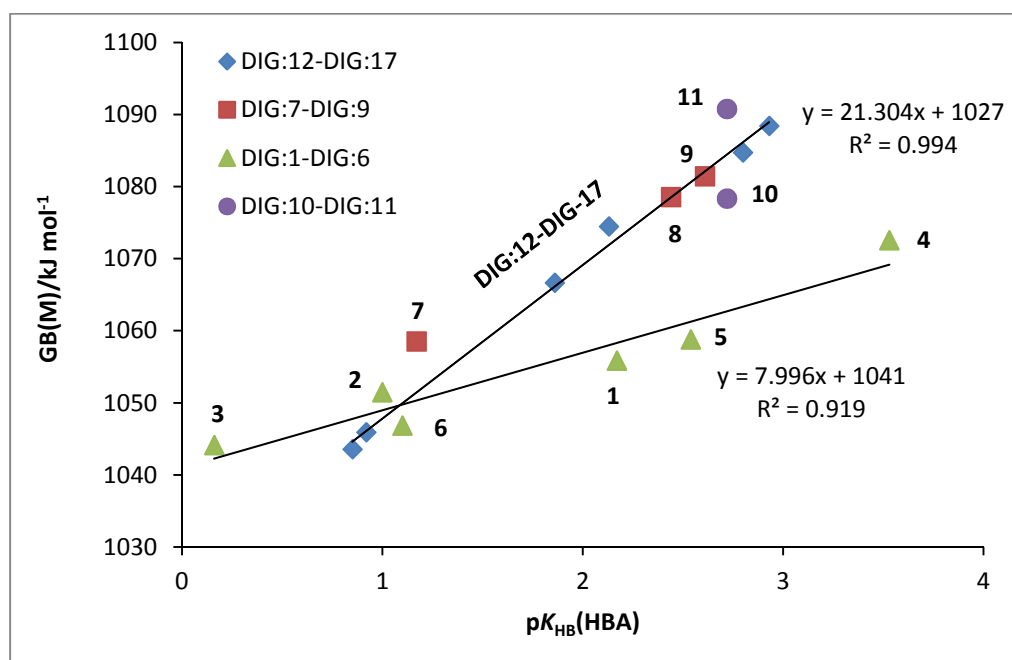


Figure S2. Correlation of the calculated gas-phase basicity (GB) against pK_{HB} (HBA) in DIG series of bases. $M = \text{DIG}:X$ where $X = 1-17$.

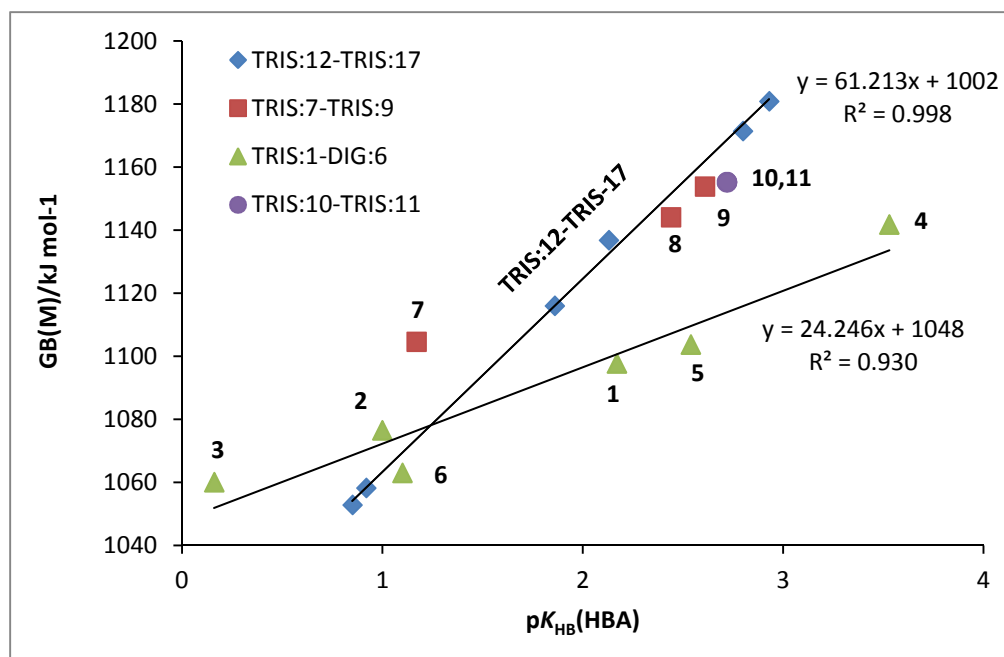


Figure S3. Correlation of the calculated gas-phase basicity (GB) against pK_{HB} (HBA) in TRIS series of bases. $M = \text{TRIS}:X$ where $X = 1-17$.

S4. Correlation of GB against pK_{HB} and σ^{4B}

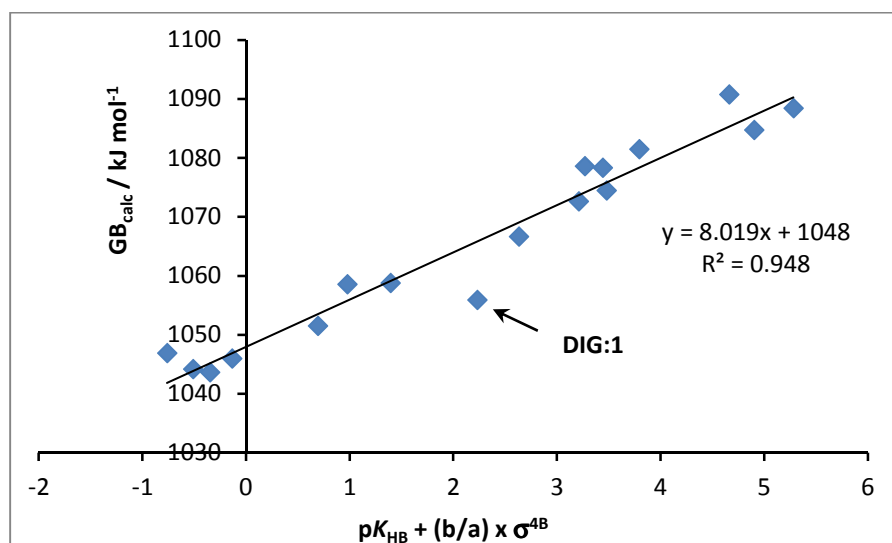


Figure S4. Correlation of the GB calculated for **DIG** series of bases against two independent variables pK_{HB} and σ^{4B}

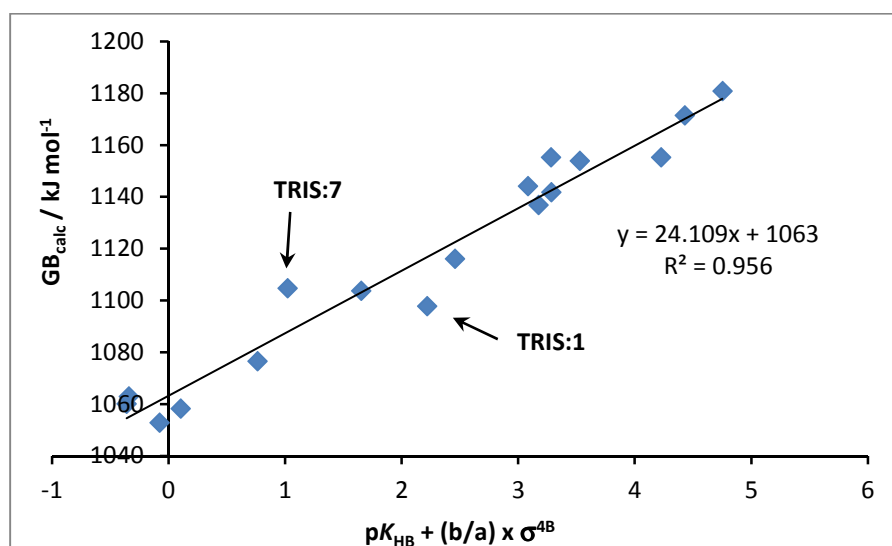


Figure S5. Correlation of the GBs calculated for **TRIS** series of bases against two independent variables pK_{HB} and σ^{4B}

S5. Correlation of PA against pK_{HB} and σ^{4B}

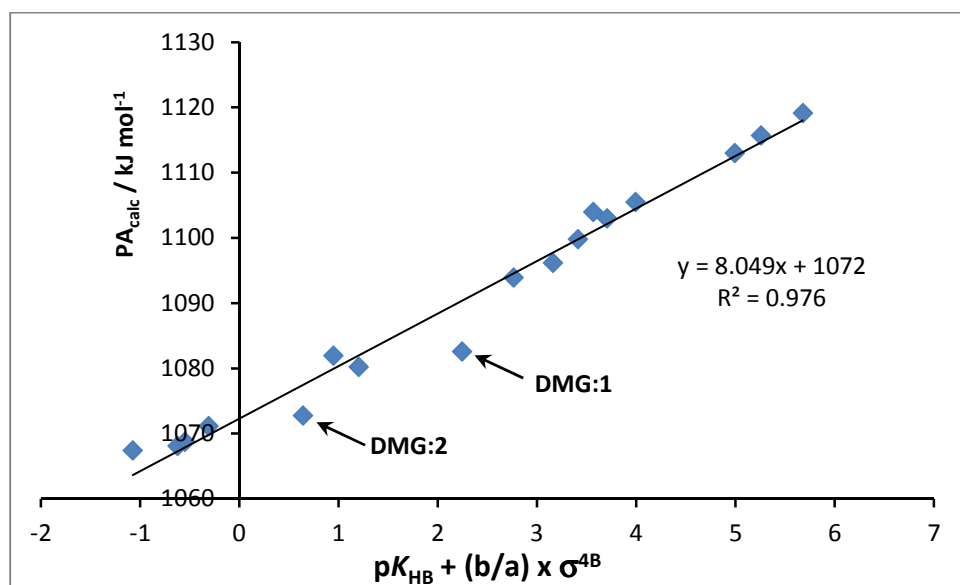


Figure S6. Correlation of the PA calculated for **DMG** series of bases against two independent variables pK_{HB} and σ^{4B}

S6. Correlation of ΔE_{HB} against $\text{p}K_{\text{HB}}$ and $\sigma^{4\text{B}}$

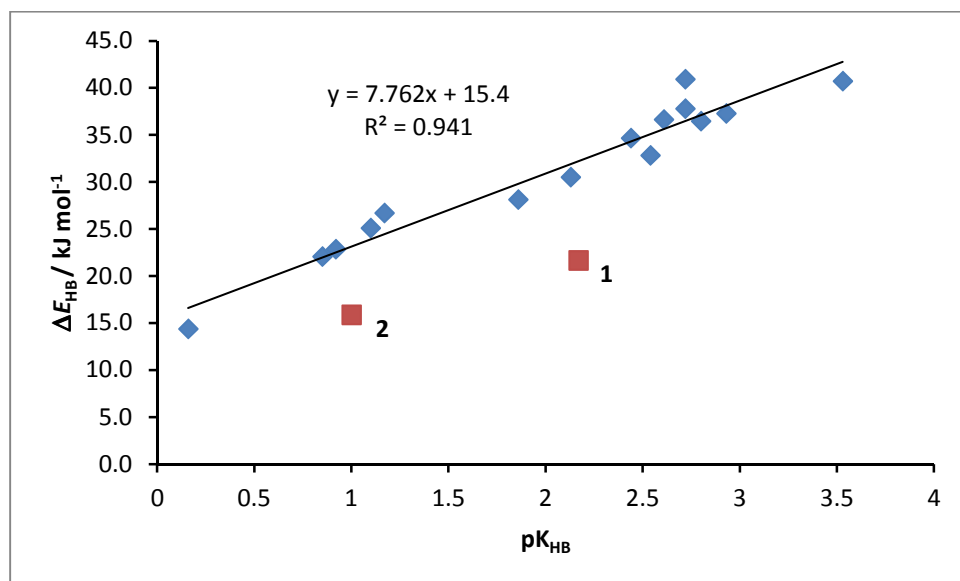


Figure S7. Correlation of the ΔE_{HB} calculated for **DIG** series of bases against two independent variables $\text{p}K_{\text{HB}}$.

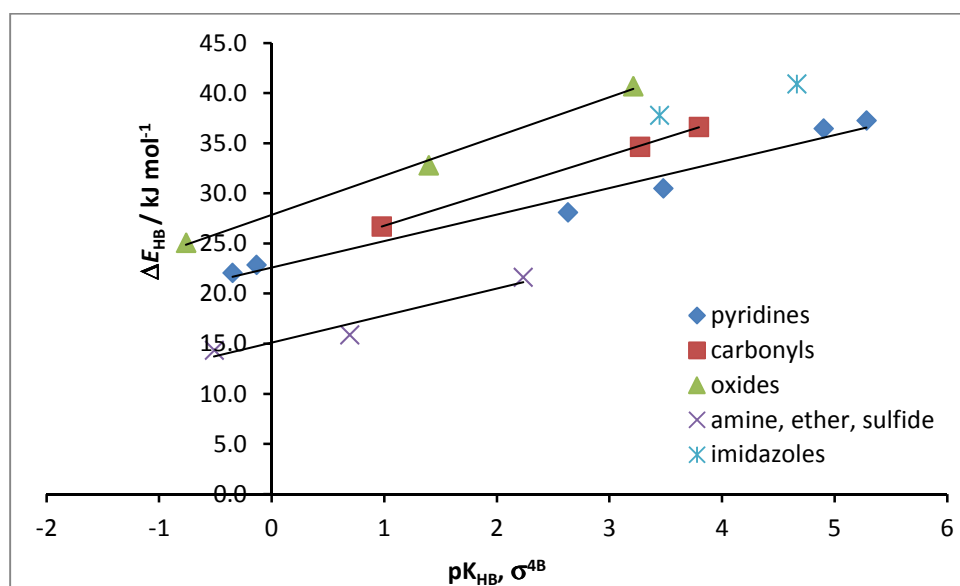


Figure S8. Correlation of the ΔE_{HB} calculated for **DIG** series of bases against two independent variables $\text{p}K_{\text{HB}}$ and $\sigma^{4\text{B}}$ as used for the correlation of GBs.

S7. Cartesian coordinated for the hydrogen bonded DMG series of bases and their conjugated acids.

DMG:1

C	2.3997254917	0.6430931643	1.4056025432
N	2.0608337101	-0.181069156	0.2471944258
C	3.2691717873	-0.5491612745	-0.4881888609
C	1.2691041395	-1.3516464232	0.668407429
C	0.7268154378	-2.2143979018	-0.4755435779
C	-0.1334120807	-1.4679990958	-1.5138783713
N	-1.3407725413	-0.8949981877	-0.9507198711
C	-1.4082244011	0.3782514298	-0.7480702873
N	-0.3646712954	1.283787878	-0.8701921663
C	-0.5195102727	2.7183436173	-0.7515000643
H	0.3997848481	3.2012956493	-1.0974648728
N	-2.6421472429	0.9503312347	-0.4400465064
C	-3.7890479754	0.0737841862	-0.2568902003
H	-0.4355898058	-2.2101466507	-2.2672764418
H	0.489939713	-0.7285241724	-2.0434092772
H	1.5467203417	-2.7292440729	-0.9944139565
H	0.1131364637	-2.999344166	-0.0154078733
H	1.8609618331	-1.9889642191	1.3547535793
H	0.4179605745	-0.9690342729	1.2433543798
H	0.5594898501	0.9002033089	-0.6611219634
H	-3.672245328	-0.6229795939	0.5853037072
H	-3.9276166109	-0.5258848241	-1.1583156887
H	-0.7082839142	3.0729847279	0.2785066083
H	-2.5936668561	1.7112143732	0.2262639643
H	-1.3432814375	3.0652930945	-1.3832552609
H	3.8136474285	0.3584625093	-0.7693149106
H	3.9502794136	-1.1882370493	0.1054461279
H	3.0090518337	-1.0832651111	-1.4051113
H	2.9483753107	1.5337838218	1.0801774848
H	1.4822617872	0.9674564894	1.9080272767
H	3.0244075845	0.1065924298	2.1444833752
H	-4.6767707866	0.6938552568	-0.0957584502

DMG:1H⁺

C	2.5545215437	0.6707254766	1.5475045314
N	2.0670455083	-0.0112782958	0.3360866111
C	3.1257957357	-0.0346535603	-0.6866014219
C	1.5879856183	-1.3648324164	0.6849014215
C	0.9518168845	-2.1389318675	-0.477292018
C	-0.111402213	-1.3835666415	-1.2873739633
N	-1.2687710428	-0.911012003	-0.5118539995
C	-1.4789967252	0.3586105291	-0.1105668942
N	-0.4689925667	1.2308880325	-0.094728083
C	-0.6466043288	2.6645390863	0.1137161354
H	0.2893659086	3.1621745301	-0.1447800973
N	-2.7234345292	0.7410901232	0.2388791547
C	-3.9318808931	-0.0628194046	0.0664749735
H	-4.7966600674	0.5886225273	0.1989764871
H	-0.5013124869	-2.040749053	-2.0712572964
H	0.31954167	-0.5139064617	-1.7889186553
H	1.717770574	-2.4712023224	-1.1879916748
H	0.5149775975	-3.0560367041	-0.0630234261
H	2.4076412435	-1.9728702473	1.1035256255
H	0.8496401425	-1.2433699929	1.4869754005
H	0.5060546336	0.8393532846	-0.0488696215

H	-3.9997700652	-0.8749653522	0.8011051073
H	-3.970405913	-0.4755576106	-0.945769636
H	-1.9989274087	-1.5818932413	-0.3179246161
H	-0.8835930338	2.9118235675	1.1573216458
H	-2.8072676384	1.6009150718	0.7618261079
H	-1.4322041547	3.0565062996	-0.5399028559
H	3.4530811765	0.9886658884	-0.889905899
H	4.000220663	-0.6207243108	-0.3612047543
H	2.7523417111	-0.4611447631	-1.6209089208
H	2.8772235082	1.6845552301	1.2929700007
H	1.7492768004	0.734401612	2.2865359442
H	3.4046598194	0.1431598387	2.0079587657

DMG:2

C	0.7862950639	1.8469537975	-0.9158742393
N	1.2025633287	0.6207876035	-0.2449882882
C	0.4028023483	-0.5197770505	-0.2137632024
N	0.7845133614	-1.7477052678	-0.2896140314
C	2.1378644396	-2.0729935221	-0.6987223292
C	3.0648289486	-2.4387981718	0.4754669417
C	3.325560504	-1.3017458523	1.4537344452
O	3.9311534106	-0.2104891448	0.758362804
N	-0.9532226528	-0.2314633355	-0.0805197946
C	-1.8916895137	-1.3321801281	0.0767912389
H	-1.7853220586	-2.0156521463	-0.7676238548
H	1.6578390556	2.5025912757	-1.000342934
H	0.3847134886	1.6695369942	-1.9228837728
H	0.0260693964	2.3923155031	-0.3430135248
H	-1.1400417375	0.5652859906	0.5165793938
H	2.0823088578	-2.9541185623	-1.3527731287
H	2.6185437105	-1.280613081	-1.296557989
H	4.0240646024	-2.7929530551	0.0754494283
H	2.616273153	-3.2673935408	1.0381052999
H	3.9968397221	-1.6375965207	2.2607900282
H	2.3845686846	-0.9691713411	1.9188244308
H	2.1979440361	0.4271821088	-0.2609976082
H	-2.9072781032	-0.9239875934	0.0838063192
H	-1.7262211563	-1.91509777	0.9939792033
C	4.2531502741	0.8657901443	1.6178894685
H	4.73484712	1.6354797757	1.0083409164
H	3.3535379982	1.2898561056	2.0905682412
H	4.9498577177	0.5512957845	2.4104005376

DMG:2H⁺

C	1.211381273	0.3630267508	0.2171170886
N	2.4731366812	0.7584826721	-0.0374844293
N	0.9742464874	-0.9190359216	0.5512759297
N	0.2072317778	1.2452880325	0.1719004713
C	0.3934334386	2.6888520886	0.0489394687
H	-0.7468330385	0.8677959618	0.0790408118
H	2.5887508008	1.6357529947	-0.5246068938
C	3.6694595942	-0.0535653952	0.18062231
H	1.7156350051	-1.5824237893	0.3733172648
C	-0.2364923276	-1.4294757374	1.21721128
H	-0.5509349701	3.1741558705	0.2988367414
H	0.6722522868	2.9892446909	-0.9695517898
H	1.1531575919	3.0385717995	0.7543577301
H	3.642865542	-0.5052142077	1.1764141344
H	3.78418903	-0.8362817764	-0.579518487

H	4.539685328	0.6018178018	0.1291605951
H	0.0980161167	-2.1155524437	2.0012788529
H	-0.7211121697	-0.5877311915	1.7160033633
C	-1.2291700416	-2.152441634	0.2965791698
H	-2.0525183896	-2.4990124478	0.9319594185
C	-1.7942283826	-1.3069968494	-0.84150725
H	-0.7633569503	-3.0468155317	-0.1354660113
H	-2.6178113863	-1.8482495701	-1.3246654679
O	-2.2744442194	-0.0697259895	-0.3085543908
H	-1.0335439941	-1.1090620514	-1.6138663262
C	-3.1642325023	0.6196049002	-1.1901948269
H	-3.4753959451	1.5324950587	-0.6784423662
H	-2.6724781002	0.8758246945	-2.1389630161
H	-4.0482239376	0.0053238308	-1.3993006707

DMG:3

C	0.5678203187	-0.6316613918	0.2489270395
N	0.4716069357	-0.6828004037	1.6368400257
N	1.7316507009	-0.6197811214	-0.3009016066
N	-0.6778625724	-0.589162432	-0.3808405059
C	-1.819749627	-1.3507277058	0.1195586518
H	-0.623030031	-0.5387356103	-1.3919673745
H	-0.3067051089	-0.1515594501	2.0082546322
C	1.6898070506	-0.593697272	2.427886375
C	1.8975155095	-0.804756044	-1.7287633053
H	-2.6001590802	-1.3335021842	-0.6464109973
H	-2.2444487402	-0.9003400127	1.0243030198
H	-1.573789526	-2.3970222886	0.3466443609
H	2.3687151686	-1.3958745736	2.132755461
H	2.2247151206	0.3568505437	2.291838277
H	1.4266927939	-0.7155853764	3.4831677293
H	2.740482314	-1.4937802796	-1.8780656333
H	1.0312909953	-1.2763899531	-2.2243866279
C	2.2497668551	0.5062395683	-2.4570331064
H	2.5388351433	0.2802347162	-3.4923867216
C	1.1447602784	1.5666259665	-2.4437331043
H	3.1298734611	0.9408460853	-1.9663437373
H	1.5247724543	2.5207638421	-2.8244268619
S	-0.2933219373	1.0609215655	-3.4836169152
H	0.79055882	1.7227502821	-1.418906939
C	-1.5105688926	2.3089109443	-2.9369598661
H	-2.4339014856	2.1303594492	-3.494344635
H	-1.713099078	2.2062725333	-1.8663086545
H	-1.1609638408	3.3232966027	-3.1519269801

DMG:3H⁺

C	1.2635129563	0.3974854426	0.2587959202
N	2.5194896562	0.7512301887	-0.0731610128
N	0.9927725957	-0.8928402301	0.5318871267
N	0.3082490942	1.3305656029	0.340729043
C	0.5574157544	2.7686228656	0.2696381594
H	-0.6717577868	1.0226510326	0.2954788637
H	2.6405047634	1.6534678619	-0.510884185
C	3.6918127857	-0.1190173741	0.0096917463
H	1.7012407938	-1.5655803599	0.2718293199
C	-0.1569415199	-1.4137311918	1.2932453196
H	-0.3508167593	3.2814869849	0.5888270697
H	0.7960474478	3.1008693057	-0.7490797691
H	1.3676468258	3.0514288545	0.9481823063

H	3.7261026668	-0.617356044	0.9828022789
H	3.7106871971	-0.8669760529	-0.7925943775
H	4.5833065367	0.5023274822	-0.0837084758
H	0.2457010187	-2.068638768	2.0730461269
H	-0.6265528256	-0.5711219939	1.805807433
C	-1.1714606867	-2.2013763914	0.4501656218
H	-1.9311642281	-2.586660956	1.1405554053
C	-1.8487439265	-1.4302592327	-0.68706846
H	-0.6755299578	-3.0792801593	0.0161491295
H	-2.5608216993	-2.0882795964	-1.1941208706
S	-2.7661891736	0.0346637012	-0.0482061194
H	-1.1129836969	-1.0993710269	-1.4296147071
C	-3.5018404715	0.6577796852	-1.6024516455
H	-4.0627373878	1.5604264117	-1.3495293561
H	-2.7326588949	0.9044578247	-2.3390979635
H	-4.1916250778	-0.0823218672	-2.0154229278

DMG:4

C	2.0104800449	0.1493052366	0.6195304155
N	3.2659464254	0.5721328418	0.1841486391
N	1.6996417229	-1.0984339374	0.4789320775
N	1.2503299058	1.1328403111	1.2280477778
C	1.704487943	2.4956201426	1.4150095552
H	0.2379634886	1.0199005388	1.1598639843
H	3.282403074	1.5072815683	-0.2025065544
C	4.1249839206	-0.3757621553	-0.5067874451
C	0.5287381485	-1.6463288211	1.1342972895
H	0.9830579771	3.0141115174	2.0526305478
H	1.7907770326	3.0785833174	0.4794282469
H	2.6784238304	2.5107368672	1.9150026618
H	4.2820924212	-1.2471745698	0.1314218272
H	3.6996129211	-0.7369338121	-1.4543927221
H	5.0878991803	0.1072598423	-0.7022008147
H	0.856209507	-2.466283097	1.7928779094
H	-0.00989497	-0.9347308953	1.7760829392
C	-0.4454532211	-2.2667201085	0.1131979672
H	-1.2552386953	-2.7818440877	0.6481629993
C	-1.0234671058	-1.2716978343	-0.9102039208
H	0.0997077125	-3.0349961079	-0.4486560434
H	-1.538330131	-1.8081644874	-1.7190701858
P	-2.1964755218	-0.021874269	-0.2506610532
H	-0.1923698821	-0.7195055435	-1.3669751056
O	-1.6177672161	0.9229118582	0.779707553
C	-3.6444791076	-0.9552448684	0.3762633847
H	-3.3501743263	-1.5441375741	1.2498210313
H	-4.4176299258	-0.2455698165	0.6865105058
H	-4.0573043321	-1.6261450544	-0.3845994977
C	-2.8194855951	0.8471565191	-1.7412223374
H	-3.555939294	1.5982322508	-1.4391940904
H	-1.9866483634	1.3607159635	-2.2316945844
H	-3.2824895683	0.1576982646	-2.4550289574

DMG:4H⁺

C	2.0583657102	0.3981837007	0.2024167153
N	3.3342608315	0.6767658301	-0.1384357851
N	1.6535619493	-0.8919846459	0.2140103976
N	1.2236653996	1.3813889887	0.5289614589
C	1.6345392907	2.770189948	0.7094403818
H	0.1985753988	1.1944722683	0.527455912

H	3.5404795404	1.6348618243	-0.381430854
C	4.3969311705	-0.3074997213	-0.325182337
C	0.5298864687	-1.4527126561	0.9834790295
H	0.7949857092	3.3058754754	1.15380697
H	1.882111676	3.2596605325	-0.2421501731
H	2.4900516653	2.8396163281	1.3890864546
H	4.4293180619	-1.0004948043	0.5209559091
H	4.2853606427	-0.8700183408	-1.2607986387
H	5.3494392854	0.2228819699	-0.3609892541
H	0.9461578396	-2.1449376628	1.7249287807
H	0.0519796088	-0.638746872	1.5270758601
C	-0.4882911111	-2.2110241875	0.1164055918
H	-1.2037542343	-2.6818921443	0.8018302013
C	-1.2369803196	-1.3833300322	-0.9461771924
H	0.0214231335	-3.0400439934	-0.3917561561
H	-1.8692228956	-2.0485869194	-1.5471141304
P	-2.2814781904	-0.0116623081	-0.2943994057
H	-0.5220832039	-0.9234299648	-1.6408547749
O	-1.4618794644	0.9776866504	0.5224558405
C	-3.6315794869	-0.7668313416	0.6712097645
H	-3.2285304829	-1.2781202415	1.5503902666
H	-4.3025624108	0.0246882283	1.0189464419
H	-4.2047624728	-1.4808626507	0.0711227628
C	-3.068443102	0.7333535375	-1.7608316038
H	-3.7254129272	1.5478666291	-1.4403955691
H	-2.3018010793	1.1501008378	-2.4212308818
H	-3.6592047514	-0.0010878249	-2.3177974203
H	2.2976714813	-1.5635279512	-0.1810519429

DMG:5

C	0.521020558	-0.7279093686	0.2975083566
N	0.5015047646	-0.6873553058	1.6908183103
N	1.6496039023	-0.5469127978	-0.3084590233
N	-0.6972038232	-1.0260022325	-0.2850635542
C	-1.9010840693	-1.3217187561	0.4635286344
H	-0.8404574888	-0.6833711048	-1.2351415535
H	-0.3395128297	-0.2880765395	2.0877162197
C	1.7221469621	-0.3418015235	2.4014275589
C	1.7803636152	-0.8284926035	-1.7244755555
H	-2.6562026582	-1.6986405091	-0.2319432634
H	-2.3396325443	-0.4486577731	0.9810611977
H	-1.7067299617	-2.096294375	1.2124826447
H	2.5141893642	-1.0336195827	2.1092597353
H	2.0790555207	0.6752083227	2.1834447005
H	1.53669486	-0.4384342899	3.4760318388
H	2.6102901254	-1.5393234129	-1.8570279506
H	0.897691915	-1.296874494	-2.181127802
C	2.1615929216	0.4409491036	-2.5132311706
H	2.3867007145	0.1809147536	-3.5569776883
C	1.1196336202	1.5614926141	-2.461805581
H	3.08451312	0.8431073865	-2.0772923275
H	1.5324294544	2.5074756485	-2.8340639137
S	-0.3437758723	1.2333366002	-3.5373524041
H	0.7674505102	1.7065451108	-1.4341699697
C	-1.2467598912	2.7759542056	-3.1289480694
H	-2.2105926294	2.7254080158	-3.6408181604
H	-1.4048585007	2.8321900099	-2.0481349762
H	-0.6819667721	3.6425393418	-3.4852678445
O	-1.1590508877	0.0890815557	-2.9416403893

DMG:5H⁺

C	1.313858898	0.4599783692	0.2654354493
N	2.5909648648	0.733076977	-0.072128315
N	0.9567286494	-0.8258969659	0.4801796373
N	0.4295197064	1.4469527144	0.3897646906
C	0.7812401684	2.8641234601	0.3744924954
H	-0.583870997	1.2175613062	0.4145669446
H	2.7734894219	1.6471489699	-0.460477364
C	3.696486581	-0.222012892	-0.0512125939
H	1.6362161994	-1.5261559941	0.2161584594
C	-0.1869363527	-1.3023113531	1.2760773842
H	-0.0940435535	3.4239984166	0.7058152344
H	1.0490091639	3.2162063788	-0.6305617539
H	1.6055525032	3.0689921644	1.065139454
H	3.7142225815	-0.7650350427	0.8984663259
H	3.6480409515	-0.933761396	-0.8849270009
H	4.6296898093	0.3362071447	-0.1363348644
H	0.2111978194	-1.9150316134	2.0925159519
H	-0.6771554537	-0.4388859211	1.724458393
C	-1.1860067138	-2.1471335978	0.4675549756
H	-1.9137298372	-2.5647854315	1.1745327737
C	-1.9193614659	-1.4285888191	-0.6717896838
H	-0.6615869073	-3.0080861482	0.0329943728
H	-2.5175728189	-2.1438456658	-1.247180139
S	-3.1007586091	-0.15544008	-0.0484468703
H	-1.2225732769	-0.9309804256	-1.3565921723
C	-3.6628377247	0.4671756708	-1.6696412106
H	-4.3251766684	1.3123670366	-1.4685347019
H	-2.8075799292	0.7978901209	-2.265342117
H	-4.2194624822	-0.3204977446	-2.1857785691
O	-2.2504925277	0.9572683612	0.5829838141

DMG:6

C	0.4932876992	-0.7960122368	0.3360315087
N	0.523185485	-0.7554309393	1.7259017731
N	1.5731029534	-0.5133610299	-0.3156007283
N	-0.7137843939	-1.2151687582	-0.2063798336
C	-1.8718012101	-1.5675945602	0.591905787
H	-0.9235308955	-0.8170746359	-1.1161906299
H	-0.3359371283	-0.4445897532	2.1606337954
C	1.7349313315	-0.3089461402	2.394196546
C	1.6820828993	-0.7987839485	-1.7329599859
H	-2.6244367058	-2.0111737002	-0.0659477935
H	-2.3471901401	-0.7124471601	1.1057366155
H	-1.5982515192	-2.311486044	1.3464007344
H	2.5738287383	-0.921599656	2.0594264349
H	1.9873730215	0.7393092517	2.1787734574
H	1.6027363719	-0.4351701388	3.4733635885
H	2.4742658442	-1.5498744976	-1.8755535342
H	0.7788896335	-1.2262187036	-2.190782644
C	2.1188549748	0.4519293388	-2.51605682
H	2.2904663188	0.2009829606	-3.5690101084
C	1.1483334071	1.6335666769	-2.4219475599
H	3.0707461549	0.802571057	-2.0995582895
H	1.5934701762	2.5454833632	-2.8342007502
S	-0.3769725816	1.3672653433	-3.3828444015
H	0.8489832334	1.8081093128	-1.3838985233
C	-1.1566031122	3.0010663153	-3.3992656159
H	-2.1036838	2.8786947644	-3.9299321651

H	-1.3406755182	3.32777751	-2.3734996443
H	-0.5149151582	3.7059899075	-3.9314880105
O	-1.2875602469	0.477233501	-2.6259211349
O	-0.0101888333	1.0247346003	-4.7664410681

DMG:6H⁺

C	1.3235823175	0.4731674252	0.5041335321
N	2.5628232272	0.8171623824	0.1037468149
N	0.9911858939	-0.835142626	0.5386444288
N	0.4615430664	1.4159593501	0.8880808326
C	0.7947104534	2.8351319518	0.9927927599
H	-0.5082045183	1.1664930756	1.1100282733
H	2.7452955123	1.7999428593	-0.0341333342
C	3.627576789	-0.1240623017	-0.234158957
H	1.6221430552	-1.4766508477	0.0799924661
C	-0.2929858551	-1.3697850285	0.9996241372
H	-0.0722666114	3.3428867649	1.4155444252
H	1.00077229	3.2786087717	0.0108106803
H	1.6490339704	2.9937171719	1.6598967948
H	3.7918771117	-0.8325535043	0.5841215851
H	3.4158244083	-0.6689879551	-1.1625961408
H	4.5475564873	0.4430148449	-0.378708181
H	-0.0943511509	-2.3704693075	1.3934943339
H	-0.6285012524	-0.7642649923	1.8432669017
C	-1.3723926536	-1.4315584295	-0.1089681858
H	-1.2174032854	-0.6272414578	-0.8375015274
C	-2.808771016	-1.3406139262	0.4343963159
H	-1.275025049	-2.3679235405	-0.6681922929
H	-3.533291616	-1.7272786676	-0.2873827167
S	-3.2403095819	0.416051819	0.6942808679
H	-2.9344751427	-1.8683882537	1.3856622381
C	-4.8414611708	0.403972784	1.5147015713
H	-5.1057125208	1.4517425341	1.6785577221
H	-5.5743551218	-0.0692053284	0.857748734
H	-4.7583821885	-0.1195723134	2.4691130352
O	-2.2481366468	0.9639549181	1.6648870192
O	-3.356760201	1.0557838273	-0.6213651335

DMG:7

C	0.9936952099	2.4768015855	0.49748517
N	0.7175144594	1.059516939	0.3410927847
C	1.6909530602	0.0966741161	0.1414492645
N	1.5901992786	-1.1707706092	0.3700582921
C	0.3920349244	-1.645444797	1.0325621124
C	-0.7924441066	-1.8576008423	0.0625214289
C	-2.1292744135	-2.0608711228	0.7791928923
C	-2.7015153348	-0.7932944195	1.4031598822
C	-4.0017817878	-0.9382168198	2.1726304981
N	2.8960903233	0.6090176456	-0.3396574151
C	3.9467481213	-0.3295699414	-0.7055669744
O	-2.159024679	0.2959053441	1.2958827709
H	-0.1841521931	0.7405975738	0.6748476085
H	2.7800753179	1.371521839	-0.9962671107
H	0.1091698711	2.9523088244	0.9294246987
H	1.1948283653	2.9776286153	-0.4619808535
H	1.8492746993	2.6597793065	1.1594365252
H	4.1931664324	-0.9453306458	0.1612580688
H	3.6566775874	-1.0093495235	-1.5192492576
H	4.8313476791	0.2414734834	-1.0049783622

H	0.6219479147	-2.6101008511	1.5063000376
H	0.0748073487	-0.9737646932	1.8493513787
H	-0.8781770116	-0.9941868911	-0.6061083999
H	-0.5786807968	-2.7231734274	-0.5749047137
H	-2.8942567453	-2.4504435926	0.090148062
H	-2.0488768682	-2.8226620746	1.5702099953
H	-4.3587866054	0.0432350032	2.4907914521
H	-4.7657756089	-1.4322080423	1.5605149627
H	-3.8441644421	-1.5705019823	3.0557582016

DMG:7H⁺

C	0.8646640713	2.4250368974	0.4845887088
N	0.7210596539	0.9710150483	0.4832360978
C	1.6877307906	0.1233089238	0.1234974866
N	1.5469778956	-1.2025550594	0.3230330701
C	0.3983174371	-1.819097169	0.9971838873
C	-0.8270865096	-2.0206485285	0.0803402146
C	-2.1436990165	-2.1030287034	0.8604073769
C	-2.599035532	-0.7664086949	1.4357603389
C	-3.9448283676	-0.7241654948	2.1133614773
N	2.835939214	0.5895886655	-0.4038102171
C	4.012562681	-0.2255544193	-0.6971299022
O	-1.9059521364	0.2414822535	1.341252537
H	-0.2010986552	0.599793929	0.7383608601
H	2.8460823031	1.5529174396	-0.7051126417
H	-0.0097601776	2.8416186888	0.9851992587
H	0.9018050233	2.8361049677	-0.532228871
H	1.7585704121	2.7295795105	1.0387979852
H	4.2872425081	-0.8261263147	0.1753578045
H	3.8568673821	-0.8794421986	-1.564424638
H	4.8430472878	0.4444510308	-0.9219420166
H	0.7443159653	-2.7762671899	1.3970115437
H	0.1496698722	-1.1925792888	1.8573818726
H	-0.891780537	-1.1914377717	-0.632580082
H	-0.6929658438	-2.9314375493	-0.512683592
H	-2.9474963451	-2.4835124631	0.216189581
H	-2.0806954172	-2.8264353255	1.6869572875
H	-4.0996323333	0.2472853225	2.5854891689
H	-4.7364270307	-0.8953783552	1.3723246664
H	-4.0332006789	-1.5229629843	2.8589173184
H	2.1915490834	-1.812149167	-0.1598745818

DMG:8

C	0.8809625014	2.4723046541	0.4293003991
N	0.6595330015	1.0423664985	0.3519666962
C	1.6605982018	0.0949271141	0.2804768345
N	1.5454425665	-1.1739895568	0.4978243506
C	0.2675322346	-1.6580019567	0.9803008199
C	-0.7517488451	-1.9025014419	-0.1553423222
C	-2.1811832498	-2.1187941701	0.3519672284
C	-2.8365373736	-0.8171018411	0.8303176704
N	-4.100749311	-0.8910370351	1.3558548605
N	2.9173266355	0.6209523065	-0.0291361014
C	4.0180089515	-0.3088230556	-0.2352404435
O	-2.2543557221	0.2682262758	0.7355290564
H	-0.2917398977	0.7177202522	0.4909069711
H	2.8861603696	1.3724192266	-0.7078176894
H	-0.0400747556	2.9448969273	0.7812215084
H	1.1276478503	2.9257323994	-0.5449832684

H	1.6887570438	2.7173756031	1.1291301721
H	4.1442994511	-0.9166071823	0.6624619316
H	3.8537749393	-0.9975277541	-1.0763458951
H	4.930988746	0.2694901881	-0.4104355304
H	0.4358651893	-2.6131801544	1.4981440801
H	-0.1815053602	-0.9797480384	1.7257073121
H	-0.744728105	-1.0547375871	-0.847235694
H	-0.4358566399	-2.7800902001	-0.7314856897
H	-2.8047690706	-2.5493932357	-0.4436399349
H	-2.1828393684	-2.8528358375	1.1697693547
C	-4.8863775429	-2.1055829861	1.4969201725
H	-5.1130148279	-2.2975238412	2.5548058826
H	-5.013938174	0.2305478779	2.8874265032
C	-4.754693292	0.3234120021	1.8246336254
H	-5.8402595903	-2.0056729919	0.9613658596
H	-4.3600513073	-2.969437427	1.0967430934
H	-4.0733202813	1.160722717	1.685883049
H	-5.6784389675	0.5042292505	1.2591781373

DMG:8H⁺

C	0.6309474243	2.3952029285	0.3431097196
N	0.5662572432	0.9377488863	0.3909926199
C	1.6143669085	0.1382975221	0.1931373798
N	1.5184719456	-1.1874018962	0.4231179493
C	0.3140213188	-1.8439246498	0.9459348357
C	-0.7650792834	-2.1082206316	-0.1244267186
C	-2.1708808653	-2.2591400401	0.4697301193
C	-2.7312197769	-0.9225595686	0.9747277179
N	-3.989277315	-0.8968144669	1.4695370946
N	2.7981089726	0.6518856137	-0.1975364131
C	4.0427810791	-0.1040730249	-0.3050677645
O	-2.035919419	0.1105359422	0.9225753778
H	-0.3657465142	0.5231117349	0.5507503034
H	2.7987845267	1.606184377	-0.5257186856
H	-0.3271637321	2.7767550695	0.6967372758
H	0.7883517062	2.7680071728	-0.6772860978
H	1.4201341594	2.7771171588	0.9996732015
H	4.231182641	-0.6622190958	0.6171576182
H	4.0377680304	-0.7918703059	-1.1601827082
H	4.860263641	0.6041150173	-0.4448605933
H	0.6422973554	-2.7799056891	1.4066990248
H	-0.0792057752	-1.215939943	1.7486105503
H	-0.775036264	-1.2879071359	-0.8486139064
H	-0.5107351758	-3.0171204906	-0.6807500956
H	-2.8401300164	-2.6663392119	-0.296631827
H	-2.166051271	-2.9916067711	1.287980856
C	-4.8858690118	-2.0461583752	1.5582143408
H	-5.2264826528	-2.168715761	2.5927073548
H	-5.459420113	0.6062349567	1.3582534674
C	-4.5633481061	0.3640354987	1.940932878
H	-5.766435274	-1.8877148798	0.9241104584
H	-4.3956646652	-2.9663475016	1.2478397335
H	-4.8464210009	0.272973323	2.9956601858
H	-3.8270171615	1.1559487028	1.825404177
H	2.2460814416	-1.7749664652	0.0418465702

DMG:9

C	0.8652966698	2.4667003826	0.446991518
N	0.6494023361	1.0376002005	0.3398339162

C	1.6557575424	0.0988469179	0.2370805446
N	1.555785387	-1.1732757274	0.4433159075
C	0.2943255998	-1.671949198	0.9534095549
C	-0.7526388756	-1.9171881701	-0.157054256
C	-2.1678351132	-2.1245932094	0.3900197113
C	-2.809951314	-0.8242815	0.8778716416
N	-4.0668008516	-0.9149458454	1.3889135817
N	2.9010945335	0.637888245	-0.0965123528
C	4.0031424508	-0.281115696	-0.3398737315
O	-2.2424576572	0.2730603452	0.8092750653
H	-0.2957125926	0.7051133409	0.5052350942
H	2.8475262113	1.396124889	-0.7662562217
H	-0.0514584386	2.9253429425	0.8273817777
H	1.0906436677	2.9439045399	-0.5210007671
H	1.6855654278	2.7002369755	1.1362939209
H	4.1560066316	-0.8977885333	0.5475922095
H	3.8233774761	-0.9619201665	-1.184276108
H	4.9073222288	0.3059915722	-0.5309775755
H	0.4834761909	-2.628972783	1.4606078451
H	-0.1426753854	-1.0025004452	1.7137318281
H	-0.7613216379	-1.0679249248	-0.8477701564
H	-0.4528925799	-2.7943575339	-0.7421778997
H	-2.8231027108	-2.562444218	-0.3767867014
H	-2.1561132806	-2.8505503255	1.2163656126
C	-4.8792364822	-2.1317382775	1.5219617827
C	-6.0517154758	-1.6792197004	2.4065144731
C	-6.2228902713	-0.196444947	2.0353031755
C	-4.7798743812	0.2907420769	1.8413876862
H	-5.2335648074	-2.476598297	0.5392435558
H	-4.3052466649	-2.9476813831	1.9724880177
H	-5.7762428125	-1.7737635966	3.4636465659
H	-6.9524019145	-2.2772488692	2.2397401213
H	-6.7584640147	0.3777702877	2.7968107144
H	-6.7802218348	-0.1058079143	1.0950310635
H	-4.3392378891	0.6580188352	2.7776444671
H	-4.6783863678	1.0877547104	1.1000714176

DMG:9H⁺

C	0.6332986461	2.3829806463	0.4198918777
N	0.569319549	0.9250085298	0.4334878565
C	1.6149211835	0.1317770575	0.2038636263
N	1.5226893391	-1.1997120483	0.4013625034
C	0.3239808044	-1.8700690336	0.9193283547
C	-0.7649774408	-2.1151585795	-0.1462992368
C	-2.1644259253	-2.2579626082	0.4630400279
C	-2.7138529894	-0.9248228847	0.9772269311
N	-3.9779867575	-0.9103299476	1.4275087246
N	2.7944075615	0.6555078903	-0.1877533068
C	4.037369533	-0.0968881541	-0.3299590364
O	-2.0216367869	0.1144110476	0.9776435272
H	-0.3634798494	0.5081110922	0.5961198237
H	2.7915505383	1.6183681769	-0.4897722634
H	-0.3231018365	2.7545373084	0.7885560239
H	0.7837920807	2.7799200436	-0.5924898264
H	1.4266327218	2.7504074966	1.0798684994
H	4.236125924	-0.680214993	0.5743422197
H	4.0231171924	-0.7611229579	-1.2035258182
H	4.853531554	0.6148592825	-0.4593786133
H	0.6577002946	-2.8145050966	1.3584117294
H	-0.0651329446	-1.2596515413	1.7374537957

H	-0.7752488507	-1.2843623569	-0.859087507
H	-0.5214951424	-3.0179413099	-0.7169910013
H	-2.8543855715	-2.6634689091	-0.2868899511
H	-2.160114446	-2.9887541628	1.2841501434
C	-4.9077618311	-2.0568258693	1.4763695379
C	-6.0812351891	-1.5256489279	2.3138082973
C	-6.0954356582	-0.0213060283	1.9948656627
C	-4.6070309245	0.3395379729	1.9059249593
H	-5.2310124237	-2.3276749127	0.4622261865
H	-4.4311007384	-2.9329983058	1.9262956087
H	-5.8808645013	-1.6867772652	3.3791766656
H	-7.0196609637	-2.0298647878	2.0695181987
H	-6.6192844345	0.57059348	2.749634149
H	-6.5844480346	0.1574065712	1.0303229098
H	-4.1875123591	0.6095951316	2.8827567335
H	-4.387091766	1.1543010801	1.2122232468
H	2.246596443	-1.7767311272	-0.0023292596

DMG:10

C	0.8376964252	1.1330688265	2.1222144683
N	0.9433294851	1.569622598	3.4462398958
N	1.8154679404	1.3594805506	1.3080535876
N	-0.362240309	0.5158003767	1.8317848026
H	0.5275399097	0.9333621412	4.1160441012
C	2.2141885063	2.1283898804	3.8835406684
H	-0.4885609847	0.1145825889	0.9045413887
C	-1.5418134324	0.5875612576	2.6701538288
H	-1.497022768	-0.0884406379	3.5400659693
H	-1.7131199806	1.6045710292	3.0431722771
H	-2.4077032421	0.2860442716	2.0739207001
H	2.1062142081	2.4627421968	4.9205373768
H	3.0494373795	1.4168816747	3.8131613262
H	2.4631776502	2.984566687	3.2540898613
C	1.6140209481	1.0417211321	-0.0916018212
C	1.8898864701	-0.4447911909	-0.4090208052
H	2.3098683087	1.6518079511	-0.6852975643
H	0.6013034683	1.3027559664	-0.4406814383
H	2.9659751816	-0.6318147056	-0.3167111571
H	1.3979535263	-1.0778410396	0.3368965514
C	1.4210996606	-0.8703333132	-1.8078944664
H	1.8717548184	-1.8390651211	-2.0721236883
C	-0.0744688154	-0.9827830767	-1.923308254
H	1.7961960026	-0.156679613	-2.5584466836
N	-0.7021428387	-1.3318459543	-3.0926623451
C	-2.0610285667	-1.362770137	-2.8340860059
C	-2.1940166963	-1.0252662644	-1.5149396663
N	-0.9577946725	-0.7911034036	-0.9549645415
C	-0.060982336	-1.6428180412	-4.3593955374
H	-2.7787376276	-1.6142671542	-3.6008772855
H	-3.1031694534	-0.9333663811	-0.9366007656
H	-0.8306079043	-1.7837309089	-5.1205673889
H	0.5938421893	-0.8237587545	-4.672806984
H	0.5335905493	-2.5601384313	-4.286709405

DMG:10H⁺

C	0.7890946439	0.9981159882	2.1027286744
N	0.9499717283	1.3455840995	3.3967559684
N	1.7858483724	1.2593706811	1.2321165851
N	-0.3515662574	0.4438640044	1.692440006

H	0.2598820691	1.0115921711	4.0522864917
C	2.1017571262	2.0649017533	3.9326218695
H	-0.4456505605	0.0676680561	0.7224819222
C	-1.514835783	0.277786856	2.5574898127
H	-1.3349953418	-0.4536498142	3.3562842657
H	-1.825075462	1.2322924662	2.9973261367
H	-2.3334045107	-0.0979364173	1.9431601007
H	1.8760798702	2.3506846874	4.9605565803
H	3.0080744729	1.4460790109	3.9433204632
H	2.2850713374	2.9789500628	3.359023175
C	1.7176759257	0.9780083225	-0.2060465284
C	1.9791702725	-0.5008436052	-0.5569140567
H	2.4535044239	1.6277487678	-0.6881223136
H	0.7345416239	1.2955980048	-0.5605331025
H	2.6922551717	1.471215006	1.6236995693
H	3.0573071217	-0.6940209043	-0.5420799184
H	1.5319110604	-1.1449549718	0.2073481639
C	1.4116714842	-0.897590377	-1.9275193502
H	1.811405045	-1.8823345924	-2.2036191944
C	-0.0910820612	-0.9445447453	-1.939348774
H	1.7733647087	-0.2052460058	-2.7027027371
N	-0.8183054063	-1.3435021352	-3.0234788675
C	-2.1531107423	-1.2679489213	-2.6745621198
C	-2.1801759592	-0.8198359358	-1.383611662
N	-0.8927739458	-0.620537283	-0.9294281427
C	-0.2902340398	-1.7816386043	-4.3114410869
H	-2.9372205728	-1.53662554	-3.3660822713
H	-3.042487678	-0.6285394766	-0.7610140686
H	-1.1260536288	-2.0295791608	-4.9665606701
H	0.2980236578	-0.9865645237	-4.7791114752
H	0.3363278338	-2.6703659241	-4.190614445

DMG:11

N	2.6866602155	0.2854841231	1.2608544248
C	2.1621059697	-0.3089478322	0.1250556359
C	3.0617804742	-0.1771604229	-0.9070319561
C	0.8032038371	-0.9475564202	0.1006349836
C	-0.3757761276	0.050613754	0.0803368595
C	-0.6079904875	0.8146522451	1.3975111925
N	-1.1207387173	-0.0448857409	2.4473600093
C	-0.392453722	-0.3911938266	3.4527843977
N	0.918591701	-0.0073458561	3.7197653113
C	1.7455893605	-0.7229781368	4.6798723192
H	1.4792930006	-0.4726533379	5.7167224861
N	-0.9470734453	-1.2474876779	4.4089976646
C	-2.3799719324	-1.497524047	4.3598514208
H	-2.6330030535	-1.9586570186	3.4034755927
H	-1.3757677024	1.5762438881	1.1959128568
H	0.3036427055	1.3716813642	1.6637577286
H	-0.2215210584	0.7722300414	-0.734253504
H	-1.2933629409	-0.506159947	-0.1477470089
H	0.689675003	-1.607428827	0.9695927294
H	0.7403991948	-1.5885577509	-0.7877074671
H	1.4485174883	0.2669980361	2.8925519996
H	-2.9822294419	-0.5821389563	4.4510647091
H	-2.6373951138	-2.1870874441	5.1702909561
H	1.6969261055	-1.8163779449	4.5710735289
H	-0.592056187	-1.0987123143	5.3446544659
H	2.7816246271	-0.4068707586	4.5315691735
N	4.1493427346	0.5082932379	-0.3969731224

C	3.8650167737	0.7592786216	0.9108733648
H	4.5546079473	1.2875406324	1.5566545279
C	5.3594049388	0.8740696571	-1.1113007404
H	3.0298250711	-0.502660714	-1.9366851875
H	6.0176358349	1.4243926554	-0.4352150726
H	5.8862493013	-0.0178397853	-1.4662058495
H	5.1239016454	1.5131195028	-1.9684684301

DMG:11H*

N	2.5471896463	0.2298529425	1.2748999774
C	2.1296334636	-0.3352200731	0.0809841149
C	3.0954514139	-0.1269285194	-0.8732300058
C	0.8034539293	-1.0248269343	-0.0516515614
C	-0.4124433452	-0.073400888	-0.0458418868
C	-0.6533345979	0.6900975895	1.2634106862
N	-1.0428733098	-0.1803004392	2.3857775594
C	-0.3417219861	-0.4411625434	3.5054438846
N	0.9528794315	-0.1378414744	3.602175472
C	1.7088037579	-0.2480617718	4.8446287597
H	1.2067262344	0.2850976159	5.6585804766
N	-0.9849831387	-0.9952134438	4.5570438089
C	-2.4256452446	-1.2172103835	4.6405529736
H	-2.760827365	-2.0376009342	3.9928674413
H	-1.4649090953	1.4124456417	1.121331887
H	0.2316262753	1.2541775058	1.5602300245
H	-0.2940286753	0.673835247	-0.8399572293
H	-1.3150941425	-0.6477100581	-0.2940479856
H	0.6918424988	-1.7673926276	0.7500482444
H	0.7905496934	-1.5896722281	-0.9898559409
H	1.5118115807	0.0383349987	2.7360535529
H	-2.9675629905	-0.3013719771	4.3858643198
H	-2.6707198719	-1.477669441	5.6710584131
H	-1.9606799951	-0.5987421021	2.3242126632
H	1.879034126	-1.2920160781	5.1416328063
H	-0.4098208206	-1.4070361387	5.2769685831
H	2.6836818525	0.2136218986	4.6824856894
N	4.1132105969	0.5718136474	-0.2555206403
C	3.7346805357	0.7609272477	1.0321816344
H	4.3547246587	1.2851752841	1.7465843673
C	5.3628400391	1.0080984993	-0.8700958081
H	3.1524719883	-0.411483675	-1.9135279345
H	5.950706622	1.5522744285	-0.1288450231
H	5.9375221994	0.1446688858	-1.2160941903
H	5.1576280348	1.6699392988	-1.7157511338

DMG:12

C	0.77327209	1.3195094149	2.2148593831
N	1.1317131201	1.827643707	3.4644596755
N	1.6297086555	1.3825778759	1.2518803238
N	-0.5317650616	0.8535938287	2.1364987653
H	0.7675688376	1.2983367237	4.2469447066
C	2.4930896932	2.3039106363	3.6560708213
H	-0.6959049982	0.1205305436	1.4462274632
C	-1.4563761563	0.8734469417	3.251230009
H	-1.2189005938	0.1513618608	4.054111973
H	-1.4964754527	1.8731009962	3.6951817147
H	-2.4561859851	0.6270782484	2.8804295871
H	2.5739183735	2.7246858742	4.6635915136
H	3.2503348686	1.5175323201	3.5265176292

H	2.7053334975	3.083413097	2.922213074
C	1.2398020037	1.0828387308	-0.1125716757
C	1.9298880925	-0.1913230179	-0.6338110857
H	1.5825757955	1.9129609531	-0.7488166729
H	0.1516714369	1.0105646932	-0.2654412522
H	3.0046426464	-0.0874012949	-0.4420380993
H	1.7998676193	-0.2600181668	-1.7229853343
C	1.4528955852	-1.5079379912	0.0243099303
H	2.1859073945	-2.2958038341	-0.1870018154
C	0.0963191819	-1.9722197455	-0.4525226445
H	1.4327370689	-1.3691068353	1.1108282723
C	-0.0235095962	-2.9097661639	-1.4895703866
C	-1.2867595946	-3.2954926918	-1.9280401661
C	-2.4100887767	-2.7347761882	-1.3202685864
C	-2.204767448	-1.8108184943	-0.2989592786
N	-0.9926893388	-1.4357882888	0.1314478815
H	0.8718135436	-3.3287152341	-1.9400343305
H	-1.3937435827	-4.0232851412	-2.7281715251
H	-3.4165314684	-3.0044744857	-1.6249429828
H	-3.0518004509	-1.347287872	0.2039871129

DMG:12H⁺

C	0.8189715305	1.1828297114	2.3146083453
N	1.167883216	1.766611316	3.4810296815
N	1.6581914533	1.2811162091	1.266085071
N	-0.3508381708	0.5504448894	2.2090134507
H	0.6519358458	1.4888669459	4.3028937062
C	2.3363401377	2.620393969	3.6786225586
H	-0.5187638495	-0.0943427132	1.4052837135
C	-1.3628921001	0.5589291063	3.2604830103
H	-1.0614175097	-0.0310577696	4.1364525971
H	-1.5967331391	1.5822468802	3.5719572355
H	-2.2699244647	0.1091154407	2.8550218182
H	2.2430629203	3.1044013366	4.6515889405
H	3.2748410984	2.0514463424	3.6695263357
H	2.3708024365	3.4025618819	2.91419414
C	1.3656730551	0.9862144971	-0.1463479139
C	2.0318098989	-0.2999386077	-0.6551193136
H	1.7288449374	1.8392883092	-0.7293525193
H	0.2821062579	0.9530555973	-0.2709801883
H	3.1105890816	-0.2387010982	-0.4617919544
H	1.9166047123	-0.321271001	-1.7457885347
C	1.4947764415	-1.6186029565	-0.0535584577
H	2.1725222851	-2.4270989587	-0.3454946781
C	0.091388831	-1.9655396156	-0.500323501
H	1.5287365891	-1.5672118065	1.041948126
C	-0.1436569318	-2.9230894462	-1.492454083
C	-1.451657229	-3.1908437263	-1.8914414795
C	-2.497291288	-2.4911181707	-1.2903222344
C	-2.1816233462	-1.5531696175	-0.312239649
N	-0.9240286304	-1.2931346426	0.0803375128
H	0.6912577905	-3.4535378036	-1.9400080401
H	-1.6509061093	-3.9349412627	-2.656966148
H	-3.5313253187	-2.6661264172	-1.5677607063
H	-2.9659939589	-0.9838534902	0.181367982
H	2.5928485272	1.6079456715	1.4680091764

DMG:13

C	0.7744233062	1.3195396245	2.2276408725
N	1.1446432798	1.8293422711	3.4706948066
N	1.6265508773	1.365164804	1.2596832912
N	-0.5376751508	0.8696704818	2.1582607537
H	0.7737037128	1.3166254651	4.2607883122
C	2.5094250382	2.299426553	3.6547430016
H	-0.7111430702	0.135280587	1.4756087538
C	-1.4620535592	0.9165540832	3.273159235
H	-1.2384337337	0.1962947444	4.0810770057
H	-1.4801602302	1.9205909579	3.7078325111
H	-2.467296983	0.6894137687	2.904842225
H	2.595476551	2.7263174809	4.6589828508
H	3.2609860018	1.5073453966	3.5286191551
H	2.7239273805	3.0729956229	2.9152835379
C	1.2280059928	1.0750322261	-0.1032510099
C	1.9192556379	-0.1935740079	-0.6352029853
H	1.5651183795	1.908997638	-0.7371840868
H	0.1388291218	1.0026504687	-0.2518121589
H	2.9940915931	-0.0895353935	-0.4467568273
H	1.7860369731	-0.2598308925	-1.7239974896
C	1.4503620956	-1.5132140499	0.0245720534
H	2.1855736087	-2.2986547886	-0.1853082776
C	0.0983085821	-1.981190113	-0.454561233
H	1.424805211	-1.3720946075	1.1103901595
C	-0.0079459075	-2.9096317752	-1.5025606524
C	-1.2758019866	-3.2814982615	-1.9215916366
C	-2.4167093257	-2.7543921557	-1.3284201704
C	-2.2090133371	-1.8395827667	-0.2994885603
N	-0.9980474293	-1.4621556621	0.1310273642
H	0.8695475029	-3.3321838492	-1.9760827964
N	-1.4177489	-4.263650117	-3.0203204647
H	-3.4058920814	-3.0476885337	-1.6549451509
H	-3.0590009955	-1.3884928653	0.2072641158
O	-2.5585607693	-4.5657295734	-3.3616122112
O	-0.3872163869	-4.7102677613	-3.5171092935

DMG:13H⁺

C	0.8257870222	1.1896747338	2.328371938
N	1.180181295	1.7779715317	3.488944593
N	1.6632761187	1.2699068496	1.2771174718
N	-0.35099836	0.5657042631	2.2298128306
H	0.6619593757	1.5117299454	4.3134264793
C	2.354242186	2.6270824369	3.6796085793
H	-0.5198942751	-0.07967502	1.4357089874
C	-1.3658872045	0.5935894484	3.279412318
H	-1.0753155493	0.0018954906	4.157563123
H	-1.5830561437	1.6219287509	3.5855434629
H	-2.2798675006	0.1584535229	2.873639106
H	2.2644922071	3.1174141519	4.6496418512
H	3.2886071777	2.0517494426	3.6733589494
H	2.3918785169	3.4042791145	2.9103755668
C	1.360200106	0.9832044482	-0.1349272246
C	2.0201646579	-0.3021748429	-0.6535693264
H	1.7227593109	1.8368751533	-0.7172734584
H	0.2755914813	0.9571154406	-0.2534911863
H	3.0995999114	-0.2458706945	-0.4645628635
H	1.9015956879	-0.3190629723	-1.7438672488
C	1.4862471454	-1.6232543706	-0.0535568616
H	2.1659366317	-2.430193738	-0.3440940852
C	0.0861156327	-1.9743764165	-0.5040395421

H	1.5139836461	-1.5727830466	1.0418549545
C	-0.1334115392	-2.9259884038	-1.5064732518
C	-1.4427971042	-3.18060885	-1.8867950311
C	-2.5097669548	-2.5156261646	-1.2985733403
C	-2.194043575	-1.5844241461	-0.3129333294
N	-0.9382177027	-1.318363228	0.0789225826
H	0.682822087	-3.4599895859	-1.9777691789
N	-1.7063507291	-4.1880539379	-2.9460986516
H	-3.5301601233	-2.7194273201	-1.5974545955
H	-2.9842312305	-1.0283910605	0.1845796352
H	2.5990117816	1.5979744119	1.4727605603
O	-2.8784604634	-4.3828639895	-3.2451900752
O	-0.7305695238	-4.7434873486	-3.4384117386

DMG:14

C	0.7729641204	1.317176441	2.2245578885
N	1.1423721399	1.8206275467	3.4706574826
N	1.625719076	1.367422258	1.2573087506
N	-0.539147813	0.8681091885	2.151564709
H	0.7709544445	1.3030324878	4.257354388
C	2.5076871121	2.287842126	3.6580706627
H	-0.7116903711	0.1369985752	1.4646341004
C	-1.4633595185	0.9069165043	3.266843784
H	-1.2390088914	0.1816780112	4.0701483599
H	-1.482668599	1.9080741646	3.7081494854
H	-2.468393588	0.6809579421	2.8971899404
H	2.5933918528	2.7105879483	4.6641182706
H	3.2582895237	1.4951906173	3.5295118669
H	2.7240406573	3.0639357322	2.9218344545
C	1.226808091	1.0815824886	-0.106696202
C	1.9175985699	-0.1854880946	-0.6428471512
H	1.5638903459	1.9175615569	-0.7380617118
H	0.1378019601	1.0092322274	-0.2551607607
H	2.9929078385	-0.0807473208	-0.4571215661
H	1.7812702718	-0.2492426012	-1.7314128775
C	1.4519529961	-1.5074386153	0.0147074548
H	2.188944408	-2.2907828755	-0.1974921849
C	0.0992706865	-1.9778242489	-0.4619216708
H	1.4287137908	-1.368868574	1.100983245
C	-0.0094092103	-2.9148691171	-1.4988399149
C	-1.277354715	-3.3086105351	-1.9399663817
C	-2.4112254959	-2.751703168	-1.3313666724
C	-2.2055759589	-1.8291737187	-0.3117099398
N	-0.995484341	-1.4496212355	0.1189766323
H	0.881818464	-3.3335297399	-1.9542129379
C	-1.4143077802	-4.2712558063	-2.9963135744
H	-3.4107856192	-3.0324718389	-1.6435193961
H	-3.055980618	-1.3714109292	0.1890717134
N	-1.5267028297	-5.0507313971	-3.8515102468

DMG:14H⁺

C	0.8235993052	1.186241481	2.324890467
N	1.1767229633	1.7740602081	3.4863313913
N	1.6616468432	1.2692403169	1.2741755353
N	-0.3516570236	0.5601751464	2.2249603635
H	0.6581193214	1.5069063292	4.3102414564
C	2.3495701125	2.6244026889	3.6782016859
H	-0.51995861	-0.084411939	1.4286550251
C	-1.3656384655	0.5830169326	3.2753440636

H	-1.0709559481	-0.0066527317	4.1535345885
H	-1.5885415827	1.6101777939	3.5814829493
H	-2.2773495238	0.142198522	2.8706107798
H	2.2589980451	3.1136148068	4.6487361133
H	3.2847130957	2.0503219211	3.6715234556
H	2.3864743345	3.4024950234	2.9098229648
C	1.3597447313	0.9824046788	-0.1380513977
C	2.0207482791	-0.3024142713	-0.656939979
H	1.7220204687	1.8365361658	-0.7199463065
H	0.2752469405	0.955005583	-0.2570699541
H	3.1001576893	-0.2452688983	-0.4677045562
H	1.902067397	-0.3184402155	-1.7472608277
C	1.487250381	-1.6242926123	-0.0582449099
H	2.1675703034	-2.4306324976	-0.3493620452
C	0.0862122419	-1.9744000715	-0.5077612396
H	1.515811546	-1.5748121858	1.0372336037
C	-0.1358875003	-2.9270945372	-1.5053099271
C	-1.448373151	-3.2026330334	-1.9103120266
C	-2.504705615	-2.5106385108	-1.3022900687
C	-2.1902737544	-1.5791713497	-0.3199849938
N	-0.9351548716	-1.3130286923	0.0747648029
H	0.6966384982	-3.4530247294	-1.9600524097
C	-1.702445751	-4.1786963976	-2.9305118701
H	-3.5339914876	-2.6963018188	-1.586847761
H	-2.9807337117	-1.0204454358	0.1746577996
H	2.5969191841	1.597951525	1.4707800851
N	-1.9050426848	-4.9689021949	-3.7580788577

DMG:15

C	0.7643293665	1.3351339075	2.1897404539
N	1.1373791546	1.8889957257	3.4161822763
N	1.598822176	1.3885767901	1.2072660499
N	-0.5307494985	0.8379948087	2.1537252641
H	0.8039527999	1.3731768295	4.2211286358
C	2.4920304518	2.3991213323	3.5631067083
H	-0.6937155413	0.0816834459	1.4875803436
C	-1.4298391023	0.8674279461	3.2886594781
H	-1.1562839884	0.1748710045	4.1060975329
H	-1.4856977514	1.8780994139	3.7053426222
H	-2.4311097079	0.5853943768	2.9483610713
H	2.5862491747	2.8498293811	4.5564901608
H	3.263309107	1.6257735143	3.4378205199
H	2.6707473507	3.161973839	2.8032445022
C	1.1875878817	1.0370323954	-0.1386996941
C	1.8922549698	-0.2394399363	-0.6344239374
H	1.5009375119	1.8529887129	-0.8076981665
H	0.0983903861	0.9386616571	-0.2660594041
H	2.968457574	-0.1078612657	-0.4689710945
H	1.7412034377	-0.344584382	-1.7178780484
C	1.458002303	-1.545707167	0.0714983241
H	2.2021333638	-2.3239809121	-0.135246295
C	0.0998843116	-2.0512255619	-0.3579408059
H	1.4594410258	-1.376895997	1.154073365
C	-0.0161207914	-3.0215607122	-1.3519848682
C	-1.2841229213	-3.4533696303	-1.7603299003
C	-2.4097313131	-2.8904376597	-1.1468427253
C	-2.190939417	-1.9276150888	-0.1636411108
N	-0.9871659215	-1.507948385	0.235835908
H	0.8633752967	-3.4528308646	-1.8189916795
O	-1.3156470294	-4.3987262165	-2.7304828578

H	-3.4209768577	-3.1771456123	-1.4083822975
H	-3.0446475609	-1.4692659251	0.333195741
C	-2.5831050962	-4.8631805586	-3.1810385052
H	-2.3700533676	-5.6019394124	-3.9550028989
H	-3.1470393993	-5.3386330941	-2.3688370978
H	-3.1784233782	-4.0474766994	-3.6097365703

DMG:15H⁺

C	0.8174537641	1.1976487681	2.2972905938
N	1.1849169511	1.8185398233	3.4395545429
N	1.6255807486	1.2905076781	1.2241346419
N	-0.3390657659	0.5368779588	2.2394103471
H	0.6995221948	1.5485589496	4.2822107844
C	2.3380909122	2.7026997685	3.5829237796
H	-0.5178400798	-0.1326219256	1.4537967835
C	-1.3188278894	0.5462590613	3.3203694544
H	-0.9764258336	-0.013618878	4.2012200501
H	-1.5707286467	1.5705718426	3.6144612169
H	-2.224972192	0.0626559857	2.9535540968
H	2.2608543451	3.2091573425	4.5458692646
H	3.2894318549	2.1556182973	3.5611332546
H	2.3332349155	3.4657988168	2.7986803132
C	1.3048792546	0.9466066951	-0.1709335885
C	1.9861580532	-0.340143307	-0.6577290209
H	1.6348021415	1.7894509185	-0.7876610069
H	0.2197328554	0.8849302315	-0.2666820323
H	3.0679155022	-0.2499885392	-0.4937694926
H	1.8441911504	-0.3971026847	-1.7439297783
C	1.493009422	-1.6514192084	-0.0057464693
H	2.1783909353	-2.4542281722	-0.2949554813
C	0.0844347388	-2.0368210216	-0.4025302638
H	1.5555766752	-1.5694440705	1.0867496264
C	-0.1482180205	-3.0227233953	-1.3513276111
C	-1.4669103097	-3.3381674024	-1.7219181596
C	-2.5142865109	-2.6316768218	-1.1117650115
C	-2.1821532464	-1.6612261433	-0.1740559663
N	-0.9278463266	-1.3562829355	0.1885908031
H	0.6701350214	-3.563932779	-1.8142055681
O	-1.6116684721	-4.3028794625	-2.6420566573
H	-3.5542953162	-2.8202185784	-1.3464109939
H	-2.9737236141	-1.0963372507	0.3137307636
H	2.5580857725	1.64118857	1.3929925898
C	-2.9297149162	-4.6720074638	-3.0622276253
H	-2.7893759741	-5.4607022951	-3.8008843508
H	-3.5166172361	-5.0560007049	-2.220460666
H	-3.4461678588	-3.8230616678	-3.5238241629

DMG:16

C	0.7790270136	1.3161828348	2.2211320281
N	1.1317645715	1.8418487053	3.4671869051
N	1.6385042532	1.3764631363	1.2606501014
N	-0.5205648269	0.8391107902	2.1473193213
H	0.7738715811	1.3136338971	4.2535177301
C	2.491031337	2.3252388936	3.6545759857
H	-0.6871359924	0.1015846885	1.4592558206
C	-1.4477459228	0.870420411	3.2588571829
H	-1.2052185032	0.1655339203	4.0757234556
H	-1.5003660849	1.8772678255	3.685524208
H	-2.4433243711	0.6052479561	2.8896963844

H	2.5712072197	2.7515441523	4.6600158548
H	3.25239608	1.5422589319	3.5276304818
H	2.6990788627	3.1022654564	2.9167534581
C	1.2555753028	1.0567631627	-0.101577603
C	1.9387374609	-0.2304525459	-0.5996368782
H	1.6088677731	1.8748781566	-0.7478692684
H	0.1682483644	0.9890482906	-0.2595105311
H	3.0128032262	-0.1328328296	-0.3989957882
H	1.8186130422	-0.3103557434	-1.6893940231
C	1.4437878005	-1.5364838813	0.0646601993
H	2.1705091672	-2.3327259784	-0.1377699532
C	0.0813920883	-1.9893029655	-0.4122559408
H	1.4201525515	-1.3915808227	1.1504303914
C	-0.0263332487	-2.9225203351	-1.4432083494
C	-1.2929084812	-3.3281223595	-1.91956094
C	-2.4124843181	-2.7296074773	-1.2953453656
C	-2.2006955751	-1.8122880312	-0.2783933249
N	-0.9979761593	-1.4331186243	0.1762604136
H	0.8831816085	-3.3277201715	-1.8700791748
N	-1.430104294	-4.2540392595	-2.9271339023
H	-3.4263969851	-2.9680138494	-1.5914198096
H	-3.0587730067	-1.3481716199	0.2059835339
C	-2.7515240794	-4.5694592239	-3.4460236544
C	-0.2514889375	-4.7614634619	-3.6117920003
H	-2.6604786314	-5.3407995939	-4.2124199816
H	-3.4064999737	-4.9583372154	-2.6562065318
H	-3.2427417152	-3.6944887714	-3.8967828824
H	0.3135966379	-3.9629912135	-4.1143883487
H	0.4262383071	-5.2708262754	-2.9150163304
H	-0.5604451429	-5.4865329592	-4.366432874

DMG:16H⁺

C	0.8169071367	1.191264748	2.3000648282
N	1.1670901733	1.7765749059	3.4675381158
N	1.6461562482	1.3131961128	1.2453324802
N	-0.3399289245	0.5389312747	2.2009976434
H	0.663573835	1.4846407599	4.2918976708
C	2.3245443079	2.6446452165	3.659773015
H	-0.5140837743	-0.1066408269	1.386163905
C	-1.336967178	0.5192445188	3.265166418
H	-1.0071157348	-0.0597317004	4.138685787
H	-1.5996450078	1.5348989526	3.5799510864
H	-2.2338309805	0.0391008007	2.8717927445
H	2.2339303027	3.1216510652	4.6365510122
H	3.2718625491	2.090293891	3.6381863288
H	2.3413584863	3.4320461507	2.8999841597
C	1.3532052427	1.0038463119	-0.1637535929
C	2.0299524701	-0.2794830332	-0.6659075929
H	1.7060866763	1.8569393566	-0.7532136845
H	0.2701485979	0.9548139193	-0.2849473887
H	3.1089859064	-0.2069672521	-0.4758578956
H	1.9107930777	-0.3077517831	-1.7561127764
C	1.5045862602	-1.6002331001	-0.0601894755
H	2.182535183	-2.4053750608	-0.3609639692
C	0.0941428643	-1.9484142843	-0.4885041253
H	1.5518817844	-1.5498351512	1.0351375309
C	-0.132510411	-2.9087015341	-1.4647296189
C	-1.4529661294	-3.2103573796	-1.888985145
C	-2.4882108156	-2.4719693683	-1.2586469704
C	-2.1612607695	-1.5359898149	-0.2973690888

N	-0.9066357392	-1.2579087325	0.1045202553
H	0.7167445261	-3.4262022764	-1.8929152909
N	-1.7102239754	-4.1494738585	-2.8407020577
H	-3.5291849629	-2.6253780664	-1.511175488
H	-2.9541589517	-0.9685138203	0.1856627874
H	2.5778828711	1.6503866695	1.4426359354
C	-3.0856145561	-4.4237630198	-3.2474649861
C	-0.6141491901	-4.885383313	-3.4630378512
H	-0.0407553126	-5.4556057839	-2.7213214462
H	-1.0232265036	-5.5898319038	-4.1870314749
H	0.0725080098	-4.2133136741	-3.9935496642
H	-3.0832267542	-5.2012874709	-4.0111703873
H	-3.6910326318	-4.7781736605	-2.4039087841
H	-3.5648262062	-3.532374785	-3.6714809493

DMG:17

C	0.7835100123	1.289889074	2.3448876139
N	1.1279197617	1.6909089172	3.6390010887
N	1.6413918306	1.4636946761	1.3969993217
N	-0.5076562707	0.8006871689	2.2210846577
H	0.7824341243	1.0767116341	4.3662433853
C	2.4781945801	2.1779973988	3.8754938796
H	-0.6622546561	0.1340729722	1.4610732765
C	-1.433070808	0.700566177	3.3300249825
H	-1.174592496	-0.0780540192	4.0716783645
H	-1.5055640878	1.6577913676	3.8564419495
H	-2.4236260745	0.4534228274	2.9357129981
H	2.5527653514	2.4972139553	4.9203264649
H	3.2541953335	1.4278472916	3.6659533672
H	2.6693865587	3.0326318485	3.2239183654
C	1.2637512983	1.2806151328	0.0084040394
C	1.9667050255	0.0628957036	-0.6199085393
H	1.6043599516	2.1667878967	-0.5488638201
H	0.1775682371	1.2128364036	-0.1574472639
H	3.0388402391	0.154186918	-0.4060538712
H	1.8504200885	0.0973202175	-1.7124798484
C	1.4893590324	-1.3132203059	-0.1000120274
H	2.2261040831	-2.0734253647	-0.3871689009
C	0.1320748589	-1.7301975699	-0.6221757984
H	1.4652456977	-1.2865145839	0.9950841288
C	0.0326576605	-2.5425371898	-1.7508752474
C	-1.2319903426	-2.9044759825	-2.2659498032
C	-2.3581599805	-2.404745368	-1.5709687085
C	-2.1537841583	-1.6043138119	-0.4588699496
N	-0.9529811569	-1.2592275864	0.028718992
H	0.9420874627	-2.8829398855	-2.233453708
N	-1.3618108427	-3.6964808519	-3.3727404075
H	-3.3679669506	-2.6447257693	-1.8825070146
H	-3.0149141708	-1.2151577141	0.0828905855
C	-0.2294532428	-4.2924697991	-4.0841307563
C	-0.8923653741	-5.2727083407	-5.0630182775
C	-2.25001673	-4.6143903196	-5.3568891635
C	-2.6466380857	-4.0018705284	-4.0055286257
H	0.3531941648	-3.5232226016	-4.6150079122
H	0.4500340946	-4.7973748461	-3.3869915737
H	-1.0407837823	-6.2433272618	-4.5750641871
H	-0.2887586902	-5.4375965278	-5.960176933
H	-2.9994993534	-5.317326361	-5.7318647909
H	-2.1302658227	-3.8209714145	-6.104037865
H	-3.2292573974	-4.7104225127	-3.3960082437

H -3.2510919731 -3.0943360645 -4.1234002241

DMG:17

C	0.8206743605	1.134192433	2.4115172485
N	1.1436347158	1.598190383	3.6401038562
N	1.6749231056	1.3602640657	1.394488217
N	-0.3334592817	0.4983717294	2.2202784809
H	0.6214095659	1.2251447046	4.4187965011
C	2.2958925934	2.4400124021	3.945730775
H	-0.4898492855	-0.0630032551	1.3400205103
C	-1.3539858137	0.3736059638	3.2545219879
H	-1.042972241	-0.2898297569	4.0732614927
H	-1.6252345904	1.352939995	3.6632880092
H	-2.2410497632	-0.0644144972	2.795273246
H	2.1819294394	2.8171447913	4.9629157236
H	3.2437656251	1.8887935384	3.8913191177
H	2.3306838517	3.2994065671	3.2691212982
C	1.4169676819	1.1941099855	-0.045205296
C	2.1042613121	-0.0352516932	-0.656195198
H	1.7856903705	2.1005421679	-0.5373921504
H	0.3373152354	1.1614105807	-0.1975343426
H	3.1783016775	0.0132755045	-0.43274926
H	2.0128688807	0.0464306446	-1.7464137811
C	1.5607701606	-1.4076222268	-0.1999867054
H	2.2428713776	-2.1817558158	-0.5657835555
C	0.1596495921	-1.70269596	-0.6937424393
H	1.582873039	-1.4691150656	0.895563759
C	-0.0472077866	-2.5515048949	-1.7712496155
C	-1.3594397126	-2.7954984005	-2.2550044913
C	-2.4082170797	-2.1250011677	-1.5725055281
C	-2.1001802631	-1.2992038289	-0.5102553746
N	-0.85295139	-1.0724442387	-0.0535893319
H	0.8073250697	-3.021533696	-2.2435475988
N	-1.5959923102	-3.6180836182	-3.3041786041
H	-3.443395714	-2.2591692908	-1.8607686902
H	-2.9014954297	-0.7839715649	0.0157000956
H	2.6024020552	1.6710859043	1.6471808684
C	-0.5516892584	-4.3926426605	-3.9917196474
C	-1.3434565848	-5.3500134514	-4.8940395035
C	-2.6257622976	-4.5637827449	-5.2098607002
C	-2.9266034778	-3.8309591244	-3.895114912
H	0.0981560497	-3.7268478437	-4.5783592412
H	0.0766112684	-4.9245263447	-3.268393022
H	-1.5855431562	-6.26630668	-4.3438037582
H	-0.781709363	-5.6343216921	-5.7875294146
H	-3.45492196	-5.2017977621	-5.5262109279
H	-2.4384003528	-3.8360673701	-6.0076318853
H	-3.5525920213	-4.4387236436	-3.2259240228
H	-3.4362128943	-2.8747740721	-4.0573921899

DMG:18

C	-0.7661306886	-0.0591099069	1.8428474504
N	-0.4885505783	0.2505526639	3.172609015
N	0.178188793	-0.0484402446	0.9708625762
N	-2.1073823896	-0.3581064951	1.600189099
H	-1.04054722	-0.2802487395	3.8356285483
C	0.906900301	0.4060456015	3.5610538926
H	-2.3215925781	-0.4003047012	0.6141117089
C	-3.1868118635	0.1832963884	2.4196995721

H	-3.2422415049	-0.320213879	3.3924199902
H	-3.0924980937	1.262685859	2.6001770828
H	-4.1343897521	-0.0082063384	1.9087888785
H	0.9412911153	0.6850541051	4.6185193963
H	1.5032663726	-0.5029938575	3.4007437317
H	1.3570415748	1.2019939431	2.9651107234
C	-0.149886927	-0.2406043838	-0.4291589845
C	1.0764702477	0.0230057871	-1.308180698
H	-0.5045984946	-1.2707238466	-0.6205661427
H	-0.9684973616	0.4295465809	-0.7631694688
H	1.4261438179	1.0453862204	-1.1161024966
H	1.8837317328	-0.6438804466	-0.9803367379
C	0.8004338932	-0.1717282062	-2.8012655413
H	0.4686510159	-1.1955303859	-3.0166462734
H	1.6984124974	0.0172446024	-3.4001859226
H	0.0168960906	0.5099406794	-3.1563323997

DMG:18H⁺

C	-0.8539275968	0.0962786738	1.866462285
N	-0.6902920512	0.8034241596	2.9972346616
N	0.0653726784	0.1595428597	0.8934872088
N	-1.9627968134	-0.6424074384	1.6955130186
H	-1.2945294656	0.5809016092	3.7750840353
C	0.3985052732	1.7512968445	3.234689548
H	-1.9658195445	-1.2977007527	0.9272921048
C	-3.0977940551	-0.669704578	2.6180577509
H	-2.856939486	-1.1944512003	3.5505697163
H	-3.4342064578	0.3479931065	2.8378221942
H	-3.9171479036	-1.1993743086	2.1313131756
H	0.1689360289	2.3108246628	4.1419025904
H	1.3606665302	1.2446521116	3.3775392436
H	0.4702629283	2.4620377966	2.405987214
C	-0.0675905974	-0.4370258544	-0.4469114543
C	1.0526276301	0.0574494964	-1.3653213774
H	-0.0317945104	-1.5332043309	-0.3726174398
H	-1.0433289093	-0.150373946	-0.8570806951
H	1.0069405748	1.1520488861	-1.4250179958
H	2.0226428301	-0.2042695206	-0.9208406656
C	0.9488521593	-0.5495566661	-2.7678595812
H	1.0209070383	-1.6424720431	-2.7383358815
H	1.7597256176	-0.1804708645	-3.4018633853
H	0.0019818724	-0.2823346348	-3.2500647436
H	0.9605212295	0.5702419315	1.1223014727

S8. Cartesian coordinated for the „open chain“ DMG series of bases and their conjugated acids.

DMG:1_oc

C	-1.0769840916	0.0282108885	2.11717851
N	-0.8436116334	0.3620077378	3.4491979178
N	-0.1043971886	0.0297287514	1.2762734567
N	-2.4075034369	-0.2820563975	1.8353998119
H	-1.414858985	-0.157974043	4.1043130682
C	0.5375813399	0.5329804154	3.8798589642
H	-2.5914834128	-0.3356332377	0.8439619651
C	-3.5167669616	0.2523415501	2.6184781212
H	-3.5965847304	-0.2469006369	3.5917446649
H	-3.4388025958	1.3335545617	2.7955602707
H	-4.4463056773	0.0482088107	2.0801575884
H	0.5357102961	0.8344643075	4.9316776139
H	1.1430524262	-0.3761448634	3.7589708574
H	1.003318865	1.3184922556	3.2821621974
C	-0.386609866	-0.1898666018	-0.12992002
C	0.8787006533	0.0398036403	-0.9636037318
H	-0.7492067803	-1.2192482958	-0.3100504837
H	-1.1829512136	0.4840080052	-0.5060516936
H	1.2163966584	1.0740660892	-0.8285054556
H	1.6649310236	-0.6062484589	-0.5569782411
C	0.6545380544	-0.2280113138	-2.454242821
H	0.3721895334	-1.2927565196	-2.6043798194
N	1.7901049209	0.1444242688	-3.3007639269
H	-0.2048285897	0.3674714718	-2.7912574785
C	1.419195619	0.1368487802	-4.7086999216
C	2.9612833184	-0.6917953121	-3.0744020141
H	2.2649027056	0.4806919243	-5.3149443372
H	1.1206777773	-0.8647144078	-5.0807514601
H	0.5809030222	0.8223329203	-4.8760220918
H	3.7800475264	-0.3522710945	-3.7182820714
H	3.2970206605	-0.6090750987	-2.0373951554
H	2.778094462	-1.7641264936	-3.2925632758

DMG:1_ocH⁺

C	-1.048600989	-0.0769270918	2.1984732003
N	-0.8687711634	0.5443662274	3.376272592
N	-0.118807842	0.0186477029	1.2383780601
N	-2.1833574724	-0.7588913085	1.9701034749
H	-1.4891990383	0.293545802	4.1324007551
C	0.255556614	1.4275198503	3.6862900125
H	-2.2046070732	-1.3594090596	1.1586805012
C	-3.3273424799	-0.8035847434	2.8806467099
H	-3.1178508337	-1.4029754624	3.7750482789
H	-3.6226914744	0.2092763148	3.1706598321
H	-4.1636096819	-1.2618714688	2.3519961462
H	0.0408555901	1.9314284795	4.6290295041
H	1.1948399243	0.8725439402	3.7988892929
H	0.3641089386	2.1904147041	2.9096002143
C	-0.2563972723	-0.4867407834	-0.1383167401

C	0.8758717719	0.0547641141	-1.0127255208
H	-0.2375448866	-1.5858786783	-0.1344386403
H	-1.2271199485	-0.1594738247	-0.5293724257
H	0.8387921375	1.1499950987	-0.997629708
H	1.8467856344	-0.2502495231	-0.6018283874
C	0.7819692494	-0.471188595	-2.4539295409
H	0.7840555293	-1.5677537999	-2.4213969888
N	1.9163521927	-0.0510578171	-3.2647444911
H	-0.1900862755	-0.1692300213	-2.8975501171
H	0.7919261546	0.3696550728	1.5026867362
C	2.0740340566	-0.8976040261	-4.4463802911
C	1.8513152155	1.3581194505	-3.6434426114
H	2.9744687763	-0.5953929036	-4.9895207474
H	2.1980448283	-1.9420403972	-4.1419314899
H	1.2178438372	-0.8372962287	-5.1442130937
H	2.7454631399	1.6188646167	-4.2170934057
H	0.9644537534	1.5985742905	-4.2610018593
H	1.834723967	1.9996703646	-2.7567731592

DMG:2_oc

C	-0.7674322292	-0.0533201709	1.8357141633
N	-0.4870913542	0.2525654449	3.1648576642
N	0.1765160507	-0.0394598448	0.9624885459
N	-2.1082913111	-0.3516653448	1.5931946589
H	-1.0401322576	-0.2756992523	3.828859906
C	0.9089566853	0.4074728296	3.5521411628
H	-2.3265818344	-0.3858924847	0.6078481647
C	-3.1872018322	0.1734142155	2.4237997003
H	-3.2392480446	-0.3464703437	3.3881194752
H	-3.0945124975	1.2498186251	2.6215415217
H	-4.1354611485	-0.0118242933	1.9119722817
H	0.9440767429	0.6878424501	4.6091566648
H	1.504083837	-0.5024374198	3.3927800013
H	1.3592331902	1.2021320462	2.9547301095
C	-0.1557785255	-0.2305199635	-0.4365673826
C	1.0782394557	0.0208579649	-1.3083224161
H	-0.5223549351	-1.2570567839	-0.6245304235
H	-0.9677252343	0.4483444731	-0.7686763867
H	1.437568648	1.0422788622	-1.1378746497
H	1.8819437306	-0.6544887162	-0.9938154995
C	0.8070701781	-0.1767208268	-2.7932295117
H	0.453461529	-1.2054825172	-2.9901997038
O	2.0025578389	0.0722055187	-3.5114025185
H	0.0089070269	0.5063406946	-3.1378768322
C	1.8478354606	-0.0920706869	-4.9019634573
H	2.8159257215	0.1204696196	-5.3641237079
H	1.5465642799	-1.1204461256	-5.1633565029
H	1.0957196804	0.6001650586	-5.3165539069

DMG:2_och⁺

C	-0.856241068	0.091009926	1.8631173427
N	-0.6874232457	0.8026029132	2.9899062603
N	0.0597570429	0.1499062519	0.8865829011
N	-1.9662922264	-0.6475356891	1.6990549679
H	-1.2887126596	0.5837472103	3.7710979611
C	0.4016660138	1.7527932978	3.2183642369

H	-1.9716080424	-1.3078922063	0.9352556356
C	-3.0974036709	-0.6709011831	2.626555959
H	-2.8524038283	-1.1911389664	3.5605237881
H	-3.4332935421	0.3477055264	2.8429701783
H	-3.918611615	-1.2031322929	2.145768433
H	0.174458877	2.3172530966	4.1230986725
H	1.3645391055	1.2475307978	3.3608939904
H	0.4700903609	2.458660889	2.3852829232
C	-0.080951168	-0.4448905393	-0.4529176734
C	1.0450209566	0.0505565867	-1.3599476056
H	-0.0523490058	-1.5413129478	-0.3784352051
H	-1.0563408443	-0.1517208516	-0.8595306456
H	1.0100610411	1.1435924089	-1.434119379
H	2.0182690685	-0.2224178385	-0.93236542
C	0.9642281887	-0.5364277562	-2.7691949253
H	1.0037416879	-1.6399310577	-2.7300843803
O	2.0537987	-0.0168978844	-3.4873059722
H	0.0062633187	-0.2619163444	-3.2461166621
H	0.9562994143	0.5608215342	1.1095554388
C	2.1064130872	-0.4731590036	-4.8303586181
H	2.9840333824	-0.0108356959	-5.2860212113
H	2.2080414625	-1.5676588494	-4.8798952995
H	1.2084471879	-0.1748736387	-5.3919522418

DMG:3_oc

C	-0.7927234001	-0.051224372	1.903169959
N	-0.5443063765	0.2470759492	3.2397484006
N	0.172052328	-0.0320872011	1.0525926433
N	-2.1266211742	-0.348385311	1.6259426073
H	-1.1148775863	-0.2814993396	3.8883599093
C	0.8416809224	0.4007360851	3.6621274791
H	-2.3218231285	-0.3764204662	0.6356100727
C	-3.226442463	0.1643191453	2.4364778644
H	-3.3003493657	-0.3672063	3.3930250139
H	-3.1409734649	1.238487264	2.6488368122
H	-4.1616425847	-0.016895617	1.8998826324
H	0.8505155381	0.6747394556	4.7212916563
H	1.4410441623	-0.5078920743	3.5119820995
H	1.305825644	1.199435262	3.0809115674
C	-0.1249284969	-0.2139598358	-0.3543866861
C	1.1359250028	0.0384824703	-1.1908157602
H	-0.4880807989	-1.2379043381	-0.5614753256
H	-0.9229367727	0.4708741835	-0.7067372458
H	1.491115859	1.0561203039	-0.9902278378
H	1.9226068524	-0.6436711778	-0.8482685089
C	0.8912242019	-0.1486560171	-2.689351488
H	0.547179333	-1.1696759068	-2.8982789262
S	2.4349128697	0.1587167512	-3.6364152571
H	0.1177017258	0.544979301	-3.0429967485
C	1.8176574282	-0.1373408999	-5.3302384283
H	2.6591381555	0.0156051305	-6.0112443967
H	1.4527746852	-1.1628492043	-5.4479134699
H	1.0211997555	0.5664497881	-5.5928975172

DMG:3_och⁺

C	-0.8816678447	0.0921563567	1.9298889552
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N	-0.7434069728	0.796759725	3.0650473121
N	0.061853895	0.154839082	0.9798777628
N	-1.9880910202	-0.6430843226	1.7301071775
H	-1.3664575344	0.5740834095	3.8279369344
C	0.3385260138	1.7461093904	3.328666842
H	-1.9714549776	-1.3021391048	0.9653091709
C	-3.1464035169	-0.6670795332	2.6235036289
H	-2.9308508874	-1.1920380418	3.5620879717
H	-3.4856272676	0.3515905454	2.8342787188
H	-3.9544451527	-1.1948147169	2.116170595
H	0.0859521983	2.3058917327	4.229570602
H	1.2971878836	1.2403280889	3.4955747227
H	0.4298751113	2.4560930556	2.5013187728
C	-0.0438518968	-0.4245034065	-0.370010522
C	1.0903128146	0.1042753592	-1.2525586209
H	0.0032464041	-1.5209582965	-0.311500159
H	-1.0153500986	-0.1410002553	-0.7916655235
H	1.0306766262	1.1983961491	-1.2983016388
H	2.0557493683	-0.155047114	-0.7978622845
C	1.0319095155	-0.4726544858	-2.6706660103
H	1.1126987745	-1.5661330905	-2.6425978163
S	2.4188797371	0.2206882491	-3.6507658978
H	0.0796107455	-0.2133020321	-3.1491311538
H	0.9534029652	0.5595998445	1.2326860397
C	2.1087918684	-0.6012236344	-5.2519813398
H	2.8915433001	-0.2580876444	-5.9327845877
H	2.1749510173	-1.689054926	-5.1599224345
H	1.1359369103	-0.3161526897	-5.6624937679

DMG:4_oc

C	-1.4857770847	-0.1394408719	2.6533338609
N	-1.2321656941	0.1459578248	3.9912858393
N	-0.5132297177	-0.1833514656	1.8127877595
N	-2.8335984789	-0.3541475673	2.3660462557
H	-1.8405302021	-0.3435403283	4.6361091586
C	0.1552937747	0.2233803418	4.4281302604
H	-3.019730993	-0.3836693123	1.373970842
C	-3.9041405632	0.2497645843	3.1537925808
H	-4.0267665214	-0.2581417395	4.1180043486
H	-3.744873592	1.3186643208	3.3487566795
H	-4.8433126187	0.1257416893	2.6079168826
H	0.1683198678	0.5030373989	5.4857643611
H	0.7037049752	-0.7189444415	4.2904854442
H	0.6703981717	0.990835578	3.8477595995
C	-0.7969358319	-0.3410046493	0.401455247
C	0.4687778523	-0.0638816346	-0.4193125269
H	-1.1515141876	-1.3641797393	0.1755827456
H	-1.5939330253	0.3436135965	0.0464622761
H	0.7919932008	0.966463114	-0.2340051434
H	1.2663273015	-0.7160907888	-0.0433978755
C	0.2595967679	-0.281328188	-1.9248184193
H	0.0206924227	-1.3323246425	-2.1415078027
P	1.697974975	0.2348046224	-2.9527089996
H	-0.5912244512	0.3178389527	-2.2781181844
C	1.2228853722	-0.2559364208	-4.6576161355
C	3.0504625091	-0.9282912837	-2.5165812828
H	3.9056025634	-0.7419580816	-3.1738303178

H	3.3678686181	-0.7480835028	-1.4854574887
H	2.7423937499	-1.9747079042	-2.6183333787
H	2.0544417946	-0.0455865042	-5.337547312
H	0.9662683085	-1.3187806744	-4.7246825131
H	0.3625766754	0.340258157	-4.9776439871
O	2.0692067217	1.6848378382	-2.8158492286

DMG:4_ocH⁺

C	-1.5778277516	-0.0008423957	2.6443156534
N	-1.5305990899	0.8283085359	3.7003331196
N	-0.5984908354	0.013641453	1.731214278
N	-2.6286697771	-0.8236515856	2.4871657405
H	-2.1770349397	0.6546448387	4.4562074153
C	-0.5143409873	1.8619524399	3.9014069958
H	-2.5466978936	-1.5462869512	1.786834053
C	-3.8124259554	-0.8381992599	3.3460765594
H	-3.595694377	-1.2532661687	4.3379259821
H	-4.2239956121	0.1708641338	3.4452568878
H	-4.5673722997	-1.4657034134	2.8716592533
H	-0.8279015814	2.4862382173	4.7384405387
H	0.4657283884	1.4323369605	4.1409779217
H	-0.4366391923	2.4982642962	3.0145165121
C	-0.6270989038	-0.6757846509	0.4286782737
C	0.5491547152	-0.1979354144	-0.4255462211
H	-0.574483386	-1.7626150518	0.5823695156
H	-1.5761152865	-0.4414383675	-0.0689511964
H	0.5235676557	0.8950253416	-0.5079109507
H	1.4883177676	-0.4620365391	0.0795459734
C	0.5363678072	-0.7830806586	-1.844374148
H	0.7253658462	-1.8636545068	-1.8465461861
P	1.7739552303	0.1180998055	-2.9042272239
H	-0.4465770649	-0.6205787608	-2.3056228887
H	0.2275184084	0.5586630419	1.9380042377
C	1.2825784391	-0.2811511303	-4.6182513609
O	1.7975128489	1.5809256548	-2.5605957262
C	3.3640350234	-0.7550868823	-2.6515529906
H	4.1272511578	-0.2833795683	-3.2783281429
H	3.6824449307	-0.6613242963	-1.6087072165
H	3.2957403874	-1.8160839825	-2.9142897988
H	2.0241303227	0.1302784287	-5.3100511029
H	1.2072422457	-1.3617866117	-4.7815612472
H	0.3174368731	0.1856155289	-4.83710393

DMG:5_oc

C	-0.7896787426	-0.0560906797	1.8881424123
N	-0.5419935629	0.2491773931	3.2223168158
N	0.1819552928	-0.0717516399	1.0448538692
N	-2.1287413963	-0.3206387148	1.6042603618
H	-1.1315202742	-0.253844739	3.8740686265
C	0.8441200861	0.3764464342	3.6529855415
H	-2.3184014777	-0.3543385144	0.6130277939
C	-3.2202134934	0.2295815064	2.4018567384
H	-3.3158503111	-0.2914980285	3.3622009598
H	-3.1060476082	1.3027020562	2.6051397464
H	-4.155926706	0.0695371368	1.8595230654
H	0.8516218048	0.6603313837	4.7094758605

H	1.4236320112	-0.5469529225	3.5158272141
H	1.3299559825	1.1590623224	3.0676382262
C	-0.1045827988	-0.2567213493	-0.3624429613
C	1.1641679306	-0.0011669278	-1.1860441339
H	-0.4640204249	-1.2822024139	-0.5700127478
H	-0.8989132134	0.4254533342	-0.7273807074
H	1.4974944264	1.0288011063	-1.0186184415
H	1.9587090719	-0.6586974871	-0.8125871852
C	0.9488160164	-0.226340294	-2.6812224444
H	0.7113345109	-1.2735551151	-2.9096334613
S	2.4813114733	0.2010911793	-3.6220826468
H	0.1466179594	0.4131295357	-3.0709562615
C	1.773851353	-0.1036063592	-5.2909994961
H	2.5486086382	0.1515306697	-6.01813556
H	1.5007355225	-1.1583620971	-5.394856271
H	0.9036846876	0.5420664502	-5.4425262328
O	2.6941282417	1.694001774	-3.4877826811

DMG:5_ocH⁺

C	-0.873939969	0.0878567218	1.8965555349
N	-0.7777055268	0.8857954175	2.9725284183
N	0.1111073181	0.0606466283	0.9886154881
N	-1.9780316161	-0.6553614208	1.7118673263
H	-1.434165128	0.7315251808	3.7241868333
C	0.3001136578	1.8492933323	3.2010957828
H	-1.9352812678	-1.377471721	1.0074100082
C	-3.1723483412	-0.597379132	2.5550279267
H	-3.0028682074	-1.0489619533	3.5401197538
H	-3.5054181528	0.4383095573	2.6711079423
H	-3.966270786	-1.1544075508	2.0567731298
H	0.0161410524	2.4811792709	4.0430080541
H	1.2474420767	1.3544696437	3.4467147414
H	0.4294576112	2.4902650035	2.3238737554
C	0.0483112529	-0.5990591933	-0.3271999479
C	1.2280445282	-0.1349717708	-1.183588079
H	0.0692766157	-1.6903051816	-0.1995117509
H	-0.8981873826	-0.3241374514	-0.8076610551
H	1.2120257421	0.958654669	-1.2670683068
H	2.1694388132	-0.4179953039	-0.6925017689
C	1.1925599393	-0.7074797715	-2.5997757913
H	1.4026590582	-1.7822158616	-2.6333911255
S	2.5062877285	0.1774610221	-3.5889109968
H	0.2262064618	-0.5099271981	-3.0780034106
H	0.9835071563	0.5104477134	1.2310939234
C	1.8764231622	-0.3184890028	-5.2365850626
H	2.5442817727	0.1236848731	-5.9795603455
H	1.897430618	-1.4091988225	-5.3247877182
H	0.8638886225	0.0711487601	-5.3751806174
O	2.227247327	1.6518885416	-3.3968146423

DMG:6_oc

C	-0.7903379131	-0.0483727383	1.9009050019
N	-0.5325285577	0.257711301	3.2319156866
N	0.170779327	-0.036020531	1.0448608107
N	-2.1252363649	-0.3445654352	1.6322782699
H	-1.1052992015	-0.2557100248	3.8903079424

C	0.8554438063	0.4144901902	3.6475324739
H	-2.3294976301	-0.3792128123	0.6442591762
C	-3.2209525143	0.1605371137	2.4532058143
H	-3.2911205334	-0.3812558296	3.4043351758
H	-3.1321374773	1.2321694709	2.6757279039
H	-4.158767687	-0.013648506	1.9190614584
H	0.868109467	0.69647824	4.7043898132
H	1.4529674633	-0.4958500143	3.5021016953
H	1.3176539249	1.2086495566	3.0587153171
C	-0.1278402408	-0.2235683252	-0.3579366528
C	1.13567037	0.0446049034	-1.1865600685
H	-0.4777109636	-1.2522763826	-0.5657203024
H	-0.9325779476	0.45150878	-0.7150007528
H	1.4775665483	1.0673366643	-0.9982394796
H	1.9309507873	-0.628903186	-0.852111819
C	0.8895535743	-0.1495872485	-2.6839272882
H	0.5896881817	-1.1773659554	-2.9176281267
S	2.4066545823	0.1777846202	-3.6375094424
H	0.128144526	0.5404377175	-3.0646727112
C	1.8923010904	-0.1058164024	-5.3517039044
H	2.7771010388	0.0787753131	-5.9655561271
H	1.5644652104	-1.1407455138	-5.4700940768
H	1.0992586367	0.5960951671	-5.6179614642
O	2.7367957647	1.6065515316	-3.5041525411
O	3.3998917318	-0.8541736642	-3.2963197825

DMG:6_ocH⁺

C	-0.8814484192	0.0712167214	1.9417768706
N	-0.7163590803	0.8034130367	3.054752273
N	0.0556091543	0.0896409942	0.9824487354
N	-2.005774394	-0.6441579959	1.7711574054
H	-1.3284001884	0.6070808979	3.8338512318
C	0.3791164556	1.7494546651	3.275505394
H	-2.001516337	-1.3430367118	1.0422021437
C	-3.1608227062	-0.6080826263	2.6693496169
H	-2.9623854077	-1.1250181697	3.616073973
H	-3.4560901708	0.4271453615	2.86338294
H	-3.991875791	-1.1102412563	2.1732456649
H	0.1390739536	2.3457124657	4.1562160817
H	1.3327320795	1.2386675333	3.4551182584
H	0.4727535496	2.4259214695	2.4209959011
C	-0.0757224358	-0.4976541697	-0.3606339511
C	1.0171711434	0.0743506659	-1.2661125636
H	0.0074481513	-1.592010792	-0.3035998834
H	-1.0684109553	-0.244829463	-0.7508595596
H	0.9092121748	1.1626736723	-1.3294091262
H	2.0035778551	-0.1383760436	-0.8350249675
C	0.9762506553	-0.511565999	-2.67969935
H	1.1341096741	-1.5947469786	-2.6816371793
S	2.3505381548	0.2525137367	-3.6260862164
H	0.0427664401	-0.2731864922	-3.1990410339
H	0.9621019508	0.4675589667	1.2247598075
C	2.2418318868	-0.5093068129	-5.2577269912
H	3.0520763853	-0.0703529216	-5.84551743
H	2.3874977749	-1.5877374814	-5.1685547788
H	1.2785405069	-0.2665704522	-5.7109698556
O	2.031904301	1.6823087513	-3.7512113256

O 3.5967576384 -0.1884375721 -2.9817490853

DMG:7_oc

C -1.0109170784 -0.0966146574 2.0629275518
N -0.7475616013 0.2047566788 3.3963777917
N -0.0571352509 -0.0752871093 1.200879575
N -2.3477470622 -0.3994796907 1.8028407991
H -1.3066480494 -0.3275821292 4.0519941367
C 0.643441194 0.3634602591 3.800454532
H -2.5534166345 -0.4288454261 0.81458201
C -3.4386609837 0.1178333773 2.6226171114
H -3.5007015854 -0.4071538715 3.5835647605
H -3.3521674782 1.1935278167 2.8269490268
H -4.3799633449 -0.0681419089 2.0983005903
H 0.665335551 0.638634718 4.8591633112
H 1.2437658896 -0.5432926597 3.6430772777
H 1.0972976829 1.1627554384 3.2120383395
C -0.3677448519 -0.2603576724 -0.202906862
C 0.8767391387 0.0034396191 -1.056031575
H -0.7260102355 -1.2880907087 -0.4028750228
H -1.1797869089 0.414610399 -0.5445113978
H 1.2316014862 1.0222441949 -0.8662283681
H 1.681774976 -0.6614633166 -0.7254010928
C 0.623397704 -0.1891684034 -2.5505335036
H 0.2624475219 -1.2083372575 -2.7618323114
C 1.8447466017 0.0632382553 -3.4285803299
H -0.1840754105 0.4724243442 -2.9029854012
C 1.6520489969 -0.1251094795 -4.9265742417
H 2.5874804091 0.0860114822 -5.4487868352
H 1.3325835624 -1.1512369478 -5.1480596858
H 0.8648572088 0.5412346309 -5.3011693199
O 2.918053554 0.3978055328 -2.9645929096

DMG:7_ocH⁺

C -1.0752703581 -0.0614492457 2.0892917242
N -0.6785005371 0.2037372759 3.3450707659
N -0.1725608243 -0.1540567055 1.1037877271
N -2.3843611828 -0.1923126196 1.8158723363
H -1.3546763089 0.07034615 4.0830758129
C 0.6980386867 0.5112732385 3.7347698554
H -2.6303892592 -0.5756090233 0.9147400187
C -3.463582849 0.0329651883 2.7772828502
H -3.5145267807 -0.7611687435 3.5321497722
H -3.3415707406 1.0046959669 3.2652139371
H -4.4071147605 0.0448947312 2.2309762791
H 0.6860919869 0.8732523978 4.7631740477
H 1.3455650515 -0.3726192596 3.6882399141
H 1.1036134844 1.3044963165 3.0997339662
C -0.4769962016 -0.2664419495 -0.3335899953
C 0.8029247367 -0.0582443531 -1.1431614197
H -0.9069644337 -1.2554172725 -0.5469923465
H -1.2230582436 0.4960035098 -0.5884027813
H 1.22511218 0.9266549458 -0.9148918561
H 1.5558909944 -0.7967690826 -0.8418896237
C 0.5766993438 -0.1740608731 -2.6514608313
H 0.1468504335 -1.1507984541 -2.9170076246

C	1.8882352836	0.0041863906	-3.4281994688
H	-0.145297595	0.5750772708	-3.0064324336
C	1.8034796848	-0.0566057881	-4.9377647423
H	2.7979733752	0.0723742731	-5.3681719365
H	1.3851529633	-1.0171997171	-5.2632897682
H	1.1362686409	0.7271552287	-5.3177554122
O	2.9333037584	0.1837022937	-2.8343566481
H	0.8014367937	-0.2262988898	1.3662595807

DMG:8_oc

C	-1.0042712645	-0.0901777261	2.1138256642
N	-0.8732968399	0.4304859922	3.3988767088
N	-0.0097816216	-0.0471904715	1.300597617
N	-2.2657042618	-0.6232871055	1.8439732038
H	-1.3888634264	-0.0867184059	4.1007848877
C	0.4525566352	0.8511452288	3.8335256203
H	-2.4000212248	-0.8190564045	0.8623337565
C	-3.4692733214	-0.1585943492	2.526159244
H	-3.5175511192	-0.5372973207	3.5542392685
H	-3.5499640593	0.9362588618	2.5625360254
H	-4.3391424454	-0.5601724049	1.9991131563
H	0.3680745796	1.26902691	4.8412003379
H	1.1854968188	0.0325410944	3.8342934137
H	0.8232776606	1.6214115739	3.1550227154
C	-0.1993421101	-0.4716105806	-0.072839299
C	1.0503977214	-0.1544165503	-0.8998901072
H	-0.4016869335	-1.5581210953	-0.1320819679
H	-1.0721903214	0.0245117731	-0.5460076919
H	1.2501470185	0.9207955902	-0.8533924924
H	1.9164166886	-0.6414209431	-0.4409428007
C	0.913154081	-0.5975497241	-2.3577311922
H	0.7176218314	-1.6787169383	-2.4041213115
C	2.1607541897	-0.2715177617	-3.1855815011
H	0.0380056003	-0.1144687219	-2.8164221788
N	2.1557947242	-0.6363444514	-4.5164542923
C	3.3174351918	-0.3294980391	-5.3367348812
C	1.0611988554	-1.2857706483	-5.2130576477
O	3.1263233988	0.2919130431	-2.6798305032
H	3.042919888	0.3428196326	-6.1614617991
H	4.0638094147	0.1529170748	-4.7073953998
H	3.737576633	-1.2479690024	-5.7687492113
H	0.6738913349	-0.6436113846	-6.0176434528
H	1.4014561046	-2.2252275506	-5.6711603342
H	0.2403085789	-1.5167391948	-4.5366905553

DMG:8_ocH⁺

C	-1.0847385493	0.0102841436	2.0906151882
N	-0.6624876987	0.2275575523	3.3476424399
N	-0.2006263679	-0.0849752065	1.089965178
N	-2.4013516995	-0.0713165797	1.8331250784
H	-1.3328639823	0.0972184266	4.0913301935
C	0.7295896792	0.4737264348	3.7253498477
H	-2.6708905047	-0.4137610765	0.9223943735
C	-3.4591437363	0.1544399086	2.8173436093
H	-3.5179306457	-0.6579523082	3.5520308168
H	-3.3064663074	1.1097077528	3.328806897

H	-4.410622929	0.2030917048	2.2870950418
H	0.7454642467	0.8006714656	4.7653650438
H	1.3448632703	-0.4299401624	3.6388613619
H	1.1538442913	1.2735217636	3.111019239
C	-0.5276243257	-0.1463505171	-0.345803773
C	0.7577443149	0.0054287281	-1.1596085335
H	-1.015418921	-1.1046800258	-0.5747258545
H	-1.2318075511	0.6628351914	-0.5752376711
H	1.2410758455	0.9555270145	-0.9096536582
H	1.4661121169	-0.7845815679	-0.8861402725
C	0.5122156826	-0.0537940177	-2.6695028626
H	0.020689856	-0.9978604722	-2.9401196217
C	1.8577292569	0.0704373875	-3.4100329088
H	-0.1661311283	0.7524533006	-2.9772969242
N	1.8386703051	0.0695564177	-4.7748436653
C	3.0987954748	0.1977782289	-5.5018887506
C	0.6504586348	-0.0310114981	-5.6082357994
O	2.8949687166	0.1638368065	-2.75663154
H	0.7761462273	-0.1823291468	1.3334666383
H	3.0855520224	1.098857512	-6.1273755465
H	3.9119721948	0.2650824557	-4.7815428381
H	3.2516003846	-0.6735748925	-6.1501454647
H	0.5299753436	0.8739045912	-6.2183130232
H	0.7368739998	-0.8876857448	-6.2886005057
H	-0.2501045174	-0.1628095705	-5.0102827334

DMG:9_oc

C	-1.190185319	0.1088738746	2.2883195624
N	-1.2652002131	0.7910873056	3.5006435346
N	-0.1098156344	0.1536502348	1.5939171435
N	-2.3581006109	-0.5775633702	1.9513860307
H	-1.8151779641	0.3104232705	4.2024951586
C	-0.0441773342	1.3922214921	4.021800944
H	-2.3531304187	-0.9017100013	0.9949532485
C	-3.6722297495	-0.1584702	2.4279361127
H	-3.8129196382	-0.4105177908	3.4859153261
H	-3.852607305	0.9183997133	2.3078005518
H	-4.4323040038	-0.7092517702	1.8669604655
H	-0.2876573736	1.9151764837	4.9515672
H	0.7515307132	0.6580464268	4.2093974334
H	0.3387410752	2.1108847796	3.2951697972
C	-0.0868589001	-0.4518568803	0.2765604708
C	1.2331744719	-0.1280784236	-0.4296428336
H	-0.1989942412	-1.5511920047	0.338709913
H	-0.9239819937	-0.0979071534	-0.3601267319
H	1.3459258875	0.958017888	-0.5059105698
H	2.0647214357	-0.4730500197	0.1938080216
C	1.3268134617	-0.758715111	-1.8192650453
H	1.2230436095	-1.8520932393	-1.7541252676
C	2.6350768358	-0.4208147595	-2.5355165791
H	0.4876861353	-0.4228338485	-2.4482601796
N	2.8445293984	-1.0388074646	-3.7381683747
O	3.4607017969	0.3624368861	-2.0727236077
C	1.9581653607	-1.9985107156	-4.4048010125
C	2.5775714238	-2.1402489207	-5.8050000341
C	4.0774254103	-1.9120311793	-5.5506798506
C	4.0904103376	-0.8088608412	-4.4830650038

H	1.9499373959	-2.9651569613	-3.8779567586
H	0.9254053316	-1.6345775812	-4.4408922682
H	2.1849464921	-1.3574271594	-6.4651750972
H	2.3540225073	-3.1084705063	-6.2631820125
H	4.6282266806	-1.629428131	-6.4527264341
H	4.5341073295	-2.8264653181	-5.1525239672
H	4.0868979759	0.1944735929	-4.9307628707
H	4.9477686331	-0.8573185965	-3.8062794157

DMG:9_ocH⁺

C	-1.2635581674	0.1484329528	2.3146464047
N	-1.1604790445	0.8392193836	3.4628883414
N	-0.198368204	0.003967391	1.5173673537
N	-2.4503500147	-0.3654231008	1.948824446
H	-1.9215515328	0.7609922573	4.1216903995
C	0.0409657389	1.5526930575	3.8970902417
H	-2.4502540673	-1.0187407329	1.1791344245
C	-3.7065460603	-0.1575558887	2.6676969609
H	-3.7273966853	-0.6951425882	3.6235873118
H	-3.8777642288	0.910066043	2.8360717177
H	-4.5189426313	-0.5364028551	2.046949058
H	-0.2210862176	2.1610725603	4.7630823361
H	0.843807014	0.8652257411	4.1894497371
H	0.3928856202	2.2216475502	3.105982999
C	-0.2083742863	-0.5754553764	0.161905668
C	1.1555639072	-0.3501179254	-0.4898867485
H	-0.4327817733	-1.6501202851	0.2204153952
H	-1.0016134495	-0.0881376273	-0.418375462
H	1.3778187847	0.7216062845	-0.5205882107
H	1.9394696866	-0.81117375	0.1223159661
C	1.2397445672	-0.9170597099	-1.908314266
H	1.0373204839	-1.9969870451	-1.9129674802
C	2.6377873285	-0.6466098555	-2.4884427331
H	0.4776869282	-0.4596011559	-2.5543290809
N	2.8878644476	-1.1288223657	-3.7295515805
O	3.4742353707	-0.0207158543	-1.8377195187
C	1.970394311	-1.8969898057	-4.5852563607
C	2.6968220561	-1.9337245183	-5.939665106
C	4.1835732588	-1.9041037573	-5.5464290525
C	4.216361399	-0.9486740516	-4.3462123656
H	1.8230833994	-2.9119572199	-4.1874648101
H	0.9879704918	-1.4165623572	-4.6522098866
H	2.4412930191	-1.0403805663	-6.5211792697
H	2.4205234858	-2.8099427796	-6.5325118498
H	4.8336691091	-1.5718514683	-6.3600748934
H	4.514038879	-2.9041248914	-5.2416908537
H	4.3450433159	0.0968197214	-4.6536599056
H	4.9992865331	-1.1751176178	-3.6182280266
H	0.7052332275	0.2675852068	1.8870846998

DMG:10_oc

C	-1.8538517721	-0.0760471608	2.7596961959
N	-1.5498979365	0.073843601	4.1098458189
N	-0.9049675668	-0.1684602138	1.8964159971
N	-3.2210482914	-0.1086157616	2.4868663231
H	-2.2037469048	-0.3891216925	4.7292768349

C	-0.1575825687	-0.0519804165	4.5186507688
H	-3.4224450782	-0.0291453168	1.5004737046
C	-4.204107213	0.5405989156	3.3485954007
H	-4.3680250864	-0.0314252225	4.269955636
H	-3.9226895658	1.564654966	3.6282747305
H	-5.159742438	0.5686459048	2.8181910314
H	-0.0954233485	0.1394722238	5.5940821935
H	0.2697344152	-1.0397797446	4.2960346106
H	0.4393364682	0.6909933729	3.986802938
C	-1.2304977963	-0.1885057898	0.4840737061
C	0.0457508715	-0.0477537489	-0.3517088596
H	-1.7369002679	-1.1312484775	0.2026254486
H	-1.9250130756	0.6268433767	0.1969338998
H	0.524181763	0.9096891633	-0.1152739691
H	0.7472196651	-0.8310012528	-0.0379754757
C	-0.2201313723	-0.1288813453	-1.8671731671
H	-0.7090273808	-1.0862104646	-2.1028592082
C	1.0015576431	0.0597750787	-2.7150245739
H	-0.9198429792	0.6604272761	-2.161593788
N	1.9689682264	-0.9021282443	-2.9025736974
C	2.9392867115	-0.3398700462	-3.7129277937
C	2.506480668	0.9321153172	-3.9803177559
N	1.302975812	1.1735598314	-3.3599412544
C	2.0219488977	-2.2360206862	-2.3298988167
H	3.8146884384	-0.8964477747	-4.0148746322
H	2.9866441462	1.684928106	-4.5915660782
H	2.5506381154	-2.903827336	-3.0153364604
H	2.5380698734	-2.2411537545	-1.3628171449
H	1.0096949275	-2.6213486833	-2.187689563

DMG:10_ocH⁺

C	-1.7431234793	-0.1795334739	3.015100254
N	-1.4444251383	0.3080137794	4.231302886
N	-0.8493485145	-0.1041053974	2.0216203675
N	-2.9581514687	-0.7070955066	2.7872625835
H	-2.0552837952	0.0565267377	4.9948882606
C	-0.2134643175	1.0287990322	4.5571516374
H	-3.0810271052	-1.2240665169	1.9287267944
C	-4.0589000228	-0.7123675858	3.7499948587
H	-3.8806192339	-1.412456235	4.5753950882
H	-4.2244968984	0.2947871747	4.1443815089
H	-4.9640948924	-1.0243745739	3.228320562
H	-0.3295267402	1.4660626932	5.5491842335
H	0.6595980445	0.3652784114	4.5728256836
H	-0.0501290158	1.8422261143	3.8439211121
C	-1.100628892	-0.4355524824	0.6081283457
C	0.0782917819	0.0469769062	-0.2368088739
H	-1.2312886934	-1.5216176675	0.4986361768
H	-2.0297579126	0.0577099617	0.2971645893
H	0.2014430196	1.1283657692	-0.1158168693
H	1.0066396479	-0.4128034349	0.1215371387
C	-0.0849890109	-0.2785215486	-1.7263795786
H	-0.2374700577	-1.3608689045	-1.8582482324
C	1.1267704096	0.1784353436	-2.4879538775
H	-0.9924149467	0.2050827099	-2.118393172
N	1.2570421172	0.0733652401	-3.8488249719
C	2.5002941582	0.5909201572	-4.1646835758

C	3.0565090743	0.9838581803	-2.9758695572
N	2.1943100067	0.7235306804	-1.9349452853
C	0.2917420505	-0.4829866224	-4.784442998
H	2.8546008731	0.6267518458	-5.1842585371
H	4.0231476539	1.438501006	-2.8088555546
H	0.1013009813	0.1429673993	2.262742017
H	0.681208111	-0.3782275768	-5.7981450406
H	0.1193164308	-1.5465649652	-4.587060868
H	-0.6628442252	0.0503143492	-4.7242991061

DMG:11_oc

C	-1.8697887238	0.0165446325	2.8862601693
N	-1.6237648841	0.3515286477	4.2166680385
N	-0.8915723718	-0.0868641564	2.0598493026
N	-3.2216894344	-0.1774701442	2.5952898366
H	-2.2440398739	-0.1115169491	4.8702055463
C	-0.2375867136	0.4061381019	4.6614636324
H	-3.3946712313	-0.2440070562	1.6023208483
C	-4.2789195798	0.5077281646	3.332923491
H	-4.4175361846	0.0724612995	4.3297651712
H	-4.0943103771	1.5837280442	3.4544456062
H	-5.2192121856	0.3690713549	2.7921341588
H	-0.2242847443	0.7171219493	5.7105473089
H	0.2879183107	-0.5532888142	4.5554873987
H	0.3014310137	1.1420631914	4.0621700976
C	-1.1680023519	-0.3022497628	0.6519386682
C	0.1057136807	-0.1147992985	-0.1776233774
H	-1.5604091774	-1.3215369628	0.476621792
H	-1.940320809	0.3920207521	0.2624311326
H	0.4767526519	0.9070923059	-0.0396330496
H	0.8814984045	-0.7850473897	0.2128944832
C	-0.1109296207	-0.381198692	-1.6776273013
H	-0.4365839828	-1.4196900196	-1.8274805977
C	1.111910707	-0.1214920455	-2.5069960383
H	-0.9266768301	0.2593323571	-2.0419895388
C	1.9182486919	-1.0246419747	-3.1600377684
N	2.9220106333	-0.2845959506	-3.7583437221
C	2.6724610866	1.0202223019	-3.4385206983
N	1.5994139956	1.1589667236	-2.691791355
H	1.874224856	-2.1002246865	-3.2544791286
C	4.0122568317	-0.7918053232	-4.5692338133
H	3.3121966967	1.8218693007	-3.7866981474
H	4.6369807681	0.0465744012	-4.8865819439
H	4.6315168348	-1.491748766	-3.9978647879
H	3.6325562411	-1.3019067789	-5.4612828373

DMG:11_ocH⁺

C	-1.7439993364	-0.1241824808	3.0171152157
N	-1.5519196469	0.5565547113	4.1606350226
N	-0.8839125105	0.0096114078	2.0006760281
N	-2.8273790438	-0.9079475918	2.8820571291
H	-2.1043010642	0.284814529	4.9608201931
C	-0.4791098264	1.5271986595	4.3756984112
H	-2.8482586369	-1.5295254241	2.0867187259
C	-3.9031838299	-1.0207586584	3.8654958696
H	-3.5829898718	-1.5599196854	4.7655290063

H	-4.2771337089	-0.029049129	4.1380368838
H	-4.7222878832	-1.5775020577	3.409471341
H	-0.6740766498	2.0451850504	5.3151034086
H	0.503607773	1.0451275376	4.445275899
H	-0.4728933498	2.2702998674	3.5726249664
C	-1.0455334591	-0.5745076365	0.6569474918
C	0.0228226571	-0.0162705773	-0.2826614051
H	-0.9559705079	-1.6685896588	0.716003604
H	-2.0501277376	-0.3283339629	0.2915374141
H	-0.0933847479	1.0715468378	-0.3647041194
H	1.0198200642	-0.2089206896	0.1325421048
C	-0.0306245703	-0.6542655977	-1.6811348739
H	-0.0422586265	-1.7489527016	-1.569341587
C	1.154151253	-0.2462224804	-2.5088975482
H	-0.9602868721	-0.380115552	-2.1946641564
C	1.1978950575	0.1909159127	-3.8116467183
N	2.5326195586	0.3997105769	-4.0954881655
C	3.2215796028	0.0870401318	-2.9604182068
N	2.4284502711	-0.3045217832	-1.9844805148
H	0.4268894517	0.3621235895	-4.5488963335
C	3.0918148409	0.854513396	-5.3600609176
H	4.2997559605	0.1662817475	-2.9075892495
H	0.0027184371	0.4573255667	2.1910971752
H	4.1761704408	0.931659366	-5.258564068
H	2.8629083649	0.1443805057	-6.1604262306
H	2.6922144292	1.8375490041	-5.6269953851

DMG:12_oc

C	-1.6763595432	-0.2754938887	2.7796555879
N	-1.4148867	0.0302194446	4.1131343879
N	-0.7163893631	-0.285211972	1.9248182399
N	-3.0191005508	-0.5492447601	2.5162769026
H	-1.9898306134	-0.4867420716	4.7674440589
C	-0.0237514641	0.1591171344	4.5259738864
H	-3.2177461747	-0.5941978409	1.5270712562
C	-4.0998796024	0.0252254983	3.3118118125
H	-4.1817783555	-0.4657661369	4.2889793654
H	-3.9846246138	1.1042789079	3.4813627091
H	-5.0429237343	-0.1516712621	2.7874506208
H	-0.002699576	0.4349328954	5.5846047207
H	0.5580925373	-0.7607068923	4.373917612
H	0.4516923113	0.9479454523	3.9403301359
C	-1.01667481	-0.4721302281	0.5188970384
C	0.2205471764	-0.1654410053	-0.3309811287
H	-1.3399279174	-1.5101088362	0.3153079761
H	-1.8446542166	0.1786688041	0.1712451937
H	0.5179657418	0.8767361873	-0.1674817019
H	1.050930303	-0.789341736	0.0227653138
C	-0.0131299414	-0.3974033621	-1.8351035022
H	-0.2724021807	-1.4496302463	-2.0122300788
C	1.1893123885	-0.0193593497	-2.6692937746
H	-0.8645271791	0.2103963955	-2.1663013874
C	2.079690519	-0.9851033687	-3.158673832
C	3.1896301515	-0.5783952576	-3.8961152342
C	3.380743521	0.7832802038	-4.1246303803
C	2.4421931634	1.671922734	-3.5985963252
N	1.3728940008	1.2947691995	-2.8900215213

H	1.8987310598	-2.0384465939	-2.962462859
H	3.8906931568	-1.3116728857	-4.2868112998
H	4.2287732328	1.1500718774	-4.69529891
H	2.5526851588	2.7442159371	-3.7570136778

DMG:12_ocH⁺

C	-1.779645001	-0.0748172041	2.7925380247
N	-1.620064206	0.5996412054	3.9442305922
N	-0.8689389163	0.0334154909	1.8170607248
N	-2.8789207809	-0.8248926852	2.6057384434
H	-2.215193337	0.3430330807	4.7184425739
C	-0.5375739406	1.5478656785	4.2067756332
H	-2.8768243231	-1.4550683978	1.8168703413
C	-4.0043724912	-0.9017630454	3.5362968722
H	-3.7464222377	-1.4521916504	4.4493556167
H	-4.3563831266	0.1021292367	3.7925209633
H	-4.8191478973	-1.4295081019	3.0398118933
H	-0.7653920007	2.0740338647	5.1341713615
H	0.4298055795	1.0447634565	4.3249174681
H	-0.4770975934	2.286823762	3.4022224152
C	-0.9909652652	-0.5333861455	0.462169775
C	0.1199699419	0.0178758118	-0.4313963754
H	-0.9229725192	-1.6295532074	0.5104520052
H	-1.9772846663	-0.2651010526	0.0644866228
H	0.0303638083	1.1099369253	-0.4909852072
H	1.0997209333	-0.209229603	0.0054845419
C	0.0896962297	-0.586938364	-1.842919419
H	0.0632138227	-1.6835383839	-1.7615417763
C	1.3120145632	-0.1945863431	-2.6549668477
H	-0.8224600825	-0.287248875	-2.3722429337
C	1.2032415853	0.2266684529	-3.9836343584
C	2.3656441872	0.5369498204	-4.6893134356
C	3.5947342955	0.4205418707	-4.0434894765
C	3.6016718475	-0.0002423082	-2.7129349793
N	2.4936946405	-0.3030350181	-2.0267800706
H	0.2286059722	0.3064638853	-4.4568345979
H	2.3100598604	0.8647523131	-5.7235057345
H	4.5255237869	0.6510141378	-4.551895028
H	4.5404692347	-0.1007912001	-2.1713211733
H	0.02452391	0.4443675155	2.053090339

DMG:13_oc

C	-2.3921995913	0.0377162474	3.5097868004
N	-2.1209073368	0.3201754302	4.8450167463
N	-1.4439143575	0.0796971871	2.641397071
N	-3.7273585544	-0.2706547936	3.2550678801
H	-2.67435271	-0.2214248567	5.4975749891
C	-0.7292982787	0.4835510643	5.2440963884
H	-3.944122224	-0.2916203394	2.2692148295
C	-4.8164366282	0.2131741862	4.0972174055
H	-4.8670371601	-0.3395452193	5.043356307
H	-4.7360234867	1.2832058017	4.330689328
H	-5.7599443261	0.0348063434	3.574547282
H	-0.7039366855	0.7368459356	6.3080827272
H	-0.1215411164	-0.414262398	5.0651429804
H	-0.2858621304	1.2996339365	4.6707771122

C	-1.7612936959	-0.0893343144	1.2382406528
C	-0.5202609809	0.1993447846	0.3871074872
H	-2.1071385921	-1.117914392	1.0228347305
H	-2.5770193868	0.5835934867	0.9044087283
H	-0.1950806232	1.2304018115	0.5680199899
H	0.2940537088	-0.4526336151	0.7269027527
C	-0.7674896556	-0.0032313623	-1.1200892733
H	-1.0711885929	-1.0405823034	-1.3104642707
C	0.4516420408	0.3295009808	-1.9453587195
H	-1.5880260925	0.6472003312	-1.4455931442
C	1.3310125128	-0.6716873712	-2.3829605468
C	2.4490972667	-0.2807060212	-3.1061197832
C	2.6933769515	1.0571338978	-3.3890196481
C	1.7562838591	1.9714055452	-2.9072487555
N	0.6686755159	1.6306655145	-2.2082993235
H	1.1555151897	-1.719353552	-2.1723445216
N	3.3962343008	-1.3093114505	-3.5881125372
H	3.5643361782	1.3602151429	-3.9555351305
H	1.8883511504	3.0345667625	-3.0979336
O	4.3786590191	-0.9230703269	-4.2174634925
O	3.1405043712	-2.4829724122	-3.3286717566

DMG:13_ocH⁺

C	-2.1461452122	-0.2575802631	3.8373727819
N	-2.0075538512	0.4419309134	4.9760012975
N	-1.2134956419	-0.1727250343	2.8783834142
N	-3.2433398933	-1.0080762169	3.6436777655
H	-2.6199598185	0.2053611354	5.7432740244
C	-0.9318745477	1.3985421218	5.2376090352
H	-3.225471263	-1.6597917721	2.872638606
C	-4.3918138731	-1.055681737	4.5487730153
H	-4.1607575299	-1.5900613719	5.4782904909
H	-4.7388853167	-0.0432965507	4.7761011186
H	-5.1999198955	-1.5850515458	4.0432349158
H	-1.1807719452	1.9485278208	6.1455480741
H	0.0328353565	0.8999369502	5.3911090912
H	-0.8544188441	2.1160891734	4.4154006305
C	-1.3128901392	-0.7665769095	1.5344470168
C	-0.1961818485	-0.2244209374	0.6410579443
H	-1.2388486668	-1.8613000498	1.603251402
H	-2.2951051272	-0.5123150175	1.118242205
H	-0.2888757361	0.8663067438	0.5661966892
H	0.7804990713	-0.4439003039	1.0885980497
C	-0.2250709777	-0.8491289598	-0.7629903344
H	-0.2186521169	-1.9443276338	-0.6693906221
C	0.9742600041	-0.4365138051	-1.5950323633
H	-1.1497155674	-0.5790832539	-1.2856253439
C	0.8225339002	0.0488307824	-2.8970680242
C	1.9775814073	0.3749816384	-3.5968320723
C	3.2328767461	0.2263464984	-3.025522295
C	3.26840393	-0.2600693508	-1.7169175945
N	2.1770598479	-0.5832841331	-1.0153532057
H	-0.1477420209	0.1711937265	-3.3625136829
N	1.8601215499	0.8956098239	-4.9796283703
H	4.1307083272	0.4801933683	-3.5746868217
H	4.2220735109	-0.396374057	-1.2125058267
H	-0.3223811175	0.2352151851	3.1278659897

O	2.902553813	1.1636175911	-5.5668833617
O	0.7269172226	1.0221468479	-5.435113883

DMG:14_oc

C	-1.6634820205	-0.2934091157	2.7527734665
N	-1.3612186801	-0.0828130419	4.0947054824
N	-0.7241371221	-0.2713089988	1.874096671
N	-3.0173885481	-0.5115924076	2.502986401
H	-1.9384263127	-0.6174220373	4.7322724993
C	0.0419774548	-0.0170582076	4.4809269173
H	-3.2448561271	-0.4738598163	1.5200443022
C	-4.0667688879	-0.0025152176	3.3798854414
H	-4.1420933485	-0.5947471124	4.3001200059
H	-3.9191455013	1.0486354516	3.6613540571
H	-5.024457587	-0.0989109813	2.8614308673
H	0.0943290191	0.1917739617	5.5535711994
H	0.5937956853	-0.9409327455	4.2586678953
H	0.526025822	0.7938863777	3.9338207972
C	-1.0669811789	-0.3621553332	0.4695527805
C	0.1792363405	-0.115718364	-0.3871701531
H	-1.4797435076	-1.3572340661	0.2174014368
H	-1.842191097	0.3737672812	0.1743622065
H	0.5714497258	0.8838801862	-0.1676491809
H	0.9548626016	-0.8319686254	-0.0888449247
C	-0.1002578415	-0.2345460182	-1.8973124974
H	-0.4641786419	-1.2434532366	-2.1307385357
C	1.1215956443	0.0727075852	-2.7293774899
H	-0.8901183613	0.4733137719	-2.1769241687
C	1.9039431209	-0.9473977963	-3.284018418
C	3.0463013926	-0.6055102923	-4.0187770011
C	3.3713156509	0.7484177058	-4.1757763022
C	2.5277545921	1.6864157651	-3.5845978399
N	1.4348837411	1.3721920502	-2.8820516634
H	1.6315183409	-1.9890799764	-3.1499768577
C	3.8675419787	-1.6272436055	-4.604414711
H	4.2461253008	1.0526758234	-4.7397104112
H	2.7415672426	2.7490694692	-3.6848230821
N	4.5325631094	-2.4544944331	-5.0792401901

DMG:14_ocH⁺

C	-1.7791225518	-0.0712619418	2.7898066738
N	-1.6346735563	0.6244939095	3.9300218044
N	-0.8553545894	0.0228391114	1.8232935217
N	-2.8735540344	-0.8273204518	2.6023570907
H	-2.2384941015	0.3811643611	4.7019748253
C	-0.565330181	1.5900678942	4.1842906424
H	-2.8582662274	-1.4757429059	1.8284694837
C	-4.0145738365	-0.8849192862	3.5162125173
H	-3.7733218706	-1.4222111606	4.4414436665
H	-4.3650364016	0.1246084725	3.7509393452
H	-4.8239337186	-1.4162909956	3.0147757629
H	-0.8102877884	2.1345609823	5.0966025064
H	0.405578379	1.100086934	4.3263527045
H	-0.502650056	2.3109831502	3.3637279014
C	-0.9626893059	-0.5646471771	0.4770350439
C	0.1488156886	-0.0172581872	-0.4195532494

H	-0.8867112697	-1.6595938232	0.5398107093
H	-1.9478684484	-0.3093470615	0.0685654075
H	0.0530700392	1.0733807125	-0.4918991685
H	1.1277480602	-0.235128148	0.0239733816
C	0.1199274687	-0.6396185756	-1.8245231884
H	0.1191696309	-1.7349740902	-1.7322168734
C	1.3265854129	-0.2339927573	-2.6503052234
H	-0.8015168777	-0.3635394276	-2.3500235162
C	1.1875589595	0.2527947895	-3.9509739448
C	2.3435016009	0.5821976451	-4.6738382017
C	3.5931118921	0.4124073336	-4.0653498787
C	3.6199286112	-0.0746396259	-2.7594112676
N	2.5238023238	-0.3910252039	-2.0617890909
H	0.208727276	0.3744460447	-4.4027914787
C	2.2385416272	1.0888924246	-6.012330766
H	4.5090106674	0.6548231006	-4.592485636
H	4.5705209091	-0.2182735684	-2.2505380621
H	0.0371695717	0.4307299343	2.0678427118
N	2.1459196966	1.5027135878	-7.0944851545

DMG:15_oc

C	-2.2198025797	-0.1687562203	3.4038958321
N	-1.9528128531	0.1280528092	4.7386491978
N	-1.2734758946	-0.1219795767	2.5355224747
N	-3.5524092777	-0.4985932235	3.1534277421
H	-2.4906391584	-0.4277005788	5.3928167305
C	-0.5626621583	0.3163915612	5.1315158552
H	-3.7635162265	-0.5300164701	2.166293097
C	-4.6471923309	0.0045724297	3.9772489612
H	-4.6895118746	-0.510824874	4.9442950769
H	-4.5831184931	1.0841782988	4.1692695223
H	-5.5884662688	-0.2077979865	3.4629292033
H	-0.5372809769	0.5800294941	6.193201734
H	0.0590176333	-0.5731528	4.9583752082
H	-0.1344194033	1.1335585006	4.5483278198
C	-1.5884477419	-0.3007465624	1.1312893976
C	-0.3649776824	0.0273282333	0.2696949486
H	-1.902828632	-1.3402066845	0.9209253415
H	-2.4280265445	0.3444115144	0.8018823989
H	-0.0677125128	1.0663953939	0.4520140974
H	0.4719802521	-0.6023524994	0.596460596
C	-0.6211488347	-0.1728616552	-1.2352176657
H	-0.8940105834	-1.218352549	-1.429996198
C	0.5740627579	0.2105145772	-2.0772588542
H	-1.4691843608	0.4516196805	-1.5428653814
C	1.444974044	-0.7545279612	-2.5795639717
C	2.5597098812	-0.3534744938	-3.3272211296
C	2.759547959	1.0135857617	-3.5440762269
C	1.8249968827	1.8954051207	-2.9960283808
N	0.7586750581	1.5318787671	-2.282852676
H	1.2780589403	-1.8128997717	-2.4058922305
O	3.3651408818	-1.3450745321	-3.7887767533
H	3.5977404019	1.3961162326	-4.1141707773
H	1.9521227927	2.9666019789	-3.1508229455
C	4.5061215483	-0.9818751351	-4.5546942424
H	4.9994986487	-1.919283402	-4.8167692916
H	4.2213968843	-0.4516279188	-5.4723382116

H 5.1968427274 -0.3569446705 -3.9744560736

DMG:15_ocH⁺

C -2.1911735317 -0.2436114365 3.5520066357
N -2.0419823079 0.4187520645 4.7122850462
N -1.2686298607 -0.1308187278 2.5886959402
N -3.2917904659 -0.9863637686 3.3448345878
H -2.6479391719 0.1582789702 5.476700835
C -0.9589638984 1.3599225078 4.9960768048
H -3.2849453157 -1.6052075871 2.5470667299
C -4.4291293906 -1.0666111914 4.2602884915
H -4.1857790672 -1.6286430302 5.1703011649
H -4.7785914291 -0.06361968 4.5235651465
H -5.2407771251 -1.5840151539 3.7480238536
H -1.1946313506 1.8773911046 5.9264071227
H 0.0053880043 0.8521410652 5.1192667042
H -0.8871279249 2.1067368665 4.1997272529
C -1.3761673863 -0.6854157202 1.2273159503
C -0.2497820563 -0.1332492907 0.3539818752
H -1.3152250102 -1.7823085016 1.2672972265
H -2.3553580315 -0.4074565962 0.8189779582
H -0.3369483491 0.9591075944 0.2958945741
H 0.7225047193 -0.3638205055 0.8057412672
C -0.2552971376 -0.7346895281 -1.0592512941
H -0.2801124377 -1.8313267414 -0.9802731988
C 0.9840274903 -0.3393237123 -1.8425109807
H -1.1566130047 -0.433968604 -1.6059821593
C 0.8907140668 0.1280011329 -3.1472898213
C 2.0681611416 0.4464413422 -3.8443535642
C 3.2927142803 0.2824653885 -3.1860140128
C 3.2666096059 -0.1866692011 -1.8720420472
N 2.1565279261 -0.49575269 -1.197022623
H -0.0656830527 0.2487024519 -3.6458400231
O 1.9111384938 0.8927002354 -5.1073614286
H 4.2397512236 0.5082598147 -3.6605093693
H 4.2045726289 -0.3208485 -1.3357103498
H -0.3750783459 0.2714451661 2.838915409
C 3.0742783641 1.2248890868 -5.8658066926
H 2.7071045024 1.5511521908 -6.8391496045
H 3.6354716961 2.0399710052 -5.3938416866
H 3.7260825617 0.3528123733 -5.9936461512

DMG:16_oc

C -2.5067520637 0.0808016536 3.5737168039
N -2.294684675 0.4985423921 4.8861107868
N -1.5333832679 0.0840555669 2.7349391621
N -3.820999777 -0.3121906877 3.3125645351
H -2.8377788805 -0.0180907968 5.5674647271
C -0.9251364804 0.7644825064 5.3053476602
H -3.9939901159 -0.4392279089 2.3253960899
C -4.9559886142 0.2464217085 4.0415738151
H -5.017899756 -0.1613027663 5.0575326625
H -4.9262071489 1.341982745 4.1159603941
H -5.8734676397 -0.0480749924 3.5245725571
H -0.9442252786 1.1217688555 6.3394717025
H -0.2726468997 -0.1169525879 5.2327955929

H	-0.5001520371	1.5395749544	4.6652306524
C	-1.7927507121	-0.2185216361	1.3402063684
C	-0.5753871259	0.1402283396	0.482347054
H	-2.022038384	-1.2918327449	1.2037981158
H	-2.669097739	0.3330531796	0.9430294083
H	-0.3724245453	1.2127868039	0.5781887036
H	0.3018268466	-0.3841583331	0.8818253291
C	-0.7675310008	-0.20759234	-1.0044996761
H	-0.9236456971	-1.2889014283	-1.1163954976
C	0.3998478425	0.2374343774	-1.8581613215
H	-1.6710737968	0.2926682497	-1.3763157346
C	1.3396422752	-0.6833447985	-2.3211247945
C	2.4397841829	-0.250249281	-3.0950468281
C	2.5162686341	1.1385396643	-3.3418233731
C	1.5237956726	1.9665106033	-2.8317390436
N	0.4771931365	1.5587277295	-2.1057639864
H	1.2094378591	-1.7308365536	-2.0762460172
N	3.3791592344	-1.1328281193	-3.5861638922
H	3.3260542036	1.5723281205	-3.9157055672
H	1.578895831	3.0380515083	-3.0243507766
C	4.5572988268	-0.6240382841	-4.2681076712
C	3.3371956452	-2.5293061805	-3.1854772385
H	5.1629738515	-1.4644706028	-4.6119897957
H	4.2794195924	-0.0314422663	-5.1485461238
H	5.1820897039	0.0067716842	-3.617365053
H	4.1472968071	-3.0680211713	-3.6803409404
H	3.4519046746	-2.6583850011	-2.0986191297
H	2.392033499	-2.9996351156	-3.4844680675

DMG:16_ocH⁺

C	-2.1419881429	-0.0386524125	3.9757575147
N	-1.718796706	0.2680707598	5.2146737471
N	-1.267315618	-0.1420270311	2.969367749
N	-3.4549023901	-0.2090701345	3.7433867529
H	-2.3774404495	0.1563597217	5.9713911565
C	-0.3343491168	0.5870000187	5.5617236615
H	-3.7174198481	-0.5842555564	2.8437067573
C	-4.5112780017	0.0024477303	4.7313581106
H	-4.5074956132	-0.7714303	5.5087379706
H	-4.4153802843	0.9918060048	5.1895007798
H	-5.4709061125	-0.0392760459	4.2154758796
H	-0.3166920445	0.9417481706	6.5925287145
H	0.3191713475	-0.2907535096	5.4889412079
H	0.0455349944	1.3885942186	4.920703816
C	-1.6117950556	-0.2978664126	1.5438528177
C	-0.3596884103	-0.1128178674	0.6876883034
H	-2.0503085159	-1.2921816994	1.3783568417
H	-2.3615506401	0.4593210233	1.2830260278
H	0.0815195278	0.8711240992	0.8787890594
H	0.3869871174	-0.8706081727	0.9629021425
C	-0.6548043198	-0.2051487504	-0.8163734966
H	-0.9655759579	-1.2202752623	-1.0902427426
C	0.5438606923	0.2215848911	-1.6492153331
H	-1.4971494207	0.461164495	-1.0545154267
C	0.9326861621	-0.517940837	-2.7608845475
C	2.0243759767	-0.0810802242	-3.5521938755
C	2.658327512	1.1108114653	-3.125810806

C	2.1882620118	1.7600578686	-1.9941819977
N	1.1523661776	1.3504880065	-1.2478217493
H	0.3875620669	-1.4190342321	-3.0153920506
N	2.4402809667	-0.7708286772	-4.659304917
H	3.5028540161	1.5262120018	-3.6611920113
H	2.6778534777	2.6755882116	-1.6653688882
C	3.5552416836	-0.2707742239	-5.4530588181
C	1.7493304621	-1.9850597918	-5.068097017
H	3.730950902	-0.9476149568	-6.2897859422
H	3.3469771789	0.7271249471	-5.8610674773
H	4.4788516953	-0.2152393182	-4.8622061792
H	2.2265439202	-2.3843087991	-5.9635649394
H	1.7935194355	-2.757832602	-4.2889067855
H	0.6934129993	-1.7936440948	-5.3032348658
H	-0.2823355228	-0.1243875341	3.1959187773

DMG:17_oc

C	-2.3508411503	0.1668450281	4.3736400972
N	-1.926487908	-0.122677967	5.669635157
N	-1.4867594896	0.4168545964	3.4562737059
N	-3.7375404587	0.1480850241	4.2155502096
H	-2.5438624182	0.2404095862	6.3861163418
C	-0.5120227407	0.0468837084	5.9763556176
H	-4.0161180732	0.1752727731	3.2451678897
C	-4.6069000111	-0.6642263675	5.060118077
H	-4.2560748368	-1.6990900848	5.1735279555
H	-4.7115224897	-0.2299099609	6.0616936083
H	-5.6050626779	-0.6761568252	4.6136874898
H	-0.3457004283	-0.2574590636	7.0142156686
H	0.0758602099	-0.5930043768	5.315937232
H	-0.1601205245	1.0781119931	5.8340007234
C	-1.9374679199	0.5885570812	2.0877492142
C	-0.7375261786	0.7024362598	1.1427257407
H	-2.5735524542	-0.2556190937	1.7504642201
H	-2.5568579365	1.4981421937	1.979121532
H	-0.1245840319	1.5581014935	1.4468031806
H	-0.1113282009	-0.191431151	1.2591134796
C	-1.1482942941	0.8703819619	-0.3309527485
H	-1.7302629377	-0.0023035581	-0.6568116916
C	0.0432871636	1.0652522852	-1.2430986921
H	-1.7974639613	1.7503534194	-0.4244016111
C	0.5156251395	0.0198291182	-2.0356465519
C	1.649425626	0.2093902656	-2.857098011
C	2.2424211413	1.4907606006	-2.8201367745
C	1.6863526979	2.4602252605	-1.9951069636
N	0.6145503811	2.284845424	-1.213256087
H	-0.0024167458	-0.9329707506	-2.0212801315
N	2.1440367123	-0.7944814988	-3.6481984068
H	3.1205897713	1.7249028585	-3.4111534171
H	2.139205346	3.45135093	-1.9626763429
C	3.2552603096	-0.6163278068	-4.5820814503
C	1.6311208871	-2.1641975286	-3.6376088166
C	3.2410939692	-1.9082369079	-5.4127408155
H	3.1085472084	0.2769104781	-5.2017863174
H	4.2099535361	-0.4921801888	-4.046100603
C	2.6837931403	-2.9522595183	-4.4318207036
H	1.5228064663	-2.5351169943	-2.610982204

H	0.6396645944	-2.2217565454	-4.1147606121
H	2.2606512975	-3.8303365755	-4.9285540198
H	3.4769098548	-3.2975587229	-3.7580238316
H	4.2307301526	-2.1649759456	-5.801955644
H	2.5634479408	-1.7939455813	-6.2671782626

DMG:17_ocH⁺

C	-2.4485393103	0.1633769422	4.5981782061
N	-2.0466812266	0.5217425233	5.8303668523
N	-1.5673459957	0.0879732675	3.5952278597
N	-3.7486452732	-0.0890565572	4.3683475587
H	-2.6997083246	0.3903082563	6.5887413169
C	-0.6847216517	0.931766523	6.1708320434
H	-3.9864977372	-0.4953103023	3.4753543659
C	-4.8168006041	0.0742687319	5.3526253677
H	-4.7624953652	-0.6806433694	6.1466294737
H	-4.7862831777	1.0775102678	5.7892032792
H	-5.771421716	-0.0415771962	4.8388145184
H	-0.6908144084	1.3109115943	7.1930592425
H	0.0210107885	0.0939419158	6.1189429996
H	-0.3526765673	1.73985995	5.5116572459
C	-1.8996320548	-0.1121697417	2.1720150623
C	-0.6442398318	0.0736153274	1.3212110292
H	-2.3159919749	-1.1197043811	2.0312002936
H	-2.6636126323	0.6215651625	1.885837004
H	-0.2078617776	1.0606348046	1.5084735463
H	0.1048074066	-0.6780140855	1.6057259578
C	-0.9284299758	-0.0264140477	-0.1840023828
H	-1.2427080395	-1.0413219347	-0.4554689678
C	0.2799107758	0.3871656534	-1.010290391
H	-1.7660340985	0.6424452439	-0.43209492
C	0.6444813827	-0.3365992995	-2.1400011122
C	1.7451046317	0.0908325921	-2.9238079946
C	2.4156157947	1.2535104203	-2.4726372363
C	1.9659793095	1.8892393123	-1.3260531968
N	0.920064297	1.4905355688	-0.5862777439
H	0.073354941	-1.2137442441	-2.4232670004
N	2.1357257434	-0.5791319489	-4.04327268
H	3.2779782952	1.6448918899	-2.9990850343
H	2.4821777729	2.781813591	-0.9752851935
C	3.2066876261	-0.1192271081	-4.9353744238
C	1.5212514581	-1.8280743891	-4.504777821
C	3.0484270351	-1.0056758481	-6.1788829463
H	3.0906139848	0.9457504006	-5.1670980348
H	4.1922624685	-0.2535347723	-4.4645644653
C	2.4682961777	-2.3116668237	-5.6130289277
H	1.4396020844	-2.5505439808	-3.6837231181
H	0.5065541591	-1.645767384	-4.8908886068
H	-0.5860400263	0.177535234	3.8205436778
H	1.9532070784	-2.916378153	-6.3644206011
H	3.2671899321	-2.9243422396	-5.1793730389
H	3.9934531304	-1.147956927	-6.7099932613
H	2.3377664121	-0.5464587848	-6.8756952642

S9. Cartesian coordinated for the hydrogen bonded DIG series of bases and their conjugated acids

DIG:1

C	0.842363932	1.8132385732	-1.1096468656
N	1.2168055687	0.6631441865	-0.2695741942
C	0.42150637	-0.4837375914	-0.1784046203
N	0.804105168	-1.7124458416	-0.2554737631
C	2.1224487876	-2.0526404825	-0.754653694
C	3.0945259046	-2.4861536221	0.35752176
C	3.4485854589	-1.3845915879	1.3616542777
N	4.0219111987	-0.1691619798	0.7602943768
N	-0.9235086169	-0.1920081597	0.0400537713
C	-1.9040222199	-1.2576702541	0.2639590653
H	-1.6478432235	-2.0448186377	-0.4505643191
C	1.773108355	2.9846459285	-0.783403608
C	0.8539263611	1.47631183	-2.6092206676
H	-0.1789362588	2.1027962094	-0.8389290164
H	-1.0664803693	0.6300915913	0.6168904694
H	2.0057587527	-2.907171887	-1.4363448627
H	2.5885566597	-1.2477823726	-1.3472379378
H	4.0022288457	-2.8983309041	-0.1026984607
H	2.6346300912	-3.3066313271	0.9227418221
H	4.1302479715	-1.796361583	2.1323193101
H	2.5308462306	-1.082243644	1.8785789132
H	2.2175626088	0.457415725	-0.2678491253
C	-3.3028963047	-0.7169950616	-0.0497108132
C	-1.817768162	-1.849522847	1.6786357394
H	-2.5357030087	-2.669168565	1.8055328902
H	-0.8123006143	-2.239619669	1.8565231185
H	-2.0435058516	-1.0873784863	2.4370523797
H	-4.0562867284	-1.5048447321	0.0613940747
H	-3.5761184651	0.0973729529	0.6355445887
H	-3.3521178356	-0.3292128597	-1.0724823467
H	1.4972961787	3.871753711	-1.3639315214
H	1.7269725909	3.2364037621	0.2811839617
H	2.813620691	2.7364310605	-1.0298131874
H	0.5242574623	2.3340994418	-3.2085424183
H	1.8638020696	1.2002639251	-2.9377922159
H	0.1840824629	0.6360154739	-2.8189655423
C	4.1194734797	0.8934093027	1.7585413744
H	4.515234471	1.8027917513	1.2931907896
H	3.1231361204	1.1167400051	2.1525488962
H	4.7795442	0.6273361862	2.6062502797
C	5.3210871435	-0.4074804008	0.1368725452
H	5.6983395367	0.5291493405	-0.28741297
H	6.0751589229	-0.7874147486	0.852949492
H	5.2292410641	-1.1310717124	-0.6772927458

DIG:1H⁺

C	2.5134126137	0.5757866777	1.779692979
N	2.0897043782	-0.0493183113	0.5169107621
C	3.1939689434	-0.0088619393	-0.4545131878
C	1.6190827987	-1.4237389127	0.7787197579
C	1.0536085482	-2.1507182586	-0.4469724256

C	-0.0009314555	-1.3780631105	-1.2519502833
N	-1.1838160123	-0.9667810914	-0.4823385748
C	-1.4697014964	0.2905990782	-0.0781887967
N	-0.4949373208	1.2019950836	-0.0117784074
C	-0.6997986181	2.6598329533	0.1218137597
H	-1.657500489	2.8875106265	-0.3615078653
N	-2.7428502774	0.6107623413	0.2254256672
C	-3.9588304822	-0.1839995784	-0.0594119067
C	-4.2885489749	-1.145868668	1.0911095268
H	-0.354561953	-2.0038912853	-2.078300673
H	0.4265308218	-0.4770364737	-1.6967861175
H	1.8556746786	-2.4227511338	-1.1431437472
H	0.6276426087	-3.1006012422	-0.1002150655
H	2.4280337476	-2.0394488681	1.2085736769
H	0.839588339	-1.3518396934	1.5469877659
H	0.4823545124	0.8397566493	0.0718308194
H	-3.7473445637	-0.7532724262	-0.9719423657
C	-5.1122271823	0.7802415955	-0.3499340785
H	-1.8813019138	-1.6738214964	-0.2992523586
C	-0.7523902135	3.0985790964	1.5931487225
H	-2.8793221717	1.4552848922	0.7643931933
C	0.4064949984	3.3841049857	-0.6513277616
H	3.5180793986	1.026957138	-0.5893884563
H	4.0613537851	-0.6021034213	-0.1215368932
H	2.8698639519	-0.3885079507	-1.4268874119
H	2.825280798	1.6079784314	1.5928615055
H	1.67857165	0.5847807368	2.4879044718
H	3.3563005481	0.0415312418	2.2470133427
H	-0.9496307723	4.1732077814	1.6601761562
H	-1.5356883277	2.5782056586	2.1574255732
H	0.2017347413	2.8982666888	2.0923852924
H	0.2533538522	4.4659014184	-0.5968514393
H	1.3925839092	3.1657294063	-0.2251000552
H	0.4098667838	3.0901834232	-1.7052465046
H	-5.1683835155	-1.746796971	0.8405552951
H	-3.4632027943	-1.8334461646	1.31071184
H	-4.5088143353	-0.5899026502	2.0090873437
H	-6.0166091378	0.2166471512	-0.5960381108
H	-5.3390291482	1.3980911522	0.5279540494
H	-4.8781462513	1.4388514393	-1.1916870143

DIG:2

C	0.8214055118	1.8589295453	-1.1964995007
N	1.1574440372	0.7434630884	-0.2933987438
C	0.3729618347	-0.414550955	-0.2157598224
N	0.7784180702	-1.6376796875	-0.2263940235
C	2.1361617382	-1.9676724274	-0.6154453135
C	3.03936803	-2.3186455052	0.5816288496
C	3.2669054962	-1.1700392099	1.5540700834
O	3.8812550007	-0.082392209	0.8630253
N	-0.9860892208	-0.1360244776	-0.0945599298
C	-1.9642299294	-1.2086956901	0.1072345616
H	-1.6521941014	-2.0174828365	-0.5592501366
C	1.7188931281	3.0516744181	-0.8553758465
C	0.9263319948	1.4697566463	-2.6793252569
H	-0.2168937267	2.1432936545	-0.9950502623
H	-1.1773731225	0.7045688954	0.4400901872

H	2.0892309107	-2.8568868474	-1.2592702765
H	2.6283418456	-1.183372208	-1.213301368
H	4.0099543021	-2.668151663	0.2060062973
H	2.5845821309	-3.1460248398	1.141051419
H	3.9188343142	-1.4930295156	2.3821976368
H	2.3112103159	-0.8405239096	1.9910944146
H	2.1543943967	0.5446082187	-0.2522386173
C	-3.3474538261	-0.7028846377	-0.3148694283
C	-1.9603668984	-1.7460314085	1.5459856824
H	-2.6752650718	-2.5703963136	1.6578210069
H	-0.9637769415	-2.1150814296	1.8017399549
H	-2.2427466161	-0.9596416379	2.2592430792
H	-4.0956906707	-1.4974056891	-0.2175667113
H	-3.6737620691	0.1343708782	0.3175243869
H	-3.3381602795	-0.3583164547	-1.3540981401
H	1.4695864572	3.9154647051	-1.4811245789
H	1.6062599856	3.3378342396	0.1955214574
H	2.7749585955	2.8086261396	-1.0317628201
H	0.6246970908	2.3022999227	-3.3268636761
H	1.9568239664	1.1950639063	-2.9373810398
H	0.2785929972	0.6147776306	-2.8987921951
C	4.1741223851	1.004537205	1.7191485871
H	4.658863772	1.7747323624	1.1128922301
H	3.2607404429	1.4231642674	2.1694521094
H	4.8580437236	0.7044358292	2.5283974439

DIG:2H⁺

C	0.7050305497	2.0481517711	-0.6188369065
N	1.0826197196	0.6206211987	-0.7088662868
C	0.2431197007	-0.4177387586	-0.6216534156
N	0.6534242998	-1.6468898549	-0.9996679439
C	1.8045923372	-1.9513722026	-1.8640486199
C	3.0276134391	-2.5188536155	-1.130505771
C	3.6071945356	-1.6152005129	-0.0471546057
O	3.8227845454	-0.3123009486	-0.5932962473
N	-1.0188986382	-0.2470735729	-0.1856205861
C	-2.1384449369	-1.2113638834	-0.288382996
H	-1.953312947	-1.8009629286	-1.1936680922
C	0.7809595744	2.5644705919	0.8255213416
C	1.6012718394	2.8519639227	-1.5653683889
H	-0.3270167548	2.12091386	-0.9814287379
H	-1.2099521341	0.6044503693	0.3251909245
H	1.4631337228	-2.6730225424	-2.6131174617
H	2.0702067418	-1.0383431312	-2.4000932032
H	3.7943282391	-2.7113937382	-1.889993752
H	2.7806765445	-3.4866674339	-0.6761600852
H	4.5588785617	-2.033080541	0.3068641457
H	2.9338264508	-1.5477248555	0.8225036814
H	2.0868430471	0.4022273813	-0.7562868948
C	-2.2013234429	-2.1372841742	0.9346090719
C	-3.4385240942	-0.4266626261	-0.4834686788
H	0.0825156681	-2.426120228	-0.7045977959
H	-3.0121223808	-2.8629391893	0.8164453517
H	-1.2698555665	-2.6958477229	1.0849927529
H	-2.3926792547	-1.561666352	1.8469009468
H	-4.2775922319	-1.1189066955	-0.5965891754
H	-3.6509564446	0.2071499206	0.3866172363

H	-3.3922869981	0.2051421172	-1.3755328662
H	0.4581402914	3.6093846752	0.8702374989
H	0.1471068749	1.9874086643	1.5094210842
H	1.807994814	2.5118611859	1.203469406
H	1.3148157412	3.9074048212	-1.5431050881
H	2.6530672498	2.7867415237	-1.2628014282
H	1.5130765553	2.4930221776	-2.5950432984
C	4.6979792121	0.4907526203	0.1982925859
H	4.8098772203	1.4464054731	-0.3182541451
H	4.2898596176	0.6599319385	1.2050051146
H	5.682248731	0.0147712955	0.2881803285

DIG:3

C	1.2300062163	0.2866571089	0.5992312114
N	2.5301328963	0.6543281619	0.2641147526
N	0.9735108418	-0.9365221561	0.9114738509
N	0.3300109543	1.3593241039	0.5226350522
C	0.6328317633	2.6769634488	1.1162836969
H	-0.6326906032	1.0756033564	0.6866695007
H	2.5746810563	1.3751526368	-0.4480634419
C	3.6018949071	-0.3418864313	0.174930605
C	-0.2911592128	-1.3262103412	1.5012086384
C	0.7430574068	2.6207139211	2.6473786127
C	-0.4339890251	3.6738512195	0.6555148482
H	1.5998626412	3.0017729391	0.7182274249
H	3.4554798356	-1.0061324288	1.0310798699
C	3.5174842289	-1.1862153129	-1.105391136
C	4.9510114103	0.3717629366	0.3060602197
H	-0.0713353812	-1.9833113848	2.3544179082
H	-0.8764206236	-0.4851015684	1.9101210067
C	-1.1678790093	-2.1301595283	0.5226348829
H	-2.0252345747	-2.5509301061	1.0649601716
C	-1.6574389689	-1.3421871703	-0.6958717621
H	-0.5754193687	-2.9765554282	0.1527543457
H	-2.1234566116	-2.0142711564	-1.4245561942
S	-2.8958677771	-0.0604090374	-0.2192407544
H	-0.8117696284	-0.8432596244	-1.1820455601
C	-2.9927102423	0.8625226282	-1.7927207693
H	-3.7256086457	1.6621044851	-1.6566476179
H	-2.0238187314	1.3053998149	-2.0431154157
H	-3.3257982407	0.2155366126	-2.6100115855
H	4.3096539703	-1.9445646957	-1.1260766304
H	2.5508676095	-1.6941218423	-1.1523612849
H	3.6331704523	-0.5577122182	-1.998957625
H	5.7736729841	-0.3517157307	0.2923686601
H	5.1134874349	1.0690377774	-0.5274008281
H	5.0030710955	0.9414507975	1.2395744821
H	-0.2198299072	4.675547847	1.0435877154
H	-0.4748450157	3.7245270357	-0.4375178472
H	-1.4266420637	3.3803628208	1.0201162892
H	1.0051946619	3.6031393495	3.058735397
H	-0.2096144308	2.3090306905	3.0933742749
H	1.5150256954	1.9064364695	2.9516530356

DIG:3H⁺

C	0.7157451499	1.5965364765	-1.8217303039
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N	1.1046014584	0.4011906295	-1.0388535913
C	0.267555182	-0.4439496834	-0.4251743386
N	0.7135854084	-1.6371654369	0.023862197
C	1.8942054606	-2.3771793144	-0.4522535542
C	2.9841744293	-2.568634574	0.6126185594
C	3.5731979131	-1.2873706162	1.2110681772
S	4.3385360005	-0.2315899109	-0.0900048783
N	-1.0289277389	-0.1223356666	-0.2638864909
C	-2.1433222579	-1.0330689684	0.0882075045
H	-1.8624093438	-2.0224154446	-0.2909583292
C	0.6664352943	2.854204559	-0.9422552309
C	1.6899277132	1.7504277345	-2.9933196021
H	-0.2813462592	1.3905277963	-2.2280173856
H	-1.2659639866	0.8565582097	-0.355927903
H	1.5507118304	-3.3604494967	-0.7926283997
H	2.2804584969	-1.8594109329	-1.3325074368
H	3.7816192563	-3.1658084448	0.1547644965
H	2.581747406	-3.1725431033	1.4365526368
H	4.3465855165	-1.5517558428	1.9386437544
H	2.8025169584	-0.7106932471	1.7357905024
H	2.1088625957	0.2789405226	-0.864328071
C	-2.3598466733	-1.0980691692	1.606395175
C	-3.400056914	-0.571562409	-0.6548445089
H	0.1026343631	-2.1294690173	0.6608968781
H	-3.1648039447	-1.8010120693	1.8426740381
H	-1.460793697	-1.4240739855	2.1427520738
H	-2.6421697651	-0.1155495942	2.000268074
H	-4.2306293418	-1.2493991697	-0.4385590161
H	-3.7025742777	0.4322278423	-0.3314164449
H	-3.2404531552	-0.5589792474	-1.7372106043
H	0.3398871512	3.7151596669	-1.5339669731
H	-0.0235329625	2.7467131738	-0.0966135927
H	1.6577929498	3.0803796248	-0.5348208076
H	1.4012631814	2.6096123106	-3.6057859148
H	2.7115497314	1.9224716845	-2.635713946
H	1.6891500551	0.8596420787	-3.6284918687
C	4.9972570369	1.1243878978	0.9449596714
H	5.4789865822	1.8356915416	0.2700339243
H	4.200623032	1.631777697	1.4958389693
H	5.745410165	0.7384318989	1.6418715601

DIG:4

C	-1.3678779592	-0.0473870458	-0.2129442094
N	-2.6624866616	-0.0338577152	0.3045745551
N	-0.9746303574	-1.0742070537	-0.8923312934
N	-0.6367234986	1.0897803453	0.119026412
C	-1.1882511782	2.4542401554	0.0538118732
H	0.3504168902	1.0592477446	-0.13996879
H	-2.7342962693	0.4366303705	1.1999618663
C	-3.5535098883	-1.1869792764	0.1602752099
C	0.2323547712	-1.0320689129	-1.6939170744
C	-1.39088562	2.9243778354	-1.3953773165
C	-0.2567106776	3.3889705011	0.8326604719
H	-2.1665389608	2.4482867935	0.5464715526
C	-5.0022389	-0.7180066374	0.3303814115
H	-3.4034935416	-1.5464706593	-0.861411803
C	-3.2008981737	-2.3301816744	1.1239819966

H	-0.0301851342	-1.3658909263	-2.709222589
H	0.671208885	-0.0299710829	-1.8014744605
C	1.3031679085	-2.01100324	-1.1728298674
H	2.1158348847	-2.0827752298	-1.9088066556
C	1.8693261526	-1.6678149072	0.2183590861
H	0.8467983751	-3.0065128495	-1.1105950512
H	2.4391718154	-2.5160140279	0.6220774587
P	2.9582537413	-0.188328787	0.2942817633
H	1.0350581107	-1.4878002838	0.9083722543
O	2.318028186	1.094376023	-0.1898954641
C	4.4755483124	-0.6200235152	-0.6401719572
H	4.2325365843	-0.7330195786	-1.700704125
H	5.197689134	0.1963143991	-0.5409366669
H	4.9304669519	-1.5475499626	-0.276564063
C	3.501640413	-0.1096457445	2.0438083543
H	4.2035642951	0.7210603269	2.1666273959
H	2.6318208979	0.078813256	2.6806907839
H	3.9852502359	-1.038276086	2.3650155313
H	-1.8309649414	3.9289917333	-1.4265176262
H	-0.4320840304	2.9547267733	-1.9268040345
H	-2.0596778488	2.241745814	-1.9305873558
H	-0.6229414854	4.4210791204	0.794178176
H	-0.1883736477	3.0820842649	1.8818880862
H	0.7542888262	3.3644128843	0.4102878613
H	-5.6986366986	-1.5511639528	0.1830413037
H	-5.1747739952	-0.3209097254	1.3403469494
H	-5.2446233277	0.0707077288	-0.3892463893
H	-3.8618620777	-3.1919330616	0.9689796551
H	-2.1694064104	-2.6500512369	0.9553118177
H	-3.3085305651	-2.0102930995	2.1695139191

DIG:4H⁺

C	2.0582831389	0.3838247789	0.0851894048
N	3.3361060142	0.6039471726	-0.2874510796
N	1.6055624157	-0.8931615285	0.1529049795
N	1.2499180724	1.3973907939	0.3846048608
C	1.6516383037	2.8095454547	0.5578361589
H	0.2259113497	1.2235002134	0.3799166007
H	3.5619434789	1.5446943067	-0.5810454918
C	4.4335364981	-0.3841152608	-0.3713531595
C	0.5014457696	-1.3891320923	0.9897690009
C	0.7667854322	3.4287314075	1.6446815243
C	1.5578127116	3.5784225296	-0.768347923
H	2.6893510561	2.8084979339	0.9132574849
H	4.2180266198	-1.1529719253	0.3799940816
C	4.5145402897	-1.0252361049	-1.7640913572
C	5.7422960968	0.3091470625	0.0184284077
H	0.9269993867	-2.0357338478	1.7669902611
H	0.0433337959	-0.5361885227	1.4887179318
C	-0.5441095871	-2.1934341197	0.1998208775
H	-1.2530105244	-2.6037438633	0.9297975831
C	-1.2990886808	-1.4360759457	-0.9096878425
H	-0.0546947747	-3.0647972311	-0.2550342692
H	-1.9491942026	-2.1356204465	-1.4496152224
P	-2.3174328781	-0.0046654309	-0.3528735769
H	-0.5888343133	-1.0394550431	-1.6465973464
O	-1.4758489829	1.0434979344	0.3607359611

C	-3.6554962895	-0.667255497	0.695015801
H	-3.2381161436	-1.1044220932	1.6066001898
H	-4.3175297966	0.1540410722	0.9862668058
H	-4.2416048587	-1.4264203454	0.1671471687
C	-3.1285031965	0.6212677778	-1.8619715724
H	-3.7711801979	1.4672510822	-1.5992354432
H	-2.3712930012	0.9713228191	-2.570122338
H	-3.7374947383	-0.1512715428	-2.342409489
H	2.2104921225	-1.598115723	-0.2443458384
H	1.880993188	4.6150022908	-0.6293206071
H	2.1819288209	3.1331607085	-1.5528511312
H	0.5240375529	3.5885122093	-1.1297582408
H	1.0302965174	4.4812003048	1.7856911673
H	-0.2896230935	3.3708882498	1.3620963654
H	0.8969685628	2.9097752517	2.5991909224
H	6.5670402371	-0.4087636581	-0.0047689129
H	5.9863300263	1.1129649329	-0.6874117759
H	5.6828887686	0.7326868394	1.0255034889
H	5.3045604414	-1.7825900867	-1.7867661577
H	3.5745217836	-1.508852906	-2.0544019675
H	4.7466058086	-0.2710309117	-2.5240792854

DIG:5

C	1.2427629523	0.2912619209	0.6371181526
N	2.5460406581	0.6514192061	0.2995603011
N	0.9817365295	-0.9466700643	0.8997354903
N	0.3532818941	1.3651555848	0.6087823838
C	0.6775937698	2.6918393863	1.1655250232
H	-0.6219526344	1.1135388677	0.7801774578
H	2.5964376176	1.40300931	-0.3792048587
C	3.6015788752	-0.35422939	0.1571634324
C	-0.2730950084	-1.3426135336	1.5084216836
C	0.713185663	2.6772066642	2.7016346361
C	-0.3392852453	3.7036001525	0.6266641871
H	1.6724932485	2.9746429382	0.8060925282
H	3.4543007103	-1.0522581907	0.9857090081
C	3.492757995	-1.1433998041	-1.1564497862
C	4.9625839603	0.3338937716	0.302997685
H	-0.0409291783	-2.0386594474	2.3273913062
H	-0.8428725435	-0.5162714588	1.9550613242
C	-1.1740987995	-2.1126265255	0.5199494023
H	-2.0310417833	-2.5429912909	1.0566026106
C	-1.659452651	-1.291049364	-0.6789856752
H	-0.5935836136	-2.9535272533	0.1205976302
H	-2.0680178685	-1.9366513068	-1.4666501307
S	-3.0494530499	-0.1513474478	-0.2497332361
H	-0.8380467969	-0.7003072791	-1.0984279511
C	-3.0845304111	0.7410895992	-1.8503343989
H	-3.8637907135	1.5032258651	-1.7758279645
H	-2.1138652212	1.2182173287	-2.0137078364
H	-3.3209445472	0.0453497583	-2.6609128274
O	-2.5650815074	0.8540378754	0.7928268613
H	4.2743213146	-1.9106261666	-1.2185621995
H	2.5186280623	-1.6359832437	-1.21197051
H	3.6067469346	-0.4794822047	-2.02441681
H	5.774834338	-0.3996342099	0.249916739
H	5.1264717693	1.0635668119	-0.5020934466

H	5.0322541932	0.8631679783	1.2588455191
H	-0.1414138448	4.7036387047	1.0283661543
H	-0.294640884	3.7533127857	-0.4668736019
H	-1.3579629101	3.4144846232	0.9098957924
H	0.984648869	3.6629868401	3.0993440902
H	-0.2690279333	2.4044021368	3.1058506856
H	1.4479267903	1.9492720716	3.0618721487

DIG:5H⁺

C	0.9236495109	1.3997652884	-1.8234047057
N	1.2011671721	0.114431052	-1.1399971925
C	0.2933918871	-0.6623406591	-0.5480656855
N	0.6038223109	-1.9239751641	-0.1641483157
C	1.8838606881	-2.5916556853	-0.4029923408
C	2.8914016864	-2.4199363548	0.7578095019
C	4.3457289125	-2.613189402	0.3039789678
S	4.983675363	-1.0239028063	-0.4026989556
N	-0.966876373	-0.223461295	-0.3536009688
C	-2.1436552767	-1.0296147861	0.0396761947
H	-1.9883803277	-2.0306671127	-0.3792598662
C	1.0881399838	2.5828867418	-0.859221921
C	1.8438510391	1.514239214	-3.0426723502
H	-0.1118848867	1.3544469426	-2.1814933209
H	-1.1210738001	0.7695208579	-0.4583495685
H	1.6722845042	-3.6534129286	-0.5649231302
H	2.3007071345	-2.2025456751	-1.3322726864
H	2.7691376324	-1.4263266462	1.2073941485
H	2.6676038364	-3.1409489761	1.5521890141
H	5.0040184714	-2.8528488901	1.1455730156
H	4.4357467789	-3.4055451381	-0.447507454
H	2.1941643349	-0.1647005207	-1.1237900309
C	-2.2886329984	-1.1188556225	1.5659349782
C	-3.3864505672	-0.4241408643	-0.6187310555
H	-0.0261206769	-2.3594406779	0.4940864128
H	-3.1407632612	-1.7542171811	1.8271792219
H	-1.3972721572	-1.5379694259	2.0478707653
H	-2.4603739549	-0.1264990993	1.9969416473
H	-4.2684302524	-1.0209732475	-0.3697234655
H	-3.5665518306	0.5955384693	-0.2558293536
H	-3.2863521485	-0.3972787745	-1.7079372395
H	0.8444204211	3.5213013729	-1.3673900963
H	0.4381866847	2.4954405037	0.0196186961
H	2.1224301828	2.6465906337	-0.5048186976
H	1.6507826835	2.4576130038	-3.5620697237
H	2.8957516747	1.4926888189	-2.741129395
H	1.6706622405	0.6926929585	-3.744284327
C	6.3546442875	-1.7120963178	-1.3854323186
H	6.8492172146	-0.8753359198	-1.8836760576
H	7.0602220591	-2.2129936595	-0.715905718
H	5.9548815965	-2.4064869166	-2.1292743268
O	3.9323262197	-0.5425681107	-1.4153602967

DIG:6

C	1.2838620462	0.3407286911	0.6436492104
N	2.6012068413	0.6682572523	0.3379254965
N	0.9779661241	-0.8919536944	0.8771829373

N	0.4284444515	1.4438243836	0.621167328
C	0.7795326465	2.7439213503	1.2240282386
H	-0.5507085668	1.209482813	0.7636234392
H	2.6885860146	1.4359861134	-0.3185057359
C	3.6325871719	-0.3632814153	0.1981109042
C	-0.2941947897	-1.2655196852	1.4623651745
C	0.8491239679	2.6739236625	2.7570477798
C	-0.23318091	3.7875523031	0.742719372
H	1.7698848341	3.0280079957	0.8527438482
H	3.4453967841	-1.0753275704	1.0064332331
C	3.5339742062	-1.1181646465	-1.1359289599
C	5.0078832507	0.2827344908	0.3935105764
H	-0.0885641652	-1.9333251828	2.3112232533
H	-0.8765950094	-0.4263062487	1.8699563505
C	-1.1602758757	-2.0690716355	0.4736315539
H	-2.0267066903	-2.5013366512	0.9880472858
C	-1.6389201749	-1.2810033544	-0.7525952269
H	-0.5560801966	-2.9023186394	0.0960671282
H	-2.0051062007	-1.9513275764	-1.537270784
S	-3.0480949337	-0.1912746645	-0.3676527133
H	-0.8408862795	-0.6518029432	-1.1596857311
C	-3.5049125325	0.495735943	-1.9784656157
H	-4.337507421	1.1778810017	-1.7909098367
H	-2.6562309846	1.0435228609	-2.3934581438
H	-3.8218843852	-0.3103741722	-2.6431723456
O	-4.1657934728	-1.021936804	0.1080142788
O	-2.5769970857	0.9407479644	0.4634763304
H	4.2948625116	-1.9057954496	-1.1968993339
H	2.5485078671	-1.5821837274	-1.2274345225
H	3.6880533255	-0.4383121329	-1.984973719
H	5.8000701397	-0.4722577708	0.3400671021
H	5.2113842672	1.027664398	-0.388158451
H	5.0698194885	0.7846787167	1.3644777047
H	-0.0003790567	4.7728783602	1.1610382968
H	-0.2257889453	3.861860488	-0.3498532453
H	-1.2489976454	3.5174114063	1.0552134427
H	1.145924599	3.64100923	3.1811720225
H	-0.1275910208	2.4040037621	3.1768248621
H	1.5800318049	1.9231197778	3.0752122148

DIG:6H⁺

C	0.8605729848	1.287484868	-2.0204064707
N	1.0669827077	-0.0657116534	-1.44986802
C	0.1814894036	-0.7567070765	-0.7285552721
N	0.4239171054	-2.0440007382	-0.3808730997
C	1.6280155663	-2.8056674478	-0.7165918761
C	2.7431165047	-2.6856495597	0.351963756
C	4.1620480987	-2.8769810851	-0.2088767546
S	4.7347805195	-1.2978749848	-0.9268620802
N	-0.9934242272	-0.2029182559	-0.3718754364
C	-2.1602365215	-0.8861042632	0.230465258
H	-2.170267181	-1.9043229236	-0.1762307476
C	1.2910089117	2.3720808694	-1.0228804913
C	1.6232176093	1.3794792261	-3.3453179654
H	-0.2095237106	1.3824399475	-2.2406054879
H	-1.0759623425	0.7970858463	-0.4888386372
H	1.3241744569	-3.8504570416	-0.8313331953

H	1.9793711521	-2.4748364655	-1.6943776168
H	2.690198428	-1.7084744988	0.8460056958
H	2.5826615104	-3.4312504168	1.1380184118
H	4.8730896383	-3.1269761269	0.5833348288
H	4.2111102534	-3.6432017561	-0.989594611
H	2.0121815962	-0.4404887854	-1.5711034484
C	-2.0609412113	-0.933026924	1.7620348484
C	-3.4306641695	-0.1738315605	-0.2418008879
H	-0.1696497075	-2.4293870939	0.3393153989
H	-2.9123113854	-1.4799470985	2.1793868497
H	-1.143692577	-1.4249821896	2.1064848645
H	-2.0693888297	0.0791517477	2.1806844761
H	-4.3128770104	-0.6779014192	0.1625864366
H	-3.4538615158	0.8642607652	0.1127046975
H	-3.5046982556	-0.1748607398	-1.3333996188
H	1.1159176027	3.3658188035	-1.4472139171
H	0.7403246369	2.3061683352	-0.0770983228
H	2.3581082982	2.2791858758	-0.7952470653
H	1.4705030453	2.3680100391	-3.788161858
H	2.697172226	1.2354841439	-3.1899346527
H	1.2714252632	0.6257196755	-4.0562585301
C	6.331109557	-1.6572429239	-1.6765941584
H	6.6794460873	-0.7165289496	-2.1103943237
H	7.0231792148	-1.9904819737	-0.900365325
H	6.2079522648	-2.4108853317	-2.4569300565
O	4.9073819984	-0.3342090967	0.1677481199
O	3.7888010035	-0.9579747629	-2.0273727153

DIG:7

C	0.9884968658	2.4834970636	0.5935894496
N	0.7107918848	1.0950343335	0.1900859182
C	1.6911221193	0.1133869078	0.0565653539
N	1.5721313745	-1.1412074371	0.3395881794
C	0.3824351338	-1.5835691786	1.0388101951
C	-0.8020984963	-1.8677663626	0.0894084571
C	-2.1261796177	-2.0802119516	0.8268609924
C	-2.7235312484	-0.8058192937	1.4136344176
C	-4.0100369533	-0.9562527509	2.2047189827
N	2.8979323858	0.5930987022	-0.4508513236
C	3.9817701306	-0.3329769552	-0.7954117024
O	-2.2082811748	0.290438862	1.2587392928
H	-0.1736948119	0.7535159707	0.5552863545
H	2.7832026667	1.3482535072	-1.1181901149
C	-0.2884629449	3.3055205924	0.3913038287
H	1.7576638624	2.885700778	-0.075958341
C	1.5140723248	2.5832573588	2.0340426321
H	4.0135668852	-1.0605392781	0.0199478053
C	3.7159898351	-1.0913219264	-2.1042458165
C	5.2997842817	0.4463888703	-0.8383304467
H	0.6266172011	-2.5146628256	1.5692838764
H	0.0608615643	-0.8670134294	1.8136446441
H	-0.9174876323	-1.0341383645	-0.6119241763
H	-0.5680198417	-2.7519442641	-0.5145653057
H	-2.8869156011	-2.5122068349	0.1588660375
H	-2.0181981701	-2.8125486242	1.6419034484
H	6.140092297	-0.2257512872	-1.0454007293
H	5.2853316226	1.2073263661	-1.630961316

H	5.4853178864	0.9535538887	0.1141199267
H	4.5218932593	-1.8054687963	-2.3137449937
H	2.775412257	-1.6427894396	-2.0283544056
H	3.65494061	-0.3978582841	-2.9542427463
H	1.7495829085	3.6226114681	2.2946092296
H	0.7634089306	2.2157843692	2.7445801675
H	2.4236190075	1.9858853018	2.1515038968
H	-0.1177238974	4.3539251199	0.659137982
H	-0.6185998379	3.2607508987	-0.6517658991
H	-1.1011469185	2.9218872563	1.0197595368
H	-4.3777745026	0.0253782766	2.50986458
H	-4.7747022522	-1.4712653205	1.61080811
H	-3.8319653936	-1.5716092873	3.0957830218

DIG:7H⁺

H	4.1304025361	1.0978385673	-0.2665207412
C	3.9305560844	0.0488707704	-0.0419150151
C	2.4465729808	-0.1838409156	0.0876843019
O	1.6526568377	0.7507190222	0.0739284015
C	1.9716116659	-1.6228387564	0.2542933997
C	0.4655910855	-1.7420322308	0.510470381
C	-0.3818005699	-1.461636152	-0.748993732
N	-1.7574965396	-1.0495929117	-0.4542010638
C	-2.1367299193	0.2188588041	-0.1766668431
N	-3.4480565416	0.4925616574	-0.0392639752
C	-4.5831694068	-0.399945645	-0.3664917407
C	-5.7500434129	0.4622159115	-0.8558498431
N	-1.2227410821	1.1891723952	-0.0883768227
C	-1.4994822441	2.6437673959	-0.0353524057
C	-0.3886856172	3.3791334775	-0.7916579142
C	-1.6344732392	3.1291354101	1.4147852475
C	-4.9786512023	-1.2784988511	0.8289586981
H	-0.2368710689	0.9242188602	0.0039800809
H	-3.6849308776	1.3896800749	0.3611960313
H	-2.4235885059	-1.7778997452	-0.2407597719
H	-2.4424412118	2.8062142467	-0.570826956
H	-4.2497396202	-1.0304675488	-1.1988110771
H	0.0694817118	-0.6799456193	-1.3644251329
H	-0.4458056427	-2.3553027498	-1.3768709339
H	0.1872044108	-1.0374286057	1.3017071848
H	0.2351989107	-2.7440399494	0.8882302955
H	2.278163434	-2.1898568544	-0.6374047496
H	2.5389470081	-2.071776373	1.0804210268
H	-6.5925323947	-0.1759842001	-1.1367416637
H	-6.0990667385	1.1376998115	-0.0647932966
H	-5.4657530862	1.0588480541	-1.7278511402
H	-5.7886497322	-1.9575952688	0.5448055062
H	-4.1437508723	-1.8870448046	1.1963413407
H	-5.3301124532	-0.6618827806	1.6634100452
H	-1.8759253127	4.196597225	1.4344618984
H	-2.4215383695	2.5946526275	1.9598050463
H	-0.6945401141	2.9832035848	1.9576824429
H	-0.5746780395	4.4567570535	-0.7639850071
H	0.5887517047	3.1878989346	-0.3367140006
H	-0.3503393735	3.0639006653	-1.8388737896
H	4.3597539191	-0.5904580207	-0.8222570745
H	4.4307638988	-0.2209785668	0.8971743619

DIG:8

C	0.9681692833	2.4558077848	0.6272120114
N	0.6990811989	1.0775715704	0.1861171528
C	1.6850841981	0.1031953458	0.0483052912
N	1.5754386175	-1.1532733615	0.3274319386
C	0.3933451214	-1.5998013861	1.0386872019
C	-0.8013533534	-1.8848922259	0.1030094144
C	-2.1193200264	-2.0974611307	0.8554331504
C	-2.6875634918	-0.7904960465	1.4232249444
N	-3.8455161656	-0.8589155116	2.1543196924
C	-4.4195279115	0.3617473901	2.7045278116
N	2.8875259488	0.5924054645	-0.4636551588
C	3.9770312669	-0.3253881553	-0.8106604456
O	-2.126790496	0.2914621164	1.2225815334
H	-0.1895993439	0.7266019866	0.5369778795
H	2.7605551239	1.3413983454	-1.1359546161
C	-0.2785020813	3.3020777418	0.3486873365
H	1.7918752301	2.8520023999	0.0232902872
C	1.3876649108	2.5221530297	2.1043245344
H	4.0200371267	-1.049547454	0.0073199829
C	3.7113176116	-1.0919113326	-2.1148974071
C	5.288201912	0.4649980493	-0.8647460988
H	0.6458981661	-2.5318346567	1.5642292243
H	0.0769663579	-0.8843714635	1.815099915
H	-0.923502025	-1.0574271712	-0.6027385226
H	-0.578370829	-2.7767454451	-0.494524685
H	-2.868194126	-2.5423350049	0.1860398727
H	-1.9744706743	-2.8190205438	1.6715824252
H	-4.5170854992	0.2781999937	3.7947486103
H	-3.7649993135	1.1956441283	2.4582319353
H	-5.4169806007	0.5420274164	2.2820735648
H	6.1331021207	-0.2004653161	-1.0750973034
H	5.2617716321	1.2229411218	-1.6599883292
H	5.4754956178	0.9774450308	0.0845453554
H	4.5227282156	-1.7994282049	-2.3260511303
H	2.7762478599	-1.651402723	-2.0307750168
H	3.6390069847	-0.4024890316	-2.9673648689
H	1.6112277464	3.5534515664	2.4049480367
H	0.5830715148	2.1451037792	2.747225348
H	2.2814293541	1.9137187308	2.2763631549
H	-0.11790187	4.3406343386	0.6589998581
H	-0.5257801057	3.289836939	-0.7179834296
H	-1.1415863298	2.9095013571	0.8991827794
C	-4.6047464598	-2.0691478184	2.4219911155
H	-5.6171529085	-1.9872812357	2.0029406019
H	-4.1254737712	-2.9446067265	1.9890750812
H	-4.7006477374	-2.2280496814	3.5046589705

DIG:8H⁺

C	4.1282016473	1.1174325071	-0.2031084106
N	3.6513997933	-0.2534292903	-0.0215616678
C	2.3295617465	-0.4966609624	0.136978062
O	1.4906537883	0.4237399917	0.1136860261
C	1.8760390924	-1.9465672581	0.3548130884
C	0.3639158004	-2.045098546	0.5868710865

C	-0.4590995494	-1.7931471854	-0.6930330421
N	-1.8439027782	-1.3895729102	-0.4304168512
C	-2.2280928685	-0.1235184364	-0.1465107583
N	-3.5426883438	0.1412325604	-0.0079152865
C	-4.6703989091	-0.7596965892	-0.3327377035
C	-5.8445454362	0.0923310636	-0.8228211475
N	-1.3195525468	0.849399076	-0.0550076813
C	-1.6106695443	2.2987633739	0.0146657462
C	-0.5115420224	3.0544934224	-0.7381839779
C	-1.7416212177	2.7668711428	1.4711587284
C	-5.0592134119	-1.6397239772	0.8639989629
H	-0.3256999528	0.5917688746	0.0291701167
H	-3.7857317771	1.0367486051	0.3918097361
H	-2.5034697099	-2.1212295287	-0.2084708378
H	-2.5580587806	2.4604441957	-0.5135843148
H	-4.3333587268	-1.3893132242	-1.1642672635
H	0.0003588881	-1.014855373	-1.3056989339
H	-0.5042807413	-2.6967503256	-1.3084521814
H	0.077896448	-1.3207502024	1.3556890116
H	0.1250772208	-3.0387972789	0.9823717547
H	2.1743660262	-2.5621150204	-0.504424091
H	2.4002868693	-2.3637073184	1.2222017997
H	-6.682624283	-0.5523694251	-1.1021770229
H	-6.1979080249	0.7667327532	-0.0327082317
H	-5.5649190378	0.689824592	-1.6957597847
H	-5.8634129895	-2.3264007401	0.5813112765
H	-4.2189110395	-2.2400464995	1.2324544096
H	-5.4157446628	-1.0244454606	1.6973453047
H	-1.9906103413	3.8323352447	1.5054126239
H	-2.5217273738	2.2197757026	2.0137317705
H	-0.7974999294	2.6197289421	2.0063678529
H	-0.7086500299	4.1298653877	-0.6985942167
H	0.4676938734	2.8649421493	-0.2874114409
H	-0.4730223452	2.7493240712	-1.7883156624
C	4.7045784403	-1.2643141986	0.0144782334
H	5.3173155118	-1.1880315365	-0.8909057186
H	5.3553191915	-1.104603905	0.882905394
H	4.2963811222	-2.2713207907	0.0662675175
H	4.8175962307	1.3829711588	0.6066104493
H	4.6605275011	1.2041101522	-1.1571364118
H	3.2780761824	1.7953890156	-0.1952423128

DIG:9

C	0.8149865078	2.4054794856	0.4994016537
N	0.6351692514	1.0156099695	0.049316564
C	1.6622693708	0.0757904856	0.0128197666
N	1.5712216677	-1.1819580584	0.2935512565
C	0.3455292637	-1.6641011448	0.8998545917
C	-0.7502984095	-2.0010640777	-0.1352049016
C	-2.124904879	-2.2252450248	0.5019708138
C	-2.7769574835	-0.9241383523	0.9749658642
N	-4.0068233726	-1.0272536226	1.5455659067
N	2.8896917474	0.6031833446	-0.3915659732
C	4.0374563037	-0.2784345767	-0.6255665608
O	-2.2361513738	0.1809136631	0.8454892448
H	-0.2707881989	0.6375628179	0.3204317447
H	2.799749461	1.3413309951	-1.0816069736

C	-0.4311005434	3.2042432269	0.1024193706
H	1.6753400028	2.8274210939	-0.0318195769
C	1.0966487697	2.4959524246	2.0075778723
H	4.0295916918	-0.9932691502	0.2016815413
C	3.9205874955	-1.0659796881	-1.9391520068
C	5.3202281916	0.5571336223	-0.5684820359
H	0.5812749571	-2.5812845634	1.4583303769
H	-0.0651065928	-0.9528839947	1.6349240802
H	-0.8264655501	-1.1904502233	-0.8671400897
H	-0.4525238903	-2.8982157771	-0.6905588864
H	-2.8075630768	-2.7142723053	-0.2075497603
H	-2.0438451595	-2.9145464048	1.355437889
H	6.2031404218	-0.0801308395	-0.6924351568
H	5.3413052782	1.3065489808	-1.3719381458
H	5.4016887463	1.0842916434	0.3877136295
H	4.77230905	-1.7458173186	-2.0656197201
H	3.0018367046	-1.6578556498	-1.934477655
H	3.9035641529	-0.3874871533	-2.8032289029
H	1.2557837054	3.5364943017	2.3173548575
H	0.2506943254	2.0942688566	2.5783521613
H	1.9920755991	1.9210339625	2.2651559747
H	-0.3361646486	4.2496042999	0.4171390284
H	-0.5794480477	3.1778028105	-0.9822737449
H	-1.325592903	2.7826165271	0.5755975423
C	-4.7825000676	-2.2583120676	1.7487919801
C	-5.9299541231	-1.8062755753	2.6656270047
C	-6.1524934347	-0.3400925163	2.2570772775
C	-4.7307466961	0.1747166969	1.9906076409
H	-5.1664364274	-2.6425814918	0.7922525099
H	-4.1711560672	-3.0455085009	2.2013323676
H	-5.6110253699	-1.8616320379	3.7133012771
H	-6.8212190299	-2.4305818468	2.5531679899
H	-6.6713003539	0.2447179946	3.0221066669
H	-6.7492495726	-0.2917204801	1.3381075151
H	-4.2634403894	0.5804230723	2.8976734321
H	-4.6779890046	0.9509381665	1.2226886981

DIG:9H⁺

C	4.2124775583	1.0258496369	-0.6242855423
N	3.4121135052	-0.0589523428	-0.0178192088
C	2.0706417567	-0.0525793904	-0.0787551165
O	1.4572349249	0.85612409	-0.6748626927
C	1.3274999797	-1.1956167778	0.6168315595
C	-0.1923924757	-0.9994734369	0.5862651989
C	-0.7968254371	-1.236786664	-0.8136449949
N	-2.0852121949	-0.5683624758	-1.0213136335
C	-2.2210941139	0.7234596	-1.4024060523
N	-3.4568821053	1.2010348759	-1.65385056
C	-4.7075698698	0.4194350204	-1.7648681965
C	-5.6096153453	1.0938698328	-2.8024325019
N	-1.1426521155	1.4893730299	-1.570411451
C	-1.116834424	2.8227739774	-2.2110491454
C	0.1902327956	2.9582576944	-2.9990006377
C	-1.2846183906	3.9378962432	-1.1691600373
C	-5.407165018	0.2693315799	-0.4062959871
H	-0.2420557809	1.1707114854	-1.1802252116
H	-3.5463698192	2.2039397474	-1.7383226508

H	-2.903414922	-1.0122209057	-0.6298434748
H	-1.9500982858	2.8529999088	-2.9234816631
H	-4.4223997796	-0.5671495059	-2.1479010645
H	-0.1170250849	-0.8892121628	-1.594158159
H	-0.961625956	-2.3044275404	-0.9879483195
H	-0.4210658164	0.0195273509	0.9145737782
H	-0.6622010086	-1.6785020299	1.3065417589
H	1.6087531849	-2.1496185386	0.1487880923
H	1.6719899476	-1.2656250666	1.6558245035
H	-6.5304490022	0.5173965886	-2.9283622417
H	-5.8950922148	2.1026151797	-2.4784954763
H	-5.112803227	1.1647918304	-3.7747257747
H	-6.3021434242	-0.3524979799	-0.5091323814
H	-4.7600985966	-0.1946898633	0.3474029031
H	-5.715835379	1.2467727885	-0.019601628
H	-1.2968959615	4.9163113557	-1.660068126
H	-2.2152377047	3.8339762388	-0.5986148472
H	-0.4529056441	3.9237631051	-0.4567172085
H	0.2390260348	3.9454581764	-3.4681296867
H	1.0550738449	2.8426970526	-2.3381513977
H	0.2542232147	2.1995567381	-3.7850731114
C	4.2565419655	-1.0628088175	0.6604370886
C	5.6728495146	-0.7207038648	0.1734323097
H	4.1724790512	-0.9569703592	1.7504800809
H	3.9529979433	-2.0796386943	0.3936245735
C	5.616301003	0.8000681199	-0.0476911676
H	4.1934156095	0.928371238	-1.7166891633
H	3.7782613588	1.9952412661	-0.3684565872
H	6.400606661	1.1642373343	-0.7160967246
H	5.7200115185	1.3266980281	0.9080342081
H	6.4381338476	-1.0268347013	0.8912169019
H	5.8747828775	-1.2350629954	-0.7730501333

DIG:10

H	4.529293908	-0.5211975069	0.3710521206
C	3.7849782109	0.2781522652	0.2811647593
C	2.5823429747	-0.1917330824	-0.5435217051
N	1.5872403642	0.8845193761	-0.5809186113
C	0.2542026911	0.6062462655	-0.893590732
N	-0.5370924913	1.7472763125	-1.0183310484
C	-0.4177616087	2.9165450858	-0.131986473
C	-1.1556850573	2.7006880742	1.199435202
H	-1.0445222533	3.570071321	1.8595290119
N	-0.1170229686	-0.6196606552	-1.0545650852
C	-1.5317968112	-0.9048107263	-1.1943327787
C	-2.0141169975	-0.7901312994	-2.6554936587
C	-3.539716181	-0.8768693437	-2.8036327596
C	-4.2523828746	0.354308069	-2.3158603566
N	-5.6193809512	0.4755978259	-2.3405999577
H	-2.1580530527	-0.2621852026	-0.5556095302
H	-1.704624549	-1.9370601615	-0.8576438
H	2.0922569748	-1.0249968919	-0.0328358216
C	2.9944803435	-0.6654591521	-1.9452882723
H	0.6438966895	3.0545165012	0.0911918799
C	-0.92484016	4.1590427912	-0.8724762615
H	-1.6696171576	0.1571875923	-3.0836642605
H	-1.5475403769	-1.5885520894	-3.2442214547

H	4.2806935021	1.1360218637	-0.1941197484
H	3.4752663652	0.581263321	1.2866732444
H	-2.2262443284	2.5390725898	1.0241624656
H	-0.7585843652	1.8226629969	1.7198952225
H	-3.7993345378	-1.0445420362	-3.8599416128
H	-3.9158926651	-1.7603310513	-2.2639228326
H	-1.5043850265	1.5677439361	-1.2887027577
C	-5.9263946159	1.7305275555	-1.8455855103
C	-6.5688041116	-0.5229458005	-2.8031002377
H	-6.9472568223	2.0727304617	-1.7609928838
C	-4.7253797547	2.3121287507	-1.5424620252
N	-3.6896815444	1.4532334598	-1.8371839521
H	-4.5437311061	3.2952802027	-1.1300725597
H	-6.5047975988	-1.4342280591	-2.1991394378
H	-7.5785927366	-0.1174797239	-2.7172760665
H	-6.3837734025	-0.7820618713	-3.8507833317
H	1.9284591512	1.7328642647	-1.020737876
H	-0.8375882624	5.0519080727	-0.2426033196
H	-0.3544441591	4.322285281	-1.7927364179
H	-1.9794653277	4.0418028413	-1.1497840542
H	2.1124186298	-1.0031829719	-2.4950575842
H	3.4764231515	0.1462508674	-2.5076096336
H	3.7069698995	-1.4974923188	-1.8844474974

DIG:10H⁺

N	2.585842547	0.0916922932	1.2707714043
C	2.1618770549	-0.2917488837	0.0703016061
N	3.0994091771	-0.0109249579	-0.8832469603
C	0.8231507035	-0.9114041842	-0.199575208
C	-0.3562187514	0.0824936085	-0.1015305387
C	-0.5840396827	0.6851366865	1.2913025594
N	-0.9796892135	-0.3169298898	2.2922636088
C	-0.3431433528	-0.6278981574	3.4447909057
N	0.9444082236	-0.326348099	3.6152770524
C	1.6721205854	-0.4193992193	4.8985336919
H	0.937847597	-0.2496782171	5.6950450881
N	-1.0451850166	-1.2375673975	4.4239652475
C	-2.5146596041	-1.3656697985	4.5306370307
C	-3.0223577962	-2.6555315143	3.8699541433
H	-1.3812215647	1.4357894746	1.2354982215
H	0.3137747711	1.189959271	1.6481870222
H	-0.2023785379	0.9159623148	-0.7979117108
H	-1.2721219558	-0.427135059	-0.4289653547
H	0.6660033753	-1.7307032773	0.512281989
H	0.8139910345	-1.3680499562	-1.1940484014
H	1.5314164223	-0.1453770878	2.7705938531
H	-2.9398026824	-0.493817917	4.0199787252
C	-2.9027128082	-1.2885842019	6.0102116847
H	-1.8839835288	-0.7460123444	2.1563113549
C	2.3192295159	-1.8015194802	5.0755808229
H	-0.5069792427	-1.6954627086	5.1464993779
C	2.7075613158	0.7073000371	4.9655771081
H	2.832101264	-1.8603863534	6.0410137891
H	1.5838268969	-2.6140088504	5.0346635608
H	3.0560274639	-1.9827521758	4.2857419643
H	3.2132877143	0.6886325641	5.9356407071
H	3.4691626715	0.5851714715	4.1881933249

H	2.2354399364	1.6864757895	4.8417318802
H	-4.1144475157	-2.7055508269	3.9259169183
H	-2.7359159547	-2.7239803265	2.8138728551
H	-2.616556322	-3.5364038697	4.3795797416
H	-3.9898934813	-1.3457708941	6.1154689847
H	-2.4733365013	-2.1266649343	6.5733753182
H	-2.5624364338	-0.3518187	6.4617406154
C	4.1727351543	0.5770971842	-0.2412430635
C	3.8373624121	0.6349790925	1.0834135914
H	4.4173247636	1.0324271214	1.9041229706
H	5.0551718873	0.8876629846	-0.7797732819
C	3.0206673151	-0.2927984752	-2.3143189671
H	3.9206462999	0.0936995622	-2.7939508845
H	2.9632804796	-1.3697930342	-2.4965605142
H	2.1516163644	0.1985813364	-2.7602158343

DIG:11

H	4.2474296524	-0.994449474	0.7141225309
C	3.5236634153	-0.1715896503	0.7149284031
C	2.4192772023	-0.4202107908	-0.3173605209
N	1.4414430625	0.6695272741	-0.2323751457
C	0.1526414914	0.5029762829	-0.7473532014
N	-0.6085737116	1.6745927469	-0.7150231767
C	-0.595593166	2.605755481	0.4250616271
C	-1.3924282415	2.0626823349	1.6223825563
H	-1.3489967991	2.7528700403	2.4743825427
N	-0.2077796959	-0.6475087857	-1.2033784391
C	-1.5983841798	-0.8527452568	-1.5663443408
C	-1.9097283332	-0.3865977754	-3.0018213426
C	-3.4024454158	-0.430599584	-3.3607188352
C	-4.2575883486	0.5099300042	-2.5480603297
C	-5.6164077401	0.4567025493	-2.3393199883
H	-2.2913789805	-0.3570398063	-0.8676985765
H	-1.8108821533	-1.9287705667	-1.4969980458
H	1.8690978162	-1.3272420976	-0.0528783247
C	2.9837909649	-0.5996448873	-1.7344709897
H	0.4442262996	2.7281777547	0.7422464881
C	-1.1190151537	3.9671951969	-0.0443319012
H	-1.5436243212	0.636926008	-3.1397205317
H	-1.3487163514	-1.0127273705	-3.7061589066
H	4.0759936999	0.7513449735	0.4897607986
H	3.1034589	-0.0770780586	1.7215810824
H	-2.4456954063	1.9196123252	1.3509449094
H	-0.9882027215	1.0967820429	1.9429079504
H	-3.512156051	-0.1868335049	-4.4276218955
H	-3.788847133	-1.4530359652	-3.2470547656
H	-1.5387956891	1.5799620967	-1.1194686602
N	-5.9379269795	1.5573256995	-1.5671518903
H	-6.3704965042	-0.2455252827	-2.6644618309
C	-7.2572744944	1.9270251521	-1.086813439
C	-4.7691671483	2.218074256	-1.3386088216
N	-3.7402748303	1.6234056856	-1.9090582711
H	-4.7307399747	3.1231434667	-0.7459632175
H	1.8361729293	1.5797959943	-0.4459920608
H	-7.1754695799	2.8415348834	-0.4950408836
H	-7.9383109395	2.110678077	-1.9243060195
H	-7.675284867	1.1364555129	-0.4550295066

H	2.167549241	-0.7909986508	-2.4354416013
H	3.527512885	0.2991039526	-2.0568673336
H	3.682757153	-1.4443564507	-1.7743154159
H	-1.1183212611	4.6907078738	0.7789464241
H	-0.5014229804	4.3607709762	-0.8580887681
H	-2.1461765611	3.8794393169	-0.4190143351

DIG:11H⁺

N	2.560045421	0.145562888	1.2524867883
C	2.1207992373	-0.3039662998	0.0180642215
C	3.09501638	-0.0635046035	-0.9201446803
C	0.7650321439	-0.9177087838	-0.1690213838
C	-0.4033661811	0.0861379504	-0.0734433686
C	-0.6133958474	0.7253169332	1.3057350057
N	-1.0207535481	-0.2480552845	2.3312940534
C	-0.3658768324	-0.5854395759	3.4623872044
N	0.9259038989	-0.2872962124	3.6203493565
C	1.6739746315	-0.4122666292	4.8883626932
H	0.9545185255	-0.2567100837	5.701007781
N	-1.0516224894	-1.2106873786	4.4439669872
C	-2.5178716309	-1.3686288651	4.5526384956
C	-3.00587156	-2.6481328196	3.857522831
H	-1.4024820645	1.4837166876	1.2407441332
H	0.2908870394	1.2281858955	1.6495844189
H	-0.2465838778	0.9002054239	-0.791477826
H	-1.3312607331	-0.4178690287	-0.3767846485
H	0.6181628036	-1.719937119	0.5665710941
H	0.7258834182	-1.3971163647	-1.153007358
H	1.4992303994	-0.0910118588	2.7735399534
H	-2.960324409	-0.4903053669	4.0683469007
C	-2.9011296062	-1.3402751884	6.0349597906
H	-1.9196714532	-0.6868700948	2.1906401601
C	2.3186332409	-1.8003052038	5.0246010245
H	-0.5013121576	-1.6866685093	5.1451446015
C	2.7153364003	0.7086254219	4.9631546862
H	2.8526432787	-1.880721541	5.9769828249
H	1.5789724209	-2.6088487327	4.9841959298
H	3.0358390693	-1.9688533985	4.2142376242
H	3.231862877	0.67229989	5.9270277854
H	3.4680192244	0.5944625891	4.1755999619
H	2.2463467096	1.6916167654	4.8596108315
H	-4.0961995654	-2.7209157691	3.9212234076
H	-2.7275091895	-2.6794858598	2.7975701876
H	-2.5783994971	-3.5356194181	4.3371264633
H	-3.9864330498	-1.4234311966	6.1420446085
H	-2.4524309374	-2.1842782767	6.5737983142
H	-2.5788551356	-0.4092110625	6.510727657
N	4.1416997557	0.5395433546	-0.2522988213
C	3.769058157	0.6422796775	1.0475061243
H	4.4101862576	1.084170398	1.7982143181
C	5.4091094165	0.9684897443	-0.8334448338
H	3.1393948822	-0.2665764933	-1.9800238
H	6.0163116955	1.4336614456	-0.0548487249
H	5.9504456798	0.110538389	-1.2416876175
H	5.2334358011	1.6977795646	-1.6288591564

DIG:12

N -4.8498570833	0.795225617	0.5974597149
C -4.0265272821	-0.1022268628	-0.0856443362
N -2.7830902089	0.0388095291	-0.394635525
N -4.6824179462	-1.2883664157	-0.4204683239
C -2.1139527534	1.3225457717	-0.31568391
C -1.0680516986	1.3551766651	0.8137913965
C -1.6551368781	1.3923353606	2.2453435137
C -2.1890916569	2.74831938	2.6455427554
C -6.2238012968	1.0993975014	0.1668448091
C -7.0190579861	1.6330789597	1.3629369876
C -6.2544853149	2.0745545055	-1.0218072428
H -5.8041539057	3.0365457555	-0.7462960882
H -5.6924344316	1.6665262768	-1.8686049178
H -7.2831808647	2.2643206204	-1.353024958
H -6.5787971483	2.5644306901	1.7406263243
H -8.0563314894	1.8442057074	1.0789227734
H -7.0204489308	0.9083551675	2.1835211505
H -6.6784665525	0.1594266469	-0.1598250441
C -3.9614705632	-2.4006379782	-1.04506532
C -3.0973341039	-3.179771696	-0.0423229147
C -4.9708032593	-3.305709859	-1.7591520725
H -5.6718251812	-3.7588643331	-1.0445339193
H -5.5543518901	-2.7387000961	-2.4918487301
H -4.4584474193	-4.1234760264	-2.27843129
H -2.5396605866	-3.9806497451	-0.5434125267
H -3.7201870714	-3.6427007578	0.7354134908
H -2.3816882991	-2.5039131179	0.4327326026
H -3.2971684068	-1.9414199787	-1.7821696966
H -5.3583804529	-1.5784626469	0.2782647344
H -2.7956457858	2.1820054696	-0.2167065144
H -1.5711471515	1.4688820467	-1.2612252805
H -4.3632512566	1.6041672489	0.9859254668
H -0.4510507089	0.453373234	0.7194296978
H -0.4023610984	2.2178186871	0.671612676
H -0.8745118267	1.0997227748	2.9575673672
H -2.4545815678	0.6464325117	2.3207350384
N -3.4035544857	3.103749339	2.1830860613
C -3.8819218736	4.3138676286	2.4995147853
C -3.1962044003	5.2353331523	3.2876584946
C -1.9393459504	4.8723249178	3.7706082427
C -1.4322135874	3.6173366689	3.4455120192
H -4.867155289	4.5540156148	2.1026040412
H -3.6362582825	6.2014328869	3.5148474998
H -1.365177697	5.5543259142	4.3923722998
H -0.4573303761	3.3027472634	3.8070456675

DIG:12H⁺

N -4.7441976294	0.8020625037	0.6066153816
C -4.0083278298	-0.1769225002	0.0698059737
N -2.695957709	0.0001973347	-0.1879416155
N -4.5734734141	-1.3594342618	-0.2536868076
C -1.933814995	1.2572767837	-0.2037327734
C -0.9243523688	1.3515772845	0.9485392687
C -1.5423611797	1.458744425	2.3605725081
C -2.1906746475	2.7980039627	2.6304545022
C -6.2189875638	0.7715890648	0.7239891783

C -6.6660792805	0.1275233786	2.0451993816
C -6.7699961595	2.1916899428	0.5708442057
H -6.467673654	2.8219032724	1.413643914
H -6.4253430777	2.6533055205	-0.3594570562
H -7.8635633954	2.1631801119	0.5552272067
H -6.3076235786	0.7139537798	2.8979842819
H -7.7588553561	0.085787285	2.0961689932
H -6.2845052795	-0.8936321291	2.1629828414
H -6.5889494331	0.1794797855	-0.1212414173
C -3.9836698177	-2.4405859975	-1.0738267018
C -3.1796701587	-3.4299352561	-0.2177187137
C -5.110669528	-3.1336440201	-1.8447317156
H -5.8222965822	-3.6097105113	-1.158491985
H -5.6533615232	-2.4252981857	-2.477788692
H -4.6972470953	-3.9189442889	-2.4838925326
H -2.722176141	-4.1942923277	-0.8537066798
H -3.8308984142	-3.9351115508	0.5040489616
H -2.3788497935	-2.9387700091	0.3473951798
H -3.3227920861	-1.9530992256	-1.8000292466
H -5.4675719011	-1.5638732437	0.1700179014
H -2.1655610175	-0.837424344	-0.3813119042
H -2.6384760392	2.0893562575	-0.1881605952
H -1.4026029767	1.3017695989	-1.1610911463
H -4.2575319864	1.5838820464	1.0855765456
H -0.2689846665	0.4711927894	0.914982029
H -0.2808214548	2.2195773835	0.7603578854
H -0.7503501797	1.2896899764	3.0970179145
H -2.2767120913	0.6563207232	2.5041963082
N -3.3900637218	3.0315047764	2.0571829592
C -3.9623003484	4.2325762891	2.2390222796
C -3.3917902816	5.2494051688	2.9990827025
C -2.158246872	5.0066338973	3.6009896184
C -1.5509207106	3.7673699015	3.4106199326
H -4.9214924634	4.38490786	1.7505555188
H -3.9032108593	6.1992776511	3.1139988015
H -1.6767130533	5.7679986535	4.2075594086
H -0.5891036849	3.5470414432	3.8635689991

DIG:13

N -4.8851771325	0.7786814772	0.6154288331
C -4.0465329243	-0.1074224158	-0.0682474837
N -2.8031081834	0.0504552922	-0.370007329
N -4.6872223802	-1.295893629	-0.4111162144
C -2.1480951893	1.3405611732	-0.2923193335
C -1.0790411241	1.3718724078	0.8148580547
C -1.6387263221	1.3875150114	2.2587078639
C -2.1696539226	2.7358262487	2.6805865133
C -6.2490123807	1.0881920778	0.152742828
C -7.0421490221	1.6990310012	1.3119504687
C -6.2515651278	1.9977072228	-1.0865196663
H -5.7903177109	2.9672862601	-0.8590711991
H -5.6874366218	1.5360110698	-1.903749939
H -7.2737223637	2.1836424601	-1.4388039409
H -6.5943970341	2.647540123	1.6355713254
H -8.07511645	1.9052751999	1.0104754259
H -7.0558489399	1.0239354415	2.1735534416
H -6.7209910458	0.1411130189	-0.12589398

C	-3.9603320172	-2.397174716	-1.0485947894
C	-3.0836501727	-3.1769340068	-0.0572454094
C	-4.9656771374	-3.3049617498	-1.7644391707
H	-5.6589437681	-3.7700083708	-1.050013871
H	-5.5573321384	-2.7379103522	-2.4905043214
H	-4.4481785767	-4.114007417	-2.2918403279
H	-2.5246714164	-3.9696586772	-0.5693524327
H	-3.6971572994	-3.6503556922	0.7213745019
H	-2.3689222077	-2.5002468898	0.4179020172
H	-3.3041853294	-1.9265303016	-1.7859294152
H	-5.3739336958	-1.5931974292	0.2736020562
H	-2.8359251274	2.1931220666	-0.172718428
H	-1.6257352033	1.5034309612	-1.2465038777
H	-4.4034144761	1.5883562022	1.002913811
H	-0.4582094996	0.4755615486	0.7014603771
H	-0.42222204	2.2402369578	0.668346396
H	-0.8452391159	1.0910660652	2.954023065
H	-2.4367068219	0.641084317	2.3391768694
N	-3.401275085	3.0879862175	2.2642467339
C	-3.8832681645	4.2908677139	2.6005348001
C	-3.1859944463	5.2210490031	3.367835201
C	-1.9173712098	4.842173776	3.7891002999
C	-1.3874335475	3.6043955249	3.4579810119
H	-4.8831314902	4.5232495693	2.2406371679
H	-3.5997875373	6.1859804018	3.6302454414
N	-1.1177159389	5.7772490062	4.6120577318
H	-0.3977061591	3.3259390496	3.7979827104
O	-0.0044537065	5.4044158933	4.9728777411
O	-1.6218967961	6.8653748876	4.8788294415

DIG:13H⁺

N	-4.7555164124	0.7783837163	0.6215241528
C	-4.0121789245	-0.1974799869	0.0864284882
N	-2.6959522472	-0.0174821117	-0.1496730965
N	-4.573272308	-1.3760548637	-0.2509856275
C	-1.9421705373	1.2444409244	-0.1808878766
C	-0.9269645864	1.3567511767	0.9646766627
C	-1.5359121905	1.4767834995	2.3802439025
C	-2.1788120175	2.8187481079	2.6439048377
C	-6.2329903541	0.7541191145	0.7155685743
C	-6.7056911756	0.0883120828	2.0167411143
C	-6.7715860641	2.1805270582	0.5797604315
H	-6.4772655213	2.7929524698	1.4387934984
H	-6.4116586194	2.6564014108	-0.3374908291
H	-7.8648803135	2.1607838699	0.5492810391
H	-6.3630204041	0.6583348866	2.8870652871
H	-7.7992641363	0.0487029217	2.0460512866
H	-6.3293433032	-0.9358863837	2.1241309927
H	-6.5909540146	0.1796370887	-0.1467326831
C	-3.979679776	-2.4486254519	-1.0817811197
C	-3.1932127969	-3.4558872469	-0.2307122189
C	-5.1021751529	-3.1213170505	-1.8769314322
H	-5.8248265538	-3.603772592	-1.2069319039
H	-5.6327280861	-2.3996502756	-2.5052379806
H	-4.6858979932	-3.8989170765	-2.5235571666
H	-2.7322406768	-4.212833497	-0.872934878
H	-3.8569318036	-3.9687248505	0.4740079555

H -2.3966295424	-2.9790730015	0.3523839963
H -3.3070224241	-1.9537184822	-1.7919157349
H -5.4737304384	-1.58278969	0.1583951117
H -2.1644650971	-0.8522656837	-0.3525046982
H -2.6526920293	2.0717888969	-0.1724398529
H -1.4148146125	1.2847365434	-1.1404927051
H -4.275076163	1.5546440214	1.104500832
H -0.2693674752	0.4782512353	0.9404567531
H -0.2852892768	2.2229912103	0.7625648916
H -0.7408075139	1.3120181987	3.1138766421
H -2.274215692	0.6804993533	2.5348861291
N -3.3898046564	3.0491209734	2.0956527905
C -3.9652995136	4.2478927205	2.2768108398
C -3.3881821776	5.2787931297	3.0139245314
C -2.1459042634	5.0185457271	3.5748203326
C -1.5188123313	3.7938775633	3.4009453212
H -4.9355099938	4.3928569618	1.8100104353
H -3.8750105617	6.2361801651	3.149907143
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O -2.0669863057	7.1344882054	4.5067957287

DIG:14

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N -4.6857143553	-1.2926682594	-0.4083410282
C -2.1432948706	1.3412002383	-0.3014700957
C -1.0752393217	1.3758606493	0.8066938203
C -1.6354041291	1.3934111106	2.2502135509
C -2.1677797155	2.7417788056	2.6717666279
C -6.244722403	1.0908439048	0.1577337574
C -7.032604255	1.7032321549	1.3197535497
C -6.2560965581	1.997207499	-1.0839065455
H -5.7958710167	2.9684538513	-0.8615927874
H -5.6952976223	1.5345375408	-1.9028803365
H -7.2805978802	2.1798087453	-1.4311833694
H -6.5848304299	2.6533617947	1.6383888392
H -8.0677043889	1.9065274248	1.0235306291
H -7.0400558913	1.0303998864	2.1832102033
H -6.7167160244	0.1423825739	-0.1161076364
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C -3.083532382	-3.1743645798	-0.0516387815
C -4.9682611418	-3.3050496564	-1.7556314676
H -5.6606642047	-3.7676737497	-1.0387810702
H -5.5608190131	-2.7391001176	-2.4818332892
H -4.4526499334	-4.1158699379	-2.2821888862
H -2.5251618186	-3.9684297218	-0.5623762613
H -3.6966251184	-3.6459209642	0.7284743379
H -2.3682583098	-2.4968288418	0.4214830299
H -3.3053277427	-1.9283974721	-1.783420556
H -5.3699339426	-1.5879426734	0.2797779607
H -2.8304749767	2.194529688	-0.1851277058
H -1.6197693544	1.5001261209	-1.2556989332
H -4.3950607362	1.5966162745	0.9965920071
H -0.4530247894	0.480192566	0.6950263438

H -0.4196793937	2.2449670846	0.6587265284
H -0.8420066275	1.0969574079	2.9458916583
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C -3.1831327949	5.2218951842	3.3573967211
C -1.9056548548	4.8606646302	3.8076606285
C -1.3942729263	3.6055644717	3.4590370408
H -4.8714503457	4.5359615946	2.2116893739
H -3.6157556683	6.1837691679	3.6086537422
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C -1.9431227484	1.2498615704	-0.1864640688
C -0.9247441708	1.3624482589	0.9562334908
C -1.5294757883	1.4789543516	2.3738496602
C -2.176092671	2.8187683698	2.6413985663
C -6.230285777	0.7591318571	0.7171296761
C -6.7030586157	0.1025942123	2.0229763959
C -6.7686925179	2.1847052004	0.5713631363
H -6.4730751258	2.8035151004	1.4253200502
H -6.4094291135	2.6536488019	-0.3497033846
H -7.862050446	2.1650601008	0.5422124489
H -6.3588589205	0.677675153	2.8893597881
H -7.7966765092	0.0647530378	2.053355591
H -6.3280645377	-0.921411211	2.1366184563
H -6.5888589077	0.1787102128	-0.1408985184
C -3.979777252	-2.4469650475	-1.0771188707
C -3.1873070568	-3.4511619943	-0.2279725283
C -5.1046670694	-3.1233707689	-1.8656869459
H -5.8230315217	-3.6061602004	-1.1913309256
H -5.6397396843	-2.4038158089	-2.4925757639
H -4.6900057404	-3.9012141515	-2.5130711585
H -2.7284618623	-4.2089373532	-0.8707513829
H -3.8464482128	-3.9632650264	0.48156853
H -2.388450191	-2.9716634488	0.3497993704
H -3.3112861423	-1.9520609664	-1.7911944397
H -5.4698647024	-1.5811559803	0.1679200182
H -2.1629931223	-0.8475764472	-0.3542522743
H -2.6543896328	2.0764422438	-0.1743654852
H -1.4187209214	1.2913708904	-1.1476536634
H -4.2714810101	1.5593938314	1.1050913497
H -0.26505224	0.4855528219	0.9281689616
H -0.2862071095	2.2308470968	0.753465087
H -0.731398428	1.3144214795	3.1044736573
H -2.2648454578	0.6801705562	2.5298576597
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C -3.9614117996	4.2446327683	2.2755147955
C -3.3858954839	5.2717217385	3.0145978835
C -2.13254498	5.0371221631	3.5952198558
C -1.5212702103	3.7920136236	3.4011114479

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N -0.9535711691	6.8720322554	5.0044648246

DIG:15

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N -4.6965274573	-1.2935239555	-0.4793235978
C -2.0891545268	1.2652042175	-0.2027600439
C -1.0895279698	1.2584799319	0.9684983608
C -1.7304133924	1.2877570564	2.3769548515
C -2.2658545625	2.6467555068	2.7682292052
C -6.2159322868	1.1076421977	0.1227812952
C -7.0558865961	1.5861699458	1.3119360357
C -6.1840822795	2.1470362291	-1.0101593741
H -5.7340806732	3.0859635444	-0.6635462775
H -5.5916640448	1.7779026351	-1.8541452339
H -7.195456009	2.3696085389	-1.3729063107
H -6.6201746702	2.4880116951	1.7597695214
H -8.0775236928	1.8278028994	0.9968973728
H -7.1012321393	0.8170479188	2.0898118682
H -6.6659005206	0.1931143607	-0.2749343093
C -3.9745660175	-2.3981993395	-1.115224299
C -3.151180041	-3.2211583584	-0.1128631951
C -4.9753199072	-3.2658090627	-1.8856002972
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H -5.527328862	-2.6687240634	-2.6188228463
H -4.4594680566	-4.0765060722	-2.4124384831
H -2.5936930669	-4.016371763	-0.6231497399
H -3.802330021	-3.6961053483	0.6338176332
H -2.4381116712	-2.5714415936	0.4007332148
H -3.2816237002	-1.9283513161	-1.8186313657
H -5.4042242394	-1.5917370781	0.1836116334
H -2.7607080038	2.1330118795	-0.1131124627
H -1.5050834007	1.4220958706	-1.1217648159
H -4.3804171416	1.5476356008	1.0303572672
H -0.4872332088	0.345686856	0.8841836928
H -0.4021935325	2.1097357334	0.8659532405
H -0.981443833	0.9769315727	3.1150887621
H -2.5421213934	0.5525888758	2.4139380255
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C -3.2574783785	5.1354599478	3.394400339
C -2.0111036923	4.7582681914	3.915208682
C -1.5112711182	3.492835924	3.5945357235
H -4.8969045477	4.4908073298	2.1702174975
H -3.672119986	6.1097961024	3.6285771863
O -1.3866333365	5.6672135721	4.7025834323
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C -0.1197212869	5.3287282936	5.25599212
H 0.1867430102	6.1943852117	5.8450179391
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H 0.6224829837	5.1405881466	4.4704045425

DIG:15H⁺

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C	2.164701255	1.4150188084	-0.5824771587
C	3.5431618884	1.2602878859	-0.4867973152
C	4.0312322931	0.053960976	0.0354095272
C	0.7222336079	-1.7352270199	0.6456086859
C	0.114934029	-2.4452735795	-0.5845422326
C	-0.8474510826	-1.5956368163	-1.4258327131
N	-2.0894938631	-1.2691601943	-0.7101143071
C	-2.4936874066	-0.0685957133	-0.2461245785
N	-3.7815844403	0.071837818	0.136161292
C	-4.8929351297	-0.8770976267	-0.0921666671
C	-6.184297324	-0.0755518921	-0.2789594456
O	5.3260692818	-0.2562018871	0.2020438718
C	6.3227790192	0.7021245058	-0.1673908194
N	-1.6528891923	0.9690194002	-0.192384942
C	-2.0605886977	2.3602524904	0.1013756917
C	-1.1717857633	3.3269218012	-0.6858747491
C	-2.0206131725	2.6508805032	1.6095211175
C	-5.0113495822	-1.9000909894	1.0470565621
H	-0.1386143297	3.2897628299	-0.3255736157
H	-1.1830870885	3.0947365655	-1.7551142393
H	-1.5324445487	4.3512867949	-0.5528259031
H	-1.0001904356	2.5424562381	1.9922117647
H	-2.352554228	3.6750302193	1.8083203802
H	-2.6624842048	1.971408048	2.1826985386
H	-3.0850898373	2.4743034344	-0.2717049032
H	-6.4317792079	0.4894265262	0.6285637179
H	-6.1001519322	0.6240481179	-1.1159401715
H	-7.018656312	-0.7535180986	-0.4800009878
H	-5.8135433117	-2.6132622002	0.8326767394
H	-5.2465554232	-1.3999301644	1.9930130235
H	-4.0858946679	-2.4686921627	1.1954198503
H	-4.6720305612	-1.3922516907	-1.0342525779
H	-3.9980760628	0.8767963324	0.7069050023
H	-2.7008418208	-2.0488585749	-0.513807229
H	-0.3797006147	-0.6654133135	-1.7495142562
H	-1.1310038488	-2.1477452394	-2.3288701091
H	-0.6290322258	0.7853252607	-0.2286188088
H	-0.4145187382	-3.3465173623	-0.247695704
H	0.9202422019	-2.7915017857	-1.2437349781
H	1.1988499756	-2.4902635946	1.2785541708
H	-0.0787895958	-1.2862406341	1.2463930498
H	1.7617494835	2.3402261438	-0.9876773404
H	4.1983665563	2.05961376	-0.8096250792
H	3.4636835539	-1.86534017	0.821534355
H	7.2785488374	0.2320464077	0.0628940861
H	6.27263968	0.9280664578	-1.2384325498
H	6.2161457503	1.6238673187	0.4153548632

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C -1.0791811746	1.3000926944	0.9228979561
C -1.6995964606	1.3352926108	2.3399954335
C -2.2490146501	2.6907224915	2.7271922567
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C -7.0302596517	1.5399821726	1.3973685324
C -6.2297370654	2.1349820617	-0.9418511253
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H -5.6542842544	1.7824418851	-1.8044846997
H -7.2541047095	2.3440449851	-1.2753653036
H -6.5953087888	2.4428867785	1.8434494091
H -8.0632290923	1.769526705	1.1111170201
H -7.0443198391	0.7623032276	2.1679822679
H -6.6585809526	0.1669554057	-0.2117713915
C -3.9580972535	-2.3884222238	-1.1149341149
C -3.107013197	-3.2029722492	-0.1289311363
C -4.9631296189	-3.2665767629	-1.8677078123
H -5.6739688977	-3.738551555	-1.1752358365
H -5.5362239975	-2.6743853673	-2.5886701282
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H -3.7392086966	-3.6868995906	0.6282974387
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H -3.283575155	-1.910080343	-1.8303897063
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H -0.9344602406	1.0421752467	3.0688494499
H -2.4995445104	0.5882524023	2.3974103838
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H -0.1103533165	4.4330772532	5.9075514631
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DIG:16H⁺

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C -1.9072168158	1.2422841909	-0.2613610482

C -0.8972542453	1.3385517911	0.8905117021
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C -2.1602789159	2.8273747343	2.5378517647
C -6.1764517704	0.7940495274	0.7671820298
C -6.5712695601	0.1855448609	2.1217855552
C -6.7399724782	2.2072984711	0.5961929813
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H -7.8334936029	2.1727151347	0.6131347504
H -6.1780805825	0.7959552975	2.9416621466
H -7.6611134559	0.1448578926	2.2181330685
H -6.1828723562	-0.8317256958	2.250941355
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C -3.2050067738	-3.442758616	-0.203857347
C -5.1606039132	-3.1288578482	-1.79735801
H -5.8677586947	-3.5892189228	-1.0958417518
H -5.7038616398	-2.4167659078	-2.4257815472
H -4.7698595206	-3.9247943713	-2.4377629419
H -2.7674946925	-4.2155070013	-0.843910959
H -3.8506498202	-3.9368957026	0.5305705425
H -2.3893960834	-2.9587888983	0.3459610826
H -3.3567446191	-1.9727830787	-1.7911378052
H -5.455637231	-1.546054717	0.220629007
H -2.1654751005	-0.8505575186	-0.4169737023
H -2.6004006068	2.083640106	-0.2521181347
H -1.3756712256	1.2679410197	-1.2192713355
H -4.2056537493	1.6223939939	1.0528935154
H -0.2539615087	0.4484268487	0.8700912029
H -0.2422415438	2.1951851084	0.6893312233
H -0.7179837257	1.3252642894	3.0384078346
H -2.2478266126	0.6830419035	2.4645121124
N -3.3574119327	3.0386663744	1.9434676893
C -3.9022829013	4.2589326605	2.1068021491
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C -2.0920914562	5.0746886994	3.4832848206
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C -0.2025640057	5.7813123911	4.8680228415
C -2.1204155258	7.3483257727	4.3849668546
H -1.4918262368	7.9755721212	5.0169826076
H -2.2433500876	7.8540823153	3.4187837326
H -3.1048224164	7.2642921734	4.8621644789
H 0.1059715578	6.6669612784	5.4233478633
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H 0.5768178973	5.5551836066	4.1288497008

DIG:17

N -4.812598306	0.7871647181	0.5818037044
C -4.0346924771	-0.1496555868	-0.0974322901
N -2.8065268896	-0.0383956945	-0.4731339396
N -4.7174061992	-1.3444745083	-0.344663867
C -2.1257202664	1.2427603587	-0.4883935377
C -1.0439458997	1.3377722723	0.6037993089

C -1.5770742112	1.4875547456	2.0486697199
C -2.0993426805	2.8728662798	2.36043665
C -6.210933134	1.0763322044	0.2310016359
C -6.9427754841	1.6043044301	1.4701055562
C -6.3162668967	2.0517368618	-0.953484581
H -5.8553121202	3.015776609	-0.7041531874
H -5.8019485072	1.6467912783	-1.8315981896
H -7.3636458926	2.2360521272	-1.2242130807
H -6.4835210146	2.5345408334	1.8265072766
H -7.9952228053	1.8122802472	1.2445591159
H -6.8963421629	0.8767438367	2.2870524084
H -6.6738056732	0.1322543363	-0.0713041704
C -4.0367504182	-2.4887100523	-0.9555411687
C -3.1149824905	-3.2243462929	0.0289729011
C -5.0875044281	-3.42258263	-1.5652485393
H -5.7469566466	-3.8373262187	-0.7902114996
H -5.7113643442	-2.8890320848	-2.2898197845
H -4.6073806933	-4.2672143125	-2.0723569702
H -2.5919026508	-4.0515154289	-0.4669274603
H -3.68994517	-3.6462438227	0.8648508779
H -2.3701927709	-2.5298867759	0.4255884796
H -3.4158582424	-2.0686827817	-1.7516186905
H -5.3527442601	-1.5985392347	0.404558893
H -2.7996230939	2.1102406706	-0.4189968254
H -1.611780698	1.3274535205	-1.4575067747
H -4.3036495498	1.6103521606	0.9121719563
H -0.4406422073	0.422923482	0.5514196753
H -0.3741585846	2.1795411947	0.3789654925
H -0.7692054682	1.2479079131	2.7504932361
H -2.3728372636	0.7521402063	2.2135432776
N -3.3356944796	3.1803087417	1.9133585593
C -3.7807497147	4.4204618677	2.1614961495
C -3.0706926459	5.3989706936	2.8391139039
C -1.7755924298	5.091281613	3.3165391335
C -1.3063552335	3.7842075879	3.0559770129
H -4.7795488697	4.6484836525	1.7906762789
H -3.5100389692	6.3789508634	2.9849850564
N -1.02013813	6.0066896479	3.995269657
H -0.3281848903	3.4711371744	3.4034343878
C -1.499607406	7.3385851476	4.3682063355
C -0.427458771	7.8511408797	5.34138799
C 0.8532268696	7.1527750055	4.8568804802
C 0.3578201457	5.7640607468	4.4261079745
H -1.5868858407	7.9898661406	3.4842409272
H -2.4903199768	7.2824473262	4.8352333863
H -0.6684065468	7.5326684222	6.3624997015
H -0.3518406608	8.94237846	5.3403406864
H 1.6320875375	7.097907677	5.6228859949
H 1.2690193017	7.6841668132	3.9926946865
H 0.3903407985	5.0465573431	5.2609651503
H 0.9562985128	5.3453593335	3.6081289385

DIG:17H⁺

N -4.7039147968	0.8057872164	0.5593152765
C -4.0124890675	-0.2182949033	0.0537516906
N -2.7175535593	-0.0807865624	-0.3004453729
N -4.6048458352	-1.4174505099	-0.1454178401

C	-1.9363388428	1.1579889938	-0.4275459277
C	-0.883372787	1.3132882761	0.6784078211
C	-1.444476586	1.5400126809	2.0997075863
C	-2.0820279916	2.9009724351	2.2806649083
C	-6.1652313309	0.7909843701	0.7842289156
C	-6.5096822016	0.2686142425	2.1876182284
C	-6.7330878109	2.1929863106	0.5473692281
H	-6.3779797267	2.8928493252	1.3101609236
H	-6.4523071302	2.5725815555	-0.4397673452
H	-7.8253313549	2.1629881635	0.6060865662
H	-6.0827370956	0.925536238	2.9528227586
H	-7.595143108	0.240382346	2.3280173274
H	-6.120185666	-0.7411865852	2.3635543391
H	-6.5965751629	0.1278792985	0.0250733212
C	-4.084297259	-2.5541942949	-0.9339637684
C	-3.2493318551	-3.5119710225	-0.0712639998
C	-5.2663190071	-3.2659031293	-1.5987373289
H	-5.9465151407	-3.6855594906	-0.8468315795
H	-5.8314528694	-2.5826010363	-2.2397284591
H	-4.9057719966	-4.0956372709	-2.2134728086
H	-2.8423028529	-4.3195894859	-0.6880067232
H	-3.8669676868	-3.9632978835	0.713135931
H	-2.4093346937	-3.0066452506	0.4195449651
H	-3.4581008607	-2.1231876382	-1.723674947
H	-5.4720420966	-1.5807219648	0.3459690658
H	-2.207859651	-0.939079135	-0.453571996
H	-2.6255626678	2.0025410077	-0.4382211137
H	-1.44168972	1.1271124718	-1.4048916607
H	-4.1822386211	1.6254862175	0.9493305769
H	-0.2446092454	0.4196287658	0.6853065283
H	-0.2331774679	2.1532525968	0.4044300841
H	-0.6238332514	1.4262628092	2.8152405437
H	-2.1747675746	0.7559781462	2.3374883589
N	-3.3011468511	3.0804872772	1.7194845119
C	-3.8415585587	4.3093189206	1.8342006767
C	-3.2529781391	5.3736762067	2.4882170522
C	-1.9826697081	5.1964803486	3.0943350943
C	-1.407653728	3.906337203	2.9598210991
H	-4.8120344057	4.4486050901	1.3632519247
H	-3.7637485747	6.3281586771	2.5190816839
N	-1.3567109643	6.1974316811	3.7589464822
H	-0.4408928462	3.6888134473	3.3984910562
C	-1.9556123279	7.5189135518	4.0008144184
C	-1.0143268665	8.1597047594	5.030168469
C	0.3501332367	7.5330247226	4.7030640354
C	-0.0039104123	6.0874575978	4.3244949998
H	-1.9947007998	8.1015473448	3.0688680024
H	-2.9794593504	7.4176420599	4.3774764528
H	-1.3260121794	7.8823604515	6.0435621955
H	-1.013525718	9.2509044646	4.9663905336
H	1.0568287895	7.5805832686	5.5356225924
H	0.8061154079	8.041755826	3.8461282399
H	-0.0055562094	5.4264957564	5.2035792559
H	0.691293777	5.6665150411	3.5891881495

DIG:18

C	1.2444526394	0.2488328894	0.6485435503
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N	2.5490938212	0.6443896739	0.3574600154
N	0.9803240358	-0.9853253366	0.8963920238
N	0.3193181902	1.2985526515	0.6218870101
C	0.6257717213	2.6591619253	1.1002012492
H	-0.6023676931	0.9933756401	0.9114110543
H	2.5979367111	1.397964194	-0.3201770029
C	3.6034648583	-0.3625652898	0.1824357794
C	-0.3444791452	-1.3587351832	1.3550053464
C	0.9468925117	2.7030081836	2.6014536417
C	-0.5486313344	3.5715508807	0.7353370624
H	1.506546316	3.0116232448	0.5520000949
H	3.4469080646	-1.0895363747	0.9838091523
C	3.4996771121	-1.0984887598	-1.1612250859
C	4.964678163	0.3153978933	0.3651411412
H	-1.0897735989	-1.2663750049	0.5428022008
H	-0.7049144888	-0.7065491776	2.1753350344
C	-0.3482665908	-2.8080952099	1.8514379448
H	0.0114789736	-3.4506280612	1.0380042651
C	-1.7244990368	-3.2773400029	2.3297696167
H	0.3868674407	-2.8983121922	2.6614003925
H	-1.6926523366	-4.3168012701	2.6751136071
H	-2.0907453734	-2.6635449625	3.1627348585
H	-2.4690234506	-3.2187052268	1.5254933591
H	4.2763707084	-1.8682517591	-1.2453434833
H	2.523233894	-1.5818065925	-1.2469526342
H	3.6273823067	-0.4021087938	-2.0012489338
H	5.7743866273	-0.4187457916	0.2888567054
H	5.1369927442	1.0753445959	-0.4095874462
H	5.0299229902	0.8061358077	1.341667312
H	-0.3400051911	4.6059263005	1.0281793772
H	-0.7448191853	3.5448908046	-0.3412740111
H	-1.4634602917	3.2595628171	1.2569876294
H	1.2059142906	3.7208215727	2.9173828529
H	0.0825576488	2.3744880009	3.1923731991
H	1.7917809476	2.0466569132	2.8304681212

DIG:18H⁺

C	1.1893863722	0.2672087841	0.6636597187
N	2.4555688857	0.5466108654	0.3128461439
N	0.798221279	-1.009329576	0.8241254275
N	0.3157527762	1.2588537046	0.9029053654
C	0.615885871	2.7081219141	0.9827383522
H	-0.6610560457	1.0007655586	0.9544436919
H	2.6455100662	1.4895097078	0.0014745834
C	3.5841851705	-0.4112187042	0.230622879
C	-0.4859346007	-1.4436849064	1.3953378901
C	-0.3607219598	3.3480532568	1.9726393669
C	0.5614526944	3.3736962968	-0.3992083535
H	1.6275333129	2.7886640346	1.3978416285
H	3.4030285068	-1.165360131	1.0053019027
C	3.6563522005	-1.0815447556	-1.1484671329
C	4.874768257	0.3347606694	0.5783336735
H	-1.3026743146	-1.242018725	0.6870041816
H	-0.6718610976	-0.8619990855	2.305796399
C	-0.4464019198	-2.9375048921	1.7270699769
H	-0.2191398916	-3.502935978	0.8126486787
C	-1.7727562236	-3.4269949912	2.3164398495

H	0.3718262133	-3.1232655491	2.433884647
H	-1.7181466507	-4.4959678364	2.5403611513
H	-2.0129982033	-2.9039692906	3.2488075376
H	-2.6025725085	-3.2755745807	1.6170851676
H	4.4698348079	-1.8134880329	-1.1676827572
H	2.7285443057	-1.6037989551	-1.4100789334
H	3.8504133646	-0.3389702551	-1.9300051668
H	5.7203901062	-0.3583434828	0.5603995795
H	5.0823467476	1.1246674465	-0.1542663521
H	4.8202327204	0.7831394587	1.5748435392
H	0.8358829932	4.4300220874	-0.3177590555
H	1.2436424803	2.9033291833	-1.1169045638
H	-0.4496150652	3.3177871151	-0.8168873483
H	-0.13786172	4.413513488	2.0774437038
H	-1.3949437135	3.2628276585	1.6164373394
H	-0.2884802642	2.8835402073	2.9605666248
H	1.3805090471	-1.7277347092	0.4169496638

S10. Cartesian coordinated for the „open chain“ DIG series of bases and their conjugated acids.

DIG:1_oc

C	0.7990378882	1.8727019656	-1.334228121
N	1.2053566263	0.6797081367	-0.5685991557
C	0.3797864074	-0.4358929321	-0.390152989
N	0.7663353492	-1.6611131455	-0.3336376589
C	2.1534812492	-1.986786303	-0.609122901
C	2.3303245341	-3.5068043613	-0.6943162268
C	3.7873889702	-3.9144086126	-0.9289582806
N	3.968691506	-5.3451700609	-1.1833346213
N	-0.9698032661	-0.1177399453	-0.2381788856
C	-1.9305477095	-1.1741202711	0.1233687768
H	-1.4507864832	-1.8610895126	0.8332989041
C	1.8647010866	2.9545195735	-1.1372014199
C	0.5527565232	1.5693538171	-2.8196533459
H	-0.1373185619	2.2402953515	-0.9006482128
H	-1.1082804098	0.7431299164	0.2785589553
H	2.8210815656	-1.5973273835	0.1820484693
H	2.5068287477	-1.5353556248	-1.5571281606
H	1.9417591909	-3.9385514251	0.2347949635
H	1.7099283494	-3.8972542424	-1.5097230027
H	4.1619392878	-3.3817283464	-1.8136218014
H	4.4123696656	-3.5748914065	-0.0744912009
H	2.1623093226	0.4113368605	-0.7656531345
C	-3.1425227227	-0.5193764364	0.7906257213
C	-2.3343795334	-1.9770948021	-1.11756441
H	-3.0275582888	-2.7814486092	-0.8432898006
H	-2.826984006	-1.3293349666	-1.852758296
H	-1.4499887826	-2.4255199595	-1.5756570105
H	-3.8823314177	-1.2780277633	1.0656505518
H	-2.8585416601	0.0161039542	1.7057558595
H	-3.6272251567	0.192750323	0.1107643912
H	1.5766024355	3.878335967	-1.6497456006
H	2.0085716875	3.1732382815	-0.0743152587
H	2.8290046864	2.6335697531	-1.5535331868
H	0.2164485386	2.4672233569	-3.3521445313
H	1.4735278737	1.2158850659	-3.3008446567
H	-0.2139839331	0.7968459131	-2.9304924393
C	5.3133482053	-5.6248313349	-1.6665284432
H	5.4041899916	-6.6895130554	-1.9096426505
H	5.5072564687	-5.050583254	-2.5793450763
H	6.1063092913	-5.3760544686	-0.9316781368
C	3.6597026071	-6.1687605321	-0.0219150233
H	3.7951481348	-7.2249730072	-0.2793804193
H	4.3046301856	-5.9455330779	0.8528552377
H	2.6182545555	-6.0309743955	0.2802362278

DIG:1_och⁺

C	0.7793790607	1.5201460506	-1.8870240326
N	0.9847407466	0.0834869768	-1.5870182463
C	0.1043906604	-0.7550320591	-1.0160914048
N	0.5112856824	-1.9787616539	-0.635588577
C	1.9010494058	-2.4603356884	-0.6531441117

C	2.0140949528	-3.768727122	0.1313603167
C	3.4499115362	-4.3159613309	0.1222671701
N	3.5427869877	-5.6252938874	0.7537853102
N	-1.1582415345	-0.3604491153	-0.7827744611
C	-2.177150323	-1.0798070311	0.0185306045
H	-1.6302138403	-1.6039616246	0.8108288526
C	2.1326164765	2.229300243	-1.7919806642
C	0.1133878264	1.7220577689	-3.2552010136
H	0.1312103226	1.9095345861	-1.0930198566
H	-1.4735710593	0.4707907566	-1.2640733662
H	2.232887011	-2.6149176799	-1.6902806981
H	2.5374969695	-1.6901012441	-0.2019186657
H	1.6724746934	-3.5931317213	1.1578588773
H	1.3577955187	-4.5296209884	-0.310325118
H	3.7700028352	-4.4274060636	-0.92124553
H	4.133861276	-3.5740209058	0.5855609322
H	1.8470658361	-0.3244119031	-1.9237324784
C	-3.0946142326	-0.0439630158	0.6730137809
C	-2.9574350275	-2.0879320403	-0.8365247122
H	-0.2029426067	-2.6654906106	-0.437588328
H	-3.8359185555	-0.5478782731	1.2994215316
H	-2.5284829915	0.6491639988	1.3024385239
H	-3.6415642106	0.5319829613	-0.0838732832
H	-3.6691428797	-2.6379082434	-0.2129928242
H	-3.5220103013	-1.5736720682	-1.621831872
H	-2.3017601548	-2.8192197777	-1.3234943811
H	2.0044929686	3.2995792409	-1.9759499229
H	2.5805159912	2.1022527043	-0.8019148531
H	2.8306588674	1.8476946644	-2.5475756433
H	-0.0715674332	2.7866163396	-3.4294057061
H	0.7608639277	1.3548965512	-4.0588358576
H	-0.8452957954	1.196580406	-3.3351974324
C	4.7616270521	-6.3273839009	0.3561202715
H	4.7586681843	-7.3314051428	0.7911273602
H	4.7922457696	-6.4317340615	-0.7334229901
H	5.6869423919	-5.8165900252	0.6831189642
C	3.4345751986	-5.5615141063	2.2088308305
H	3.4771399855	-6.5749590484	2.6185307658
H	4.2436694122	-4.9676391563	2.676434591
H	2.4754263989	-5.1284207591	2.5094923473

DIG:2_oc

C	0.783071619	1.8849719438	-1.3132411461
N	1.2128265743	0.6960354803	-0.5531203687
C	0.4098166427	-0.4384208508	-0.3881264991
N	0.818527472	-1.6575475962	-0.3560495525
C	2.207586524	-1.9548622946	-0.6504336309
C	2.3957542078	-3.4649308214	-0.8257742483
C	3.8396636721	-3.8536683714	-1.1118774088
O	3.9117678018	-5.2609803879	-1.2561653479
N	-0.9434414982	-0.1477970268	-0.2206628851
C	-1.8835191952	-1.2262827504	0.1299255928
H	-1.3855062372	-1.9178732261	0.8224282524
C	1.8349667256	2.9809182551	-1.1215272682
C	0.5291149259	1.5813264544	-2.7971968637
H	-0.1547990971	2.238799041	-0.8716277531
H	-1.0941791108	0.7040347852	0.3074688791

H	2.8702667884	-1.6070014149	0.163635621
H	2.5586452596	-1.4445332967	-1.569383421
H	2.0558164071	-3.9763021047	0.0818624319
H	1.7574766373	-3.8155282185	-1.6451942762
H	4.201440323	-3.3590866507	-2.0321528222
H	4.5011135915	-3.5220119625	-0.2905432108
H	2.1751106298	0.449204428	-0.7525809542
C	-3.0994274531	-0.6038497517	0.8205738085
C	-2.2863044152	-2.0131960617	-1.1216107468
H	-2.9628975264	-2.834086426	-0.8552974348
H	-2.7970723983	-1.3606960385	-1.8400426098
H	-1.3992393267	-2.4383214621	-1.5963816105
H	-3.8240405636	-1.3794612447	1.0885132795
H	-2.8152866672	-0.0806387145	1.7426906237
H	-3.6024416002	0.1124213894	0.1585733229
H	1.5300697043	3.9021381405	-1.6289674672
H	1.9839460677	3.1987779386	-0.0591582505
H	2.8004665477	2.6748096787	-1.5463030166
H	0.177185812	2.4758371944	-3.3251557562
H	1.4502264445	1.2400471751	-3.286531462
H	-0.2289140986	0.7996126914	-2.9031379137
C	5.2188514273	-5.7162227087	-1.5191100116
H	5.1712547094	-6.8048260361	-1.6119456221
H	5.6196815415	-5.2961854585	-2.456966343
H	5.9155941317	-5.4585507201	-0.70381291

DIG:2_ocH⁺

C	0.7798949946	1.5221179211	-1.8712890185
N	0.9933086152	0.0747503765	-1.6334306295
C	0.1359632203	-0.7812487896	-1.0534893224
N	0.5546823432	-2.0186787198	-0.7343995348
C	1.9430311059	-2.496743957	-0.8102799708
C	2.075651324	-3.8239157034	-0.0635363981
C	3.4963300724	-4.3852367775	-0.1109808796
O	3.4777803908	-5.6008707644	0.593619493
N	-1.1135059047	-0.3930093573	-0.7510144132
C	-2.0972195148	-1.1343862128	0.0747160517
H	-1.5159799364	-1.6857486364	0.8228268053
C	2.1374604156	2.2261806381	-1.804679238
C	0.0590893179	1.775866258	-3.2024683226
H	0.1654219651	1.881726732	-1.0374786288
H	-1.4478975483	0.4530943739	-1.1919535736
H	2.2419043848	-2.6230787592	-1.8611023084
H	2.5929665802	-1.7377970423	-0.358999569
H	1.7858533644	-3.6911080656	0.9851032396
H	1.4001101157	-4.5701880414	-0.5013305725
H	3.8161502185	-4.5381990625	-1.1574524302
H	4.2070822073	-3.6730135766	0.345251006
H	1.8353557974	-0.323590306	-2.0280417111
C	-2.9768727629	-0.1166470978	0.8050972803
C	-2.922548329	-2.1111770645	-0.7742078769
H	-0.1518999025	-2.708530058	-0.520681753
H	-3.6896544538	-0.6379753375	1.4500456348
H	-2.37768785	0.5538650984	1.4283490484
H	-3.5567320667	0.4850928464	0.0941737524
H	-3.6079927002	-2.6768226823	-0.1354544416
H	-3.5197005497	-1.5696912412	-1.5158908183

H	-2.2952910997	-2.8305661846	-1.3135323451
H	2.0039175285	3.3028642813	-1.9414957705
H	2.6254565381	2.0607523326	-0.8395483101
H	2.8031328043	1.8742566272	-2.602694834
H	-0.1294527192	2.8464996571	-3.3289475039
H	0.6718140923	1.4382432882	-4.045338555
H	-0.9038251041	1.255447467	-3.2625026452
C	4.7436919172	-6.2402096785	0.6370732464
H	4.6114004759	-7.1640710932	1.2034405173
H	5.1064104817	-6.4846781534	-0.3727090368
H	5.4946291704	-5.6126815354	1.1403513367

DIG:3_oc

C	0.8137855344	1.8573700985	-1.3157599517
N	1.2223860461	0.6605234957	-0.5563100654
C	0.3979565704	-0.4571733511	-0.386099247
N	0.7839140553	-1.6839765152	-0.3507145444
C	2.1650251493	-2.0092668307	-0.6468713656
C	2.3191445792	-3.525614224	-0.8217289241
C	3.764329125	-3.9356248308	-1.1116389653
S	3.8890041828	-5.7578717338	-1.3100093509
N	-0.9486747034	-0.1409729468	-0.2172647841
C	-1.9096254667	-1.1997184373	0.1370662622
H	-1.4236113723	-1.9003705927	0.8288995125
C	1.8898285282	2.9308850348	-1.1312275755
C	0.545261797	1.5572853349	-2.7978469018
H	-0.1137800008	2.2318766748	-0.8693601669
H	-1.0839646234	0.7170958516	0.3047164059
H	2.8379949249	-1.678463804	0.1656447143
H	2.526994193	-1.5102669418	-1.5676567166
H	1.9616688503	-4.0197509163	0.0890224113
H	1.6633227685	-3.8534037956	-1.6370719904
H	4.1240058287	-3.4562503549	-2.0310143577
H	4.4235857063	-3.6249330888	-0.2911269052
H	2.1794812087	0.3951877557	-0.7567638587
C	-3.1105348183	-0.552028002	0.8307245398
C	-2.331965723	-1.9793154125	-1.1126049834
H	-3.0234907854	-2.7867262813	-0.8435882255
H	-2.8323080592	-1.3173463819	-1.829668515
H	-1.4551962863	-2.4219978171	-1.5905338469
H	-3.8501001233	-1.3124940263	1.101133272
H	-2.8131426538	-0.0342225883	1.7516811394
H	-3.6007537367	0.1739140748	0.1696442821
H	1.6017359742	3.857694431	-1.638251669
H	2.0492860811	3.1469972226	-0.0700225587
H	2.8461541229	2.6037353859	-1.5610298301
H	0.2087623782	2.4582569703	-3.3248170247
H	1.4564064813	1.1967534784	-3.291987122
H	-0.2292550738	0.7912175252	-2.898622101
C	5.6818437076	-5.9082704988	-1.6241411989
H	5.8963829405	-6.9709985578	-1.7649757071
H	5.9746827966	-5.368175977	-2.5303273597
H	6.2674298961	-5.5417204274	-0.7748307266

DIG:3_och⁺

C	0.8109996295	1.4930558277	-1.8580259067
N	0.9930472529	0.0397490738	-1.6297828532
C	0.1156887415	-0.8023132859	-1.0594054582
N	0.5084532834	-2.0494689716	-0.7440406672
C	1.8891641299	-2.5524315699	-0.8020637619
C	1.9971469534	-3.866510476	-0.0230036642
C	3.4166048235	-4.4415359536	-0.0564164455
S	3.4466594127	-6.0082989296	0.8973851995
N	-1.1278619537	-0.3918071266	-0.7628393046
C	-2.1287726875	-1.1146382755	0.0589251333
H	-1.5604367884	-1.6832922119	0.8039428534
C	2.1820612414	2.1688097345	-1.7759786674
C	0.1057326449	1.7711713248	-3.1926651075
H	0.1975651589	1.8585983238	-1.026094324
H	-1.4438848416	0.4618544744	-1.2028703458
H	2.1926986351	-2.7083141709	-1.8472495931
H	2.5490112909	-1.7958547483	-0.3621589495
H	1.6936510598	-3.69397462	1.0165387275
H	1.3018087785	-4.6013930548	-0.4506265096
H	3.7268435928	-4.6362741782	-1.090268325
H	4.1267661941	-3.7313061697	0.3843371021
H	1.8271156833	-0.3736114764	-2.0260375887
C	-2.9848696116	-0.0810572122	0.7951224202
C	-2.9756551171	-2.0675067266	-0.7957451613
H	-0.2140509877	-2.7273450642	-0.5450559672
H	-3.7099618725	-0.5896812809	1.4365020445
H	-2.3705374642	0.5713154141	1.4228664493
H	-3.5501476098	0.5386813016	0.0879272386
H	-3.6737493856	-2.6215191981	-0.1605291812
H	-3.5604040902	-1.5084768346	-1.5342998223
H	-2.3643210544	-2.7973766218	-1.339228313
H	2.0714550473	3.2489806299	-1.9055145519
H	2.6592767042	1.9861923791	-0.808561069
H	2.8464481193	1.8093785158	-2.5717218239
H	-0.0590481608	2.8464093369	-3.313167931
H	0.7175110095	1.4262674472	-4.0332806144
H	-0.8675339758	1.2718075978	-3.2634801032
C	5.205524669	-6.4586788097	0.6984186643
H	5.3476743744	-7.3995489465	1.2355526438
H	5.4595401053	-6.6128442398	-0.3541924776
H	5.8611930652	-5.7009562284	1.1368540114

DIG:4_oc

C	0.7906469119	1.8642278135	-1.3556033192
N	1.2097088851	0.688684873	-0.5687116755
C	0.3919917103	-0.4286964528	-0.3680562002
N	0.7831611292	-1.6525526121	-0.3041591976
C	2.1604502345	-1.9869842423	-0.6033387204
C	2.303154433	-3.5051583234	-0.7694735303
C	3.7534380823	-3.9419374431	-1.0216384119
P	3.9240413094	-5.7335967504	-1.4140332917
N	-0.9549465017	-0.1145597028	-0.1996609064
C	-1.91111048225	-1.1688354034	0.179399957
H	-1.4205361276	-1.8535584677	0.8839310847
C	1.8523582559	2.9550688879	-1.1896192736
C	0.5332641282	1.5290391591	-2.8320282128
H	-0.1437003781	2.2358898345	-0.9212848927

H	-1.0919967122	0.7543075761	0.3035702942
H	2.8386913914	-1.6537056778	0.2044160835
H	2.5251105365	-1.5010245942	-1.5297511545
H	1.9086703081	-3.984131263	0.1348080543
H	1.6681915764	-3.831964786	-1.6004956428
H	4.1645570114	-3.4047341649	-1.8876438962
H	4.3937495959	-3.6978840284	-0.161921746
H	2.1678567739	0.4247834475	-0.7655956483
C	-3.1114155286	-0.5106924794	0.8641862772
C	-2.3359167552	-1.974868026	-1.0525551816
H	-3.0228282705	-2.779662463	-0.764367023
H	-2.8430618797	-1.3291350909	-1.7795191418
H	-1.4607985992	-2.4240895513	-1.52764914
H	-3.8479669684	-1.26772629	1.1518475746
H	-2.8121231867	0.0261277321	1.7735796851
H	-3.6057034935	0.2006963853	0.1904693428
H	1.5548314127	3.8671457408	-1.7175659971
H	2.0047276838	3.1959725997	-0.1326861333
H	2.8146945855	2.6314201469	-1.6086332906
H	0.1880656405	2.4142427112	-3.3797319784
H	1.4515274416	1.1701398283	-3.3138569141
H	-0.2308965471	0.7511484418	-2.920879098
C	5.7380291272	-5.9889525086	-1.5439451769
H	5.9405429665	-7.0508382252	-1.7154677691
H	6.1206934479	-5.4266951698	-2.4014999943
H	6.2657628071	-5.6658559125	-0.6400032277
C	3.4597788333	-6.6155299763	0.128057918
O	3.1561409538	-6.1765592156	-2.6278080944
H	3.6397157544	-7.6866712031	-0.0069344018
H	4.0321792819	-6.2627457899	0.9929999559
H	2.3931625615	-6.4713733636	0.3228490549

DIG:4_ocH⁺

C	0.758110072	1.5484351664	-1.8925329483
N	0.9842903437	0.1174625479	-1.5814118663
C	0.1093775844	-0.7342651935	-1.0212192687
N	0.5337198747	-1.9413352974	-0.6082487232
C	1.9305545534	-2.4024940713	-0.5854032032
C	2.0312389613	-3.6777040837	0.2552188665
C	3.4309030409	-4.306732612	0.2261232259
P	3.3692797265	-6.019106507	0.9515405002
N	-1.1687331942	-0.3690074261	-0.8296575492
C	-2.1868429476	-1.0956486538	-0.0326499543
H	-1.6439699151	-1.5806126933	0.7868914244
C	2.0907312633	2.2884373756	-1.7507028026
C	0.1375674004	1.7337184123	-3.2841102212
H	0.0731350597	1.9239099791	-1.1233031444
H	-1.4944140989	0.4409391462	-1.339503086
H	2.2800586213	-2.60185837	-1.6088685019
H	2.5508295632	-1.6051329552	-0.1599278892
H	1.7371371414	-3.4474193218	1.2868888214
H	1.320616654	-4.4250804416	-0.1208217547
H	3.7675101027	-4.4207207524	-0.8127965071
H	4.1716232873	-3.6846221866	0.7436542386
H	1.8607149335	-0.2758415835	-1.8987280895
C	-3.1492584163	-0.0684286912	0.5687344743
C	-2.9172216994	-2.1514699448	-0.8739005895

H	-0.1710387323	-2.6457726674	-0.4374849016
H	-3.8897707679	-0.5757308882	1.1933256613
H	-2.6190269542	0.6602392813	1.1893167716
H	-3.6952867088	0.4675447478	-0.2176853637
H	-3.6270927663	-2.7021406733	-0.2489874779
H	-3.4778139111	-1.679929748	-1.6884405144
H	-2.2309029064	-2.8797457065	-1.3211825084
H	1.9452471069	3.3552778232	-1.9418438493
H	2.5056926645	2.1738333461	-0.7447987996
H	2.8240753883	1.9213713962	-2.4796718652
H	-0.0586780687	2.7943945402	-3.4691790395
H	0.8189598115	1.3745916082	-4.06297669
H	-0.8088990841	1.1920918335	-3.3955004162
C	4.9185329051	-6.8074038553	0.3873080458
H	5.0110668399	-7.793910742	0.8520262279
H	4.8804983477	-6.9443346573	-0.6976478357
H	5.7995149144	-6.2097256364	0.6457208168
C	3.5821713094	-5.795263251	2.7571161764
O	2.1028291993	-6.7217565285	0.5500884738
H	3.5905635262	-6.7797569052	3.2350950037
H	4.5155569078	-5.2756583633	2.9983902725
H	2.7387480662	-5.2308437965	3.1666713597

DIG:5_oc

C	0.82405506	1.8660639508	-1.2872456193
N	1.2352263909	0.6343908036	-0.5884042661
C	0.4014402927	-0.4769546566	-0.4299629192
N	0.7769817868	-1.7078773669	-0.4257183455
C	2.1524741166	-2.0365315839	-0.7390339081
C	2.3059780713	-3.5582947074	-0.8559141654
C	3.7344564019	-3.9790111083	-1.195017588
S	3.874264605	-5.8222379744	-1.2135502014
N	-0.9398472925	-0.1540772911	-0.2369680474
C	-1.9022941328	-1.2124281142	0.1173298115
H	-1.4085471425	-1.9272830796	0.7885974289
C	1.9155110587	2.9201689344	-1.082033386
C	0.5207409831	1.6313089296	-2.7744940066
H	-0.0893590701	2.2310722911	-0.8049060344
H	-1.0622398453	0.6961016673	0.3005941556
H	2.846023413	-1.6748972066	0.0427118381
H	2.4893853871	-1.5715487012	-1.6871068052
H	2.006796424	-4.0193981418	0.0914240539
H	1.6102666046	-3.92282383	-1.6220493526
H	4.0448897884	-3.6232927586	-2.1861677494
H	4.4472440745	-3.6110164988	-0.4461726013
H	2.1846389424	0.3660699462	-0.8182459632
C	-3.0856956909	-0.5682851312	0.8433697746
C	-2.3519706753	-1.9682580131	-1.1372832132
H	-3.0445072196	-2.775073066	-0.869314324
H	-2.8598165669	-1.2912861627	-1.8348365719
H	-1.4868647759	-2.4093542569	-1.6374734067
H	-3.8245919449	-1.3285914673	1.1158837732
H	-2.7675609493	-0.0673741901	1.7666977128
H	-3.5838734531	0.1710506771	0.2033851345
H	1.6265851633	3.8697250805	-1.5444149471
H	2.0999256214	3.0906479919	-0.0166304345
H	2.8587519527	2.6014302714	-1.5457499769

H	0.1840473909	2.5572649469	-3.2560402683
H	1.4176336504	1.2825850337	-3.3021005497
H	-0.2642636664	0.8782640941	-2.890917575
C	5.6830270927	-5.873768472	-1.536838921
H	5.9773775602	-6.9260790046	-1.5422899979
H	5.9016724747	-5.4224854415	-2.5096471338
H	6.2126903989	-5.3503421309	-0.7352410928
O	3.6539217195	-6.309214263	0.202763689

DIG:5_ocH⁺

C	0.8352779525	1.484351646	-1.8391217878
N	1.000647246	0.0210475787	-1.6707758456
C	0.1304033251	-0.8282445893	-1.0996408492
N	0.5104453996	-2.095269234	-0.8590212639
C	1.8826818583	-2.6143371506	-0.966764933
C	1.9629970073	-3.9824511556	-0.286463235
C	3.3781119988	-4.5584123302	-0.2796180559
S	3.3565526812	-6.0760000492	0.8065679343
N	-1.091197357	-0.408720447	-0.7338146198
C	-2.0682700513	-1.1443595783	0.1057919816
H	-1.4787308298	-1.7439826158	0.8090647124
C	2.2201490709	2.1342623641	-1.7857139833
C	0.0843480605	1.8222166617	-3.1344734786
H	0.2608256927	1.8295208838	-0.9714728655
H	-1.4083144452	0.4692668984	-1.1220621733
H	2.1749689481	-2.6945382093	-2.0235411456
H	2.5607615917	-1.906727235	-0.4754835633
H	1.6337180028	-3.8936566617	0.7558886871
H	1.2815334641	-4.6814566226	-0.7912274621
H	3.7245983767	-4.855083921	-1.2758747496
H	4.088973113	-3.8467861196	0.1561180313
H	1.8112203753	-0.3900462483	-2.1151862185
C	-2.8773384738	-0.1228130089	0.9088437797
C	-2.9639004387	-2.057805393	-0.7420209711
H	-0.2107640833	-2.7603038197	-0.6176402493
H	-3.5842933036	-0.6414683848	1.5622604731
H	-2.2280025524	0.4990981356	1.5322456052
H	-3.460096325	0.5281278178	0.2450656377
H	-3.641346093	-2.6238412467	-0.0951826923
H	-3.5721652076	-1.4678324606	-1.4362029611
H	-2.3861713763	-2.7765930888	-1.3346665939
H	2.1239563894	3.2201365618	-1.8716803981
H	2.730324584	1.9084161908	-0.8446008038
H	2.8473684135	1.7933564352	-2.6189736262
H	-0.064225004	2.9038386003	-3.2110573217
H	0.6564152156	1.4960894675	-4.0098357132
H	-0.9003240522	1.3431263519	-3.1837407011
C	5.1740583298	-6.1977632455	1.0072123334
H	5.3677584791	-7.0656192404	1.6419118596
H	5.6431316005	-6.3440832186	0.029234751
H	5.5500569614	-5.2944188556	1.4959160281
O	2.7631654552	-5.6219644636	2.1221154473

DIG:6_oc

C	0.8013533645	1.8766840969	-1.3052105993
N	1.2203575733	0.6651755367	-0.5755550131

C	0.3988139448	-0.4530526724	-0.4049616778
N	0.7882864335	-1.6798559291	-0.3749829565
C	2.1665218604	-2.0019442759	-0.6747261213
C	2.3157258635	-3.5236611213	-0.807155958
C	3.7592566239	-3.931179567	-1.108140859
S	3.9058046863	-5.7412703948	-1.250458264
N	-0.946676332	-0.1439365299	-0.2296939563
C	-1.904286236	-1.2070419973	0.1235124686
H	-1.4105399802	-1.9128677063	0.8040354799
C	1.8795269112	2.9470352628	-1.114571393
C	0.5121634028	1.6051598279	-2.7888403679
H	-0.11968506	2.242212057	-0.8381348346
H	-1.087398201	0.715615279	0.2878637925
H	2.8490014336	-1.6482385741	0.1207112255
H	2.5179305511	-1.5291856127	-1.6135893633
H	1.9836602944	-3.9971031162	0.1221230703
H	1.6574135152	-3.8812409258	-1.6054443745
H	4.1105731738	-3.5144610901	-2.0587933397
H	4.4436400339	-3.6248775721	-0.3089674952
H	2.176391937	0.4065507433	-0.7878301487
C	-3.098292927	-0.5666126716	0.8353347152
C	-2.337818959	-1.9746833528	-1.1296233691
H	-3.0239610112	-2.786840576	-0.8616306519
H	-2.8479201357	-1.3067681303	-1.83416739
H	-1.4660977526	-2.411006931	-1.6226785194
H	-3.8343020297	-1.3304397769	1.1056168839
H	-2.7917254241	-0.0578524446	1.7582531364
H	-3.5960721771	0.1651656573	0.1863761176
H	1.5836336458	3.883442269	-1.5988390697
H	2.0542190685	3.1423790062	-0.0517495018
H	2.8297114573	2.6295934877	-1.5649364225
H	0.1665718327	2.5156246472	-3.2929924586
H	1.4170537709	1.2568158699	-3.302784308
H	-0.2622360583	0.8395793066	-2.8938531186
C	5.6654067998	-5.9908993439	-1.6039207671
H	5.8029533106	-7.0706296757	-1.6988803731
H	5.9247959223	-5.4968439173	-2.5425963093
H	6.264068633	-5.6091731319	-0.7742082654
O	3.6300921656	-6.332921892	0.0692530224
O	3.1490260739	-6.1743261187	-2.4369666656

DIG:6_och⁺

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C	0.1251368893	-0.7894169494	-1.0863909393
N	0.537438529	-2.0343554683	-0.7841586766
C	1.9229289941	-2.5200319397	-0.8454770337
C	2.0383502642	-3.8124713237	-0.0339658495
C	3.4478068056	-4.4079320772	-0.0759426703
S	3.4232493031	-5.9512651883	0.9150591833
N	-1.1211026784	-0.4018383078	-0.7747075177
C	-2.0965716226	-1.1408029078	0.0651228402
H	-1.5063412068	-1.6906566229	0.8072170831
C	2.1504132927	2.2126771814	-1.7780828523
C	0.0696404585	1.8154583757	-3.1887830671
H	0.1736330368	1.8692939948	-1.0216142099
H	-1.4575887862	0.4476621255	-1.2078329497

H	2.2191668297	-2.6976581734	-1.8893116573
H	2.5779641596	-1.7462006467	-0.4291679121
H	1.7650372085	-3.6165571982	1.0085657416
H	1.3377957096	-4.5602732133	-0.4264215282
H	3.7528022854	-4.6728698927	-1.0933538538
H	4.1916232237	-3.7402688726	0.3700839591
H	1.814405579	-0.3296877783	-2.0786378004
C	-2.9666429361	-0.1200934266	0.8026180686
C	-2.9324694298	-2.1197552504	-0.7707338013
H	-0.1761163545	-2.7232408496	-0.5895497909
H	-3.6706228016	-0.639429282	1.4587129262
H	-2.3597854235	0.5525347913	1.4161217272
H	-3.5558919126	0.4788486302	0.0970483869
H	-3.610083381	-2.6819678142	-0.1208450008
H	-3.5384705533	-1.581736202	-1.5077959573
H	-2.3134083005	-2.84318475	-1.3143452613
H	2.0283935596	3.2934483603	-1.8914929406
H	2.6345036802	2.0214316749	-0.8157182523
H	2.8142518118	1.871393555	-2.5823358885
H	-0.1027703175	2.8910970272	-3.2936528772
H	0.6778059891	1.4857387026	-4.0381116759
H	-0.9010071928	1.3110027809	-3.2596095791
C	5.1059068086	-6.5887591947	0.780656265
H	5.1219781509	-7.5124021886	1.364798358
H	5.332711805	-6.804839927	-0.2653199851
H	5.8057502694	-5.8663927282	1.2057606918
O	3.1802580765	-5.5550996319	2.3099902732
O	2.5130039738	-6.8782598547	0.2257195973

DIG:7_oc

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N	-0.037588761	-0.0028359384	1.6918519203
N	-2.3305137085	-0.6033865514	2.0339750432
H	-1.7630517231	0.2248980219	4.2876054196
C	0.0558312677	1.2486848642	4.1828719544
H	-2.2836258952	-1.0289547301	1.1157684462
C	-3.6499576729	0.002530322	2.2936518938
H	-3.7013961002	0.2322393151	3.3632095895
C	-3.8666142986	1.3071031052	1.5126652259
C	-4.7279578092	-1.0396982359	1.9836455727
C	-0.3372448092	2.3052156086	5.2197225777
C	0.9824818242	0.175837433	4.7723738721
H	0.5759872157	1.729978687	3.3504143508
C	-0.0433035052	-0.5472883071	0.3479415255
C	1.2696045378	-0.1982426669	-0.3606212025
H	-0.1561523581	-1.6479925012	0.3614400747
H	-0.8872585877	-0.1623387339	-0.2585613558
H	1.3869469066	0.8904764591	-0.3815776446
H	2.1064623937	-0.5790412043	0.2348554775
C	1.3453895938	-0.7555227895	-1.7813634908
H	1.2357034833	-1.8513879295	-1.7848890163
C	2.6338997825	-0.4072453183	-2.519604969
H	0.5058785949	-0.3879135037	-2.3934812745
C	2.8089308365	-1.0202694301	-3.9014675874
O	3.4812161001	0.3190321745	-2.0361061612
H	-4.8387636623	1.7528678492	1.7555209606

H	-3.08554908	2.0337379841	1.7560983073
H	-3.8409064047	1.1200620096	0.4315351324
H	-5.72364059	-0.6448290028	2.2114658359
H	-4.7168104646	-1.3106411305	0.9192658858
H	-4.5701856979	-1.9514924341	2.5684045942
H	0.5544944133	2.7856626165	5.6371256344
H	-0.971586123	3.0770386997	4.7718053709
H	-0.8890071971	1.8545799717	6.0563635531
H	1.9025626384	0.6277929366	5.1620402894
H	0.4934835783	-0.3541860531	5.6012118341
H	1.2536268888	-0.5477578809	3.9995585799
H	3.7165793291	-0.6304480256	-4.3668495262
H	2.8832653736	-2.1126064274	-3.8233651426
H	1.9431872271	-0.8048852658	-4.5397600266

DIG:7_ocH⁺

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N	1.5314606404	-0.3855337532	-0.2746566513
N	3.0154522735	1.3892725108	-0.1051946681
H	4.7340097311	-0.4385511721	-0.0134607256
C	3.6762119368	-2.2595167794	0.3215092942
H	2.2759372961	1.9791270297	-0.4637916167
C	4.2783461227	2.0730327445	0.260291806
C	3.9293941097	3.4295087318	0.8780852385
H	4.7486500786	1.4544533542	1.0336587114
C	5.2170781567	2.2096104525	-0.9463766652
C	4.8345428203	-2.6960568942	1.2218602323
H	2.7393399217	-2.4055255672	0.8716502415
C	3.6383672846	-3.0452552987	-0.9965689886
C	0.3145953448	0.4414741692	-0.2779839914
C	-0.9147046971	-0.457336747	-0.1421840271
H	0.373559635	1.1438942229	0.5619411168
H	0.2577136486	1.0249784485	-1.2085009049
H	-0.9318449129	-1.188483743	-0.9598328257
H	-0.8462984974	-1.033744962	0.7869510822
C	-2.2276870353	0.3268619133	-0.1572001809
H	-2.2717347175	1.0486118636	0.6709536219
C	-3.441050811	-0.6063822548	-0.0564120565
H	-2.3258034666	0.9234149075	-1.0759103379
C	-4.806086068	0.0468164773	-0.0283947878
O	-3.2879318746	-1.8109730194	-0.0035087347
H	1.4136697615	-1.3632865065	-0.5009485494
H	4.843969277	3.9424975669	1.1883019909
H	3.4222755597	4.0747443497	0.1497713784
H	3.2860648977	3.3144886481	1.7555653761
H	6.1584131034	2.6755562983	-0.6388405298
H	5.4543298105	1.2418580456	-1.4032694067
H	4.7642622791	2.8395407556	-1.7197018445
H	3.5046627087	-4.11218073	-0.7928422734
H	2.8208191304	-2.7241770868	-1.6525642458
H	4.5759507834	-2.9205940844	-1.5491738283
H	4.748653393	-3.7631202151	1.444999809
H	5.8001837042	-2.5413572204	0.7244799387
H	4.8330226169	-2.1472079702	2.1683735518
H	-4.9612362356	0.6582092524	-0.9260675874
H	-5.5806181882	-0.719842557	0.0289652909

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DIG:8_oc

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H -1.7665722595 0.2448038571 4.2752855021
C 0.0620960935 1.2504295002 4.1706047655
H -2.2809168288 -1.036328822 1.1132469745
C -3.6450679248 0.0083359217 2.2812102089
H -3.7088175406 0.2246899096 3.3530564936
C -3.8451031385 1.3236686837 1.5139721525
C -4.726037536 -1.023015229 1.9451504007
C -0.3266271324 2.3206989347 5.1948435222
C 0.9745670627 0.174151588 4.7761911744
H 0.5920783268 1.717942212 3.3365242201
C -0.0331070535 -0.587977025 0.3546509287
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H -0.8813997499 -0.216169335 -0.2547687881
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C 1.3392595426 -0.82562721 -1.775646981
H 1.2222131382 -1.9184344161 -1.7373274922
C 2.6513441869 -0.4813090533 -2.4886345882
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N 2.820378899 -0.9525312616 -3.7744791411
O 3.5145066764 0.1923051798 -1.9347313091
C 1.8794799313 -1.7836933989 -4.5019588582
H 1.6439812655 -1.3300211878 -5.4747161786
H 4.6010093702 -1.5957717968 -4.7072053951
C 4.0639003202 -0.6659975028 -4.4731770091
H 2.3004905901 -2.7820359965 -4.6927066609
H 0.9481027789 -1.9054920639 -3.95195583
H 3.8621977744 -0.1398187226 -5.4159621494
H 4.6821700762 -0.0412156229 -3.8303667153
H -4.8171371635 1.7723759823 1.752039632
H -3.0623042407 2.0421168347 1.7750013803
H -3.8088547666 1.1491710644 0.4311513725
H -5.7218873032 -0.625439288 2.1674278009
H -4.7042254813 -1.2783533365 0.8770901679
H -4.5802043629 -1.9439858302 2.5185739227
H 0.5672432226 2.7961138252 5.6134838833
H -0.9503012979 3.0946106512 4.7356701777
H -0.888185911 1.8833800989 6.0320549951
H 1.8952009133 0.6210326022 5.1703718477
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DIG:8_ocH⁺

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N 3.0188750018 1.4035520698 -0.1103488947
H 4.7191570687 -0.4419787704 -0.0407750901

C	3.6476477745	-2.2536215366	0.2981613433
H	2.2782093633	2.0005595551	-0.4543427059
C	4.2981261384	2.0718128151	0.2233633886
C	3.9816979327	3.4372418945	0.8388207116
H	4.7765220171	1.452337355	0.9911761314
C	5.2134557683	2.187118182	-1.0035230293
C	4.8066839014	-2.7059714539	1.1897950036
H	2.7128415552	-2.3953078944	0.8528142171
C	3.5957802108	-3.0299061921	-1.0249130388
C	0.3049193655	0.484084124	-0.2383454688
C	-0.926508248	-0.414295584	-0.1183100231
H	0.3738470516	1.167161658	0.6169026856
H	0.2489369002	1.0883144038	-1.1557111061
H	-0.9550289373	-1.120267314	-0.9560167248
H	-0.85315358	-1.0179556466	0.7920966794
C	-2.2368816897	0.3766530985	-0.0967233248
H	-2.2521489953	1.0648862541	0.7583515435
C	-3.4247438557	-0.6005709417	-0.013663989
H	-2.3240961032	0.9965090506	-0.9991701395
N	-4.6830108097	-0.0735718905	0.0487417765
O	-3.2079228366	-1.8106515708	-0.0066296679
C	-5.0124568482	1.3432616475	0.0426392689
C	-5.8267803468	-0.9770640613	0.1359060293
H	1.3793261723	-1.3331203757	-0.4715817843
H	4.9097318092	3.9387302203	1.1271063622
H	3.4694560581	4.0851222481	0.1164844115
H	3.3544080147	3.3371479607	1.7296123469
H	6.1684853792	2.6394700921	-0.7186346853
H	5.4253536427	1.2132590771	-1.4598666832
H	4.754430521	2.8200245232	-1.7707410547
H	3.4529217399	-4.0970114133	-0.828372817
H	2.7780552583	-2.69579306	-1.6739246148
H	4.5321492543	-2.9098117393	-1.5806107766
H	4.7134034495	-3.7739479673	1.4055015747
H	5.7713154965	-2.5551158391	0.6892502087
H	4.8138332179	-2.1639042207	2.1401815015
H	-6.4977096697	-0.8225267179	-0.7179782367
H	-5.4620716097	-2.0025935717	0.1333537084
H	-6.3893022811	-0.7885621092	1.0586551578
H	-5.6775852725	1.5750631762	-0.7991475813
H	-5.5317688789	1.6209218439	0.969306021
H	-4.1214865655	1.9627627492	-0.0482877394

DIG:9_oc

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H	-1.7588470215	0.2367312879	4.2722697829
C	0.0629263773	1.2540121454	4.1649920528
H	-2.2834621407	-1.0140027681	1.0964435214
C	-3.6479234043	-0.0150480025	2.3031289119
H	-3.7084657978	0.163303907	3.3825690913
C	-3.8711817834	1.3231104545	1.5832794869
C	-4.7169736407	-1.0491533748	1.939278381
C	-0.3259802848	2.3175701397	5.1962212369
C	0.9827232347	0.1787894672	4.7612663889

H	0.5871848291	1.7279234718	3.3309576353
C	-0.0420890959	-0.5577457981	0.3367105127
C	1.2578093725	-0.1999760529	-0.3902377515
H	-0.1411386079	-1.6595050699	0.3652062289
H	-0.8982430966	-0.1917789869	-0.2655211165
H	1.3594625004	0.8890224393	-0.4358703115
H	2.1075744531	-0.5557613071	0.2017985189
C	1.3240739171	-0.7862676877	-1.8007617183
H	1.2292444257	-1.8819235465	-1.7679872056
C	2.6151217334	-0.4168823695	-2.5325579192
H	0.4688937882	-0.4372027799	-2.4001618466
N	2.80014498	-0.9853100063	-3.763125053
O	3.4497986856	0.3487142005	-2.056385747
C	1.9003583438	-1.9151385592	-4.4541545106
C	2.4877103171	-1.9875746047	-5.8732452442
C	3.9926994641	-1.7691619436	-5.6427983541
C	4.0299139056	-0.7195350148	-4.5230196677
H	1.9068440136	-2.9057618051	-3.9739674922
H	0.8664468759	-1.5530809444	-4.4493372824
H	2.0795367184	-1.1741905108	-6.4852067739
H	2.2542971676	-2.9327440706	-6.3727932324
H	4.5218166257	-1.4412950527	-6.542514074
H	4.4599565384	-2.7010988732	-5.3015232585
H	4.0178503901	0.3046290631	-4.9204278278
H	4.901984365	-0.801243972	-3.8685475117
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H	-3.0985476787	2.0435883538	1.8676425948
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H	-4.6983498673	-1.2680677884	0.8630536825
H	-4.5549475466	-1.9866811557	2.4806432217
H	0.5676753603	2.7936371915	5.6146083812
H	-0.9533488626	3.0919393909	4.7428960273
H	-0.8838133914	1.8742343391	6.0327780439
H	1.9032468868	0.6276500246	5.1534401057
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H	1.2536627307	-0.5480844838	3.9914939285

DIG:9_ocH⁺

C	-1.3629221802	0.5054206697	2.1384863293
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N	-0.3658524494	0.5492523354	1.2399835736
N	-2.5317010067	-0.0632630448	1.7969577523
H	-2.0037267624	1.1258808455	3.94386657
C	0.1034036572	1.4470705205	3.9677388159
H	-2.6876461993	-0.218225794	0.8095360071
C	-3.6680005944	-0.3667675626	2.6973384072
C	-4.3950083589	-1.6007641344	2.1570972479
H	-3.229252908	-0.625616847	3.6683414805
C	-4.6065402556	0.8382859768	2.8507080878
C	0.0745047524	1.1581588486	5.4706663709
H	0.8893494947	0.8313075542	3.5153962065
C	0.3594344095	2.9300418786	3.6662723624
C	-0.3518154545	-0.1269231946	-0.0674836207
C	1.0601029577	-0.0628599389	-0.6495921904
H	-0.6686591605	-1.1668676348	0.0768430957
H	-1.0661919066	0.357818341	-0.7490890773

H	1.3810526631	0.9811186571	-0.738811535
H	1.7622115448	-0.5434452602	0.040648639
C	1.1711446568	-0.7221172384	-2.0255304659
H	0.9323344092	-1.7924381168	-1.9686110606
C	2.5913729875	-0.5257833202	-2.5806480183
H	0.4458166538	-0.2828323781	-2.7253320859
N	2.8899530171	-1.1691511584	-3.7353879889
O	3.4023194525	0.1876237811	-1.9906281326
C	2.0033631477	-2.0413869554	-4.5206750105
C	2.7777090313	-2.2436893963	-5.8335187082
C	4.2493247901	-2.1579940472	-5.3942992112
C	4.2379314938	-1.0581234078	-4.3244735931
H	1.842052134	-2.9999883273	-4.0056840405
H	1.0240057131	-1.5774198501	-4.6817523808
H	2.5432680541	-1.4311259652	-6.5309440479
H	2.5229906765	-3.1883955587	-6.3216587348
H	4.9287636442	-1.9284953444	-6.2194139962
H	4.5683027767	-3.1098679284	-4.9533866983
H	4.3739652035	-0.059113028	-4.7578154841
H	4.9964159762	-1.1847290486	-3.5480032473
H	0.4157978107	1.15834999	1.4380625702
H	-5.2180497695	-1.8688511623	2.8253303822
H	-4.8267690471	-1.4017506789	1.1682430906
H	-3.7206723896	-2.4589714901	2.0812352766
H	-5.4072765249	0.6032404665	3.5588573431
H	-4.084844456	1.7301549812	3.2167330625
H	-5.0677757358	1.0945583652	1.89077867
H	1.3306626793	3.2327627674	4.0698496878
H	0.361604298	3.1436951274	2.5912489344
H	-0.4103833412	3.5571741592	4.1289944495
H	1.022546092	1.4600154943	5.9244153798
H	-0.722396701	1.7267529544	5.9661860294
H	-0.0768594327	0.0928897996	5.6691696162

DIG:10_oc

H	4.4378434052	-0.6213640394	0.4069748647
C	3.7158345843	0.1981488497	0.3209135509
C	2.518584258	-0.226363701	-0.5347070134
N	1.5492552867	0.8769073831	-0.5657901063
C	0.2223297481	0.6337280169	-0.9139108978
N	-0.5434079143	1.793192517	-1.0683538861
C	-0.3731989217	2.9998253394	-0.2391614801
C	-0.6798678595	2.7485083369	1.2447472572
H	-0.5067511025	3.6535063576	1.8395046298
N	-0.1953041879	-0.5728500659	-1.0754213152
C	-1.6091609963	-0.8166289522	-1.2848671427
C	-1.8901258225	-2.3226438782	-1.2717643267
C	-3.3825305176	-2.6515925736	-1.4682788201
C	-3.6830461708	-4.1183334212	-1.5454717881
N	-3.7167821585	-4.9607122193	-0.4565840947
H	-1.9533194801	-0.4091962715	-2.2537827697
H	-2.2355980758	-0.3320195934	-0.509417514
H	1.9987277768	-1.0565651893	-0.0492180781
C	2.9425809186	-0.6801606333	-1.9388084715
H	0.6723554818	3.3166241575	-0.3240733773
C	-1.2465042834	4.1119326135	-0.8270050701
H	-1.3031645244	-2.7998324343	-2.0646787888

H	-1.5233873102	-2.7345827264	-0.322826808
H	4.2414587931	1.0522743278	-0.1279841105
H	3.395583709	0.4881234138	1.3269617138
H	-1.7277122305	2.4508736157	1.3780681791
H	-0.0410223695	1.9517403974	1.6372999713
H	-3.731899608	-2.2200335727	-2.4122093221
H	-3.9719828483	-2.1777326045	-0.6688496429
H	-1.5194989361	1.5832466955	-1.2391470669
C	-3.9911622551	-6.2276918234	-0.9401665368
C	-3.4591771253	-4.6303789372	0.934113681
H	-4.0751569407	-7.0785725664	-0.2796487821
C	-4.1162651949	-6.0866096407	-2.2970795801
N	-3.9258173902	-4.7755526352	-2.6663093447
H	-4.3422907206	-6.8511605661	-3.0287003041
H	-3.756641201	-3.59835594	1.1329527037
H	-4.0486844832	-5.2882046644	1.5784236313
H	-2.3987706208	-4.7446652998	1.1875373928
H	1.9232471361	1.7262145947	-0.9756604084
H	-1.1127091447	5.0441206894	-0.2682672329
H	-0.9948795323	4.2933789554	-1.876736826
H	-2.3103418921	3.8444694546	-0.7719038038
H	2.0652105801	-0.9881786004	-2.5131324847
H	3.4535405745	0.1300752501	-2.4767063523
H	3.6341395661	-1.5293894162	-1.8811650285

DIG:10_ocH⁺

H	4.1379301116	-0.7018240885	1.2686184383
C	3.38927623	0.0736780145	1.084431352
C	2.6142532133	-0.2469568508	-0.1959982507
N	1.5762375272	0.7948693275	-0.3854314155
C	0.3764569284	0.6350597418	-0.9683220998
N	-0.550249774	1.6055464109	-0.895268999
C	-0.4794491659	2.8450993415	-0.0874632376
C	-1.9015624254	3.230233937	0.3282940228
H	-1.8757770488	4.1259201979	0.9551465622
N	0.075784182	-0.5152558781	-1.5926414269
C	-1.256637934	-0.9125320262	-2.0739182461
C	-1.2455661683	-2.4031520051	-2.4129356607
C	-2.5924868922	-2.8996100571	-2.9517746189
C	-2.5091984931	-4.361859333	-3.2861047825
N	-3.5619144938	-5.0925700425	-3.7745870357
H	-1.9869535275	-0.6997271103	-1.2839182147
H	-1.5279462132	-0.3211595646	-2.9606838537
H	2.0782063864	-1.1912176846	-0.0453463607
C	3.5349019359	-0.3560586139	-1.419414447
H	0.0849391764	2.5899173891	0.8171531068
C	0.2286684385	3.9756757552	-0.8467718796
H	-0.4715166405	-2.6097775692	-3.1614764927
H	-0.9772014784	-2.9824988483	-1.5235161563
H	3.9213444549	1.0290037911	0.9942110697
H	2.7243144838	0.120703943	1.9520445957
H	-2.5187104099	3.4612708675	-0.54904999
H	-2.3819846008	2.4276619464	0.8958755932
H	-2.8773745539	-2.3169139779	-3.8412556716
H	-3.3825853297	-2.7196146863	-2.2068771546
H	-1.3448379901	1.5203203268	-1.5154905743
C	-3.0946386636	-6.3820884649	-3.9540777075

C	-4.9077635018	-4.6165527646	-4.0541993642
H	-3.7327386861	-7.166202147	-4.3340301772
C	-1.7815052094	-6.3629873416	-3.5638983156
N	-1.4236491382	-5.1002847472	-3.1487809898
H	-1.0750004956	-7.1814309714	-3.5572535513
H	-4.8955492674	-3.8287293067	-4.8150507533
H	-5.5061694022	-5.4484841934	-4.4284514618
H	-5.3832337703	-4.2286847726	-3.1469495576
H	1.8350454596	1.7359895101	-0.1223634579
H	0.8391904716	-1.137473794	-1.8188612566
H	2.9816067348	-0.5673908324	-2.3417664086
H	4.089962195	0.5761808715	-1.5707599956
H	4.2602828972	-1.1621417841	-1.2718459687
H	0.3076491088	4.8632845367	-0.2113373384
H	1.2406311048	3.6969387489	-1.1626806953
H	-0.3351138602	4.2508617989	-1.7447261725

DIG:11_oc

H	4.5540505894	-0.4804322649	0.2070608223
C	3.8090141594	0.3211558493	0.1535707584
C	2.5897211701	-0.1292562215	-0.6565606533
N	1.5936650107	0.9500856548	-0.6453902136
C	0.2599108642	0.6723970715	-0.9439621317
N	-0.5396755965	1.8155111283	-1.0601767281
C	-0.3786196893	3.0064952082	-0.2066155148
C	-0.631439902	2.7119082146	1.2795238193
H	-0.468436218	3.6081554349	1.8903973669
N	-0.1323298489	-0.5421770741	-1.0985829969
C	-1.5480490926	-0.8237607651	-1.2505381091
C	-1.8011619211	-2.3328252811	-1.186584339
C	-3.2889708343	-2.6972627595	-1.3340022233
C	-3.5367271302	-4.1767953389	-1.347860749
C	-4.1504127902	-4.9564068779	-0.3949370123
H	-1.9300408975	-0.4472770352	-2.217856636
H	-2.156734434	-0.3284217606	-0.4678224726
H	2.1088339495	-0.9732396183	-0.1548566099
C	2.9693466182	-0.5688146227	-2.0777578713
H	0.6544017127	3.3554366441	-0.3152661746
C	-1.301827721	4.1056404765	-0.7401607464
H	-1.2256396733	-2.8252329786	-1.9782001029
H	-1.4155764985	-2.7170073861	-0.2336991472
H	4.2951403438	1.1902170399	-0.3110791153
H	3.5214148192	0.598774158	1.172901159
H	-1.6646113892	2.3773078456	1.4373196904
H	0.0438418378	1.9271371584	1.6332958178
H	-3.6720483485	-2.2653704382	-2.2694319822
H	-3.866780449	-2.2415782497	-0.518203326
H	-1.5149148477	1.5782693047	-1.1985306613
N	-4.1071895027	-6.2543187061	-0.8709101075
H	-4.604849881	-4.7164194401	0.5556894302
C	-4.6360169671	-7.4381103281	-0.2208104435
C	-3.473509592	-6.1933159642	-2.0799382266
N	-3.1168629319	-4.9691472773	-2.4000698744
H	-3.3070634077	-7.0805382586	-2.678492452
H	1.9285382393	1.807281011	-1.0729331003
H	-1.1771757587	5.02889276	-0.1645416545
H	-1.0896587962	4.3174794077	-1.792968109

H	-2.3550734505	3.8053011073	-0.6576624814
H	2.0775537677	-0.8980297355	-2.6169333019
H	3.4374056876	0.2558302467	-2.6327909919
H	3.6842076586	-1.4001569696	-2.0505563582
H	-4.440827319	-8.306703041	-0.8542597362
H	-4.15497031	-7.5988734045	0.7500943747
H	-5.7176222296	-7.351750924	-0.0700038852

DIG:11_ocH⁺

H	4.3101421096	-0.7910303657	0.6220528141
C	3.5599580737	0.0006172953	0.5423010128
C	2.5331252109	-0.3630604698	-0.5331420086
N	1.5107211762	0.7086570736	-0.5814948925
C	0.2140387188	0.5648302693	-0.9050158904
N	-0.6482376176	1.5786457551	-0.7198811257
C	-0.3743002462	2.865964153	-0.0408393772
C	-1.6714460917	3.3522078778	0.6104644447
H	-1.489299889	4.2856291175	1.1502117498
N	-0.2405567309	-0.6092539212	-1.3719888811
C	-1.6534730112	-0.9515946085	-1.6030137161
C	-1.7820334845	-2.4449160546	-1.9029833625
C	-3.2212889266	-2.8551231967	-2.2571191488
C	-3.2775980313	-4.2711776515	-2.7540258138
C	-4.1385815496	-5.2840203763	-2.4032189712
H	-2.225267288	-0.6843130186	-0.7061781483
H	-2.047032925	-0.3684769042	-2.4485758266
H	2.0096517653	-1.2720591329	-0.2146255215
C	3.1845374459	-0.5869730198	-1.9048751984
H	0.3472970093	2.6460818806	0.7549724452
C	0.2125211043	3.9027738584	-1.0089835019
H	-1.1427660848	-2.7082583087	-2.7549164018
H	-1.4301636785	-3.0236604373	-1.0399974287
H	4.0873510192	0.9279343342	0.285575789
H	3.0861715168	0.1240803882	1.5207997731
H	-2.4395373732	3.5546770423	-0.1464011896
H	-2.0613880325	2.6161316002	1.3198723789
H	-3.5993556148	-2.1770880366	-3.0370335579
H	-3.8812886999	-2.7353835142	-1.3891654645
H	-1.5553782328	1.4866225719	-1.1580797758
N	-3.7794125888	-6.3703875907	-3.1757413734
H	-4.9575146586	-5.3329568145	-1.7001625457
C	-4.4089643757	-7.6825306005	-3.1771830227
C	-2.7267303986	-5.9658852908	-3.943386082
N	-2.394998723	-4.7113529531	-3.7184049799
H	-2.2445251653	-6.6325030771	-4.6467590025
H	1.8444515938	1.6520179253	-0.4390605628
H	0.4415607339	-1.2683975568	-1.7205200471
H	2.4501712528	-0.8285708388	-2.6817460964
H	3.7270105451	0.3084015821	-2.2275846894
H	3.8989908165	-1.4142680986	-1.8503360264
H	0.4457149925	4.8279102925	-0.4725933111
H	1.132747555	3.5513326032	-1.4898068512
H	-0.5050235941	4.1419520464	-1.8013379033
H	-3.8807944918	-8.326209288	-3.8835062242
H	-4.3583182327	-8.1354468482	-2.1823876298
H	-5.4564909031	-7.6077486932	-3.4846348569

DIG:12_oc

C -5.0672545894	-1.6228103028	-0.3089961422
N -3.8204688783	-1.0258768341	-0.8224191768
C -3.2526575352	0.1406497269	-0.2988798968
N -1.9943375609	0.378439748	-0.1759985187
C -1.0366849092	-0.6801220834	-0.4320891473
C 0.3578311728	-0.2543952019	0.038075856
C 1.4336533989	-1.3212518978	-0.2361444651
C 2.7940776395	-0.9128581176	0.2809124028
N -4.1900349943	1.0948048142	0.091745459
C -3.7519557224	2.4321396665	0.5112711616
H -3.1186695638	-1.7289850695	-1.0213756164
H -5.0183042538	1.1086690763	-0.4939164134
C -5.4654199178	-2.7715958111	-1.2399682445
H -5.8498351006	-0.8580833445	-0.3681399127
C -4.9500730803	-2.0787345506	1.152901969
H -2.8804983913	2.265314523	1.1499629709
C -3.3194174566	3.3104262779	-0.6715775121
C -4.8715159073	3.0796190944	1.3316634561
H -0.9858187001	-0.9214769606	-1.5106233189
H -1.3058376333	-1.6244266939	0.0807101277
H 0.6234863293	0.6861548337	-0.4606877982
H 0.324681308	-0.0423699339	1.1128529244
H 1.4913820999	-1.5219080334	-1.3142054071
H 1.145909006	-2.2583965491	0.2567423777
H -4.5588411699	4.0618766669	1.7028228913
H -5.7733966632	3.2309867651	0.7224316596
H -5.1420660117	2.4532203986	2.187861326
H -2.9609412382	4.2860765883	-0.321570564
H -2.5110262661	2.8228756688	-1.2223831133
H -4.1594326805	3.489788433	-1.3566169514
H -5.9033217169	-2.482620836	1.5149149144
H -4.189361222	-2.8630837257	1.2541759948
H -4.6671235516	-1.2385731713	1.7940324583
H -6.4158905119	-3.2139938897	-0.9236366677
H -5.5682096543	-2.4212117412	-2.2719587473
H -4.7095141494	-3.5682347353	-1.223172018
C 3.7891533282	-0.4198644346	-0.5743850531
C 5.0149688507	-0.027948265	-0.0405327468
C 5.2138089184	-0.1390101349	1.3345557531
C 4.1661964443	-0.6412757622	2.1076154557
N 2.9856781645	-1.0212000697	1.6079261495
H 3.5997763531	-0.3482314664	-1.6419759888
H 5.8007196711	0.3548863741	-0.6869604458
H 6.1519977418	0.1510414645	1.7982515933
H 4.2817206035	-0.7475155042	3.1857879649

DIG:12_ocH⁺

N -3.7599679407	-1.3076509059	-0.1617443498
C -3.3554025639	-0.0324650351	-0.0374177783
N -2.0517960218	0.2618715555	-0.1752018978
N -4.2377813678	0.9335396602	0.2690972625
C -0.9627250434	-0.7160739078	-0.3277897796
C 0.387103039	-0.0146088151	-0.1760031823
C 1.5718042191	-0.9654780905	-0.4026968624
C 2.8946825398	-0.2216993585	-0.4602209768

C	-5.1049857419	-1.8474500789	0.1452384985
C	-6.0548288193	-1.71421253	-1.0533153817
C	-4.9479597962	-3.3004122419	0.6005087481
H	-4.5368064167	-3.9225395974	-0.2042911671
H	-4.2929765951	-3.3756923254	1.4736497641
H	-5.9244638129	-3.7137739447	0.8675817222
H	-5.6944466405	-2.3074235518	-1.9007653621
H	-7.0515772114	-2.0780466139	-0.7849174641
H	-6.1555837396	-0.6769831943	-1.3932779241
H	-5.4845603053	-1.2620447825	0.9910759926
C	-3.9225772106	2.3323173274	0.6450543559
C	-3.7898020428	3.2336669611	-0.5902561002
C	-5.0048454678	2.8266906766	1.6081158777
H	-5.9874696427	2.8451563901	1.1202669169
H	-5.0654100061	2.1943161695	2.4989574078
H	-4.778973586	3.8478501967	1.9275693118
H	-3.5139407867	4.2482779806	-0.2865222695
H	-4.7393849994	3.288998363	-1.1336274985
H	-3.0270166422	2.8738770269	-1.2903558031
H	-2.9703407283	2.2969349178	1.1869963271
H	-5.2171699779	0.7113681761	0.1539637781
H	-1.80574274	1.2319698226	-0.3154177435
H	-1.0859820979	-1.491576786	0.4375924632
H	-1.0231255641	-1.1955223299	-1.3158741551
H	-3.1062658085	-1.950603315	-0.5892157545
H	0.4529949444	0.4344279774	0.8230643074
H	0.4702377033	0.7979926045	-0.9077502811
H	1.6080530685	-1.7319748109	0.380447346
H	1.4285062393	-1.4933214393	-1.3569138353
N	2.9211929495	0.8682458334	-1.2440493035
C	4.0738435685	1.538901961	-1.3509447664
C	5.2474638178	1.1670276902	-0.6937027317
C	5.2138237181	0.0384003557	0.1225766875
C	4.0171535857	-0.6677905924	0.244036606
H	4.0573251322	2.4158623098	-1.9955953453
H	6.1555004428	1.7481627478	-0.8193175625
H	6.1015878777	-0.2876753357	0.6570788632
H	3.9556694713	-1.552470121	0.8715530399

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C	-5.0710838019	-1.6222438103	-0.2877852235
N	-3.8285861927	-1.0332170001	-0.8207421741
C	-3.2480057901	0.1324238683	-0.3125495439
N	-1.9863564185	0.3674157118	-0.2118736357
C	-1.0326100497	-0.6906545443	-0.4753628125
C	0.3560896682	-0.2681105393	0.0166977215
C	1.4390140108	-1.3277745585	-0.2630426009
C	2.7849975471	-0.9228122741	0.2869959279
N	-4.1730289333	1.091763011	0.0902979136
C	-3.7247517212	2.4323711347	0.4888108699
H	-3.1353114025	-1.7391441682	-1.0373712416
H	-5.0170905724	1.1006987843	-0.4722756977
C	-5.4913601126	-2.7698026485	-1.2105626288
H	-5.8494325632	-0.8526132581	-0.3356418984
C	-4.9346699848	-2.0771506551	1.1727498104
H	-2.8370660079	2.2707839048	1.1059635226
C	-3.325072063	3.3006083556	-0.7129851533

C	-4.8228907308	3.0862921114	1.3327417433
H	-0.9705714244	-0.9158988869	-1.5565464533
H	-1.3035037785	-1.6430624408	0.0215151802
H	0.6232808957	0.6811935169	-0.4638578838
H	0.3079424553	-0.0737130744	1.0944221955
H	1.5177096842	-1.5037973627	-1.3433868157
H	1.149977163	-2.2756535667	0.2065551392
H	-4.5011294815	4.0720164572	1.6863768791
H	-5.7407010973	3.2318126006	0.746415721
H	-5.0702947654	2.468000406	2.2017410568
H	-2.9593859919	4.2800972433	-0.3819634649
H	-2.5310540673	2.8099720866	-1.2818167943
H	-4.1839113893	3.4716411572	-1.3761402563
H	-5.8852749275	-2.4741167538	1.5488740974
H	-4.1785658846	-2.8672326984	1.2631994839
H	-4.6368809629	-1.2386932591	1.8094315008
H	-6.4408320015	-3.2028464183	-0.8791028202
H	-5.6062180719	-2.4212335607	-2.2418555252
H	-4.7423376535	-3.5730682999	-1.2022260056
C	3.7675501795	-0.3505515381	-0.5338874244
C	4.965068104	0.0276273438	0.0572094927
C	5.1869462618	-0.1527252068	1.4164525105
C	4.1446487393	-0.7313089761	2.1411943615
N	2.9792565565	-1.1076403055	1.6051456851
H	3.6115898538	-0.2044012863	-1.5955522891
N	6.0269634136	0.6300542769	-0.7776032198
H	6.1223671275	0.1403066381	1.8751973325
H	4.2571545503	-0.9029438468	3.2098438963
O	7.0697000719	0.9587092842	-0.2162710589
O	5.7988715599	0.7631320451	-1.9777334198

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N	-3.7618719296	-1.2975036666	-0.2502272368
C	-3.3516237497	-0.0296693461	-0.0818711689
N	-2.0549096591	0.2752979374	-0.267729449
N	-4.2163960502	0.9182725273	0.3144899601
C	-0.9716615601	-0.6926348278	-0.4958913555
C	0.384575136	-0.0072033578	-0.3212033014
C	1.5574010214	-0.9635038655	-0.590802523
C	2.8916070945	-0.2423033233	-0.5892621791
C	-5.0854745148	-1.8589932922	0.1102550632
C	-6.1047032971	-1.6746568937	-1.0225971574
C	-4.8979262412	-3.3310153573	0.4858910905
H	-4.5361921641	-3.913072554	-0.370929602
H	-4.191174548	-3.4449271948	1.313327436
H	-5.8557056903	-3.7606482576	0.7922220368
H	-5.7931417974	-2.2246351887	-1.917186186
H	-7.0824096051	-2.0573628307	-0.713690213
H	-6.2292618429	-0.6231065123	-1.3061279888
H	-5.4149722192	-1.3154102009	1.0035357005
C	-3.8825889196	2.2893186598	0.7698690278
C	-3.8229065579	3.2752515618	-0.4048728188
C	-4.9083380085	2.7085778566	1.8260029912
H	-5.9172164112	2.7579779706	1.397615338
H	-4.917973886	2.0136446433	2.6710839422
H	-4.664702249	3.7050589234	2.204836743
H	-3.5314258438	4.2676598185	-0.0471812972

H	-4.8022460453	3.3637057432	-0.887627051
H	-3.1014000759	2.9693834106	-1.1713582732
H	-2.9003189918	2.2208138903	1.2514593481
H	-5.2006082472	0.7010401926	0.2347345554
H	-1.8204063909	1.2512791287	-0.3850381413
H	-1.0854319915	-1.5106772088	0.2250506064
H	-1.0476547753	-1.1146033295	-1.508662166
H	-3.1368414844	-1.9145073543	-0.7524475392
H	0.4580634192	0.3970905304	0.6961094926
H	0.4702886634	0.8351346736	-1.0181323028
H	1.5725946403	-1.7729638869	0.1478096789
H	1.4208239824	-1.4313528019	-1.575971086
N	2.9775171854	0.8469507392	-1.3708479839
C	4.1404449367	1.5042884091	-1.4256883483
C	5.2797910827	1.1255510741	-0.7123572104
C	5.1610380049	0.0018780636	0.0923223314
C	3.9679871751	-0.7054988849	0.172990564
H	4.1686884719	2.3781519933	-2.0723435809
H	6.2116608917	1.6731828969	-0.7738473683
N	6.3257587978	-0.4550364444	0.8867595252
H	3.8967207734	-1.5813892084	0.806142154
O	6.1668137519	-1.446891366	1.5929972447
O	7.3625877181	0.1913525103	0.7826846987

DIG:14_oc

C	-5.0559701049	-1.6295358324	-0.2588673552
N	-3.8363957482	-1.0258499447	-0.8282948932
C	-3.2531702672	0.1435640759	-0.3303591119
N	-1.9916106099	0.385655761	-0.2488070629
C	-1.0352298986	-0.6683770529	-0.5193201627
C	0.3508331212	-0.2522419601	-0.0145056503
C	1.4356462823	-1.3060690918	-0.3075838363
C	2.7776982022	-0.9161212151	0.2637378097
N	-4.178036014	1.0980878705	0.0837621421
C	-3.7336484657	2.4416491709	0.4761313348
H	-3.1418623874	-1.7247790642	-1.0632283405
H	-5.0299988057	1.0998207143	-0.4670078613
C	-5.4898392845	-2.7815774246	-1.169712569
H	-5.8442239405	-0.8690809919	-0.2823688869
C	-4.8701158865	-2.0833541699	1.1964442118
H	-2.8379420138	2.2861076296	1.0832531624
C	-3.353255001	3.3112126685	-0.7309099159
C	-4.8261248588	3.0893778308	1.3321317648
H	-0.9679537575	-0.8795382947	-1.6029254522
H	-1.3077498264	-1.6273805093	-0.0362285506
H	0.6190729755	0.7053965697	-0.4776615291
H	0.2983943182	-0.0764463766	1.0661651745
H	1.5229378237	-1.4595007712	-1.3908670616
H	1.1413010064	-2.2638166799	0.1384561192
H	-4.5074179188	4.0782758068	1.6796190374
H	-5.7519856655	3.2267186266	0.7566077965
H	-5.0582857578	2.4712908957	2.2054709109
H	-2.9917402583	4.294018008	-0.4052099424
H	-2.5615856122	2.8253960976	-1.3070353741
H	-4.2203309028	3.4742195527	-1.3852892944
H	-5.8029868143	-2.4950051235	1.6000849175
H	-4.099448406	-2.8615500669	1.2634587426

H	-4.5666558919	-1.240752083	1.824953588
H	-6.4240054112	-3.2260965136	-0.8109695416
H	-5.6392045706	-2.4338940733	-2.1969009018
H	-4.7314214794	-3.5758916101	-1.1841464835
C	3.7761350329	-0.3470772601	-0.5360293942
C	4.9900552683	0.0264944655	0.0544693031
C	5.1673546767	-0.1807197354	1.4289084857
C	4.1125641487	-0.7540482284	2.1357297968
N	2.950200085	-1.1150401344	1.5830446674
H	3.6160836428	-0.197747268	-1.5987576648
C	6.0363030079	0.6081396592	-0.738223977
H	6.0937314384	0.0929592316	1.9216870172
H	4.209689543	-0.935511084	3.2046607089
N	6.884085986	1.0787929251	-1.3799328776

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N	-3.7611406726	-1.2983643487	-0.2425309682
C	-3.350885864	-0.0309599961	-0.070410491
N	-2.0526309042	0.2722443627	-0.2470568
N	-4.2174530685	0.9176247428	0.3207755912
C	-0.970004521	-0.6971746513	-0.4724332663
C	0.3865468851	-0.0118045703	-0.301094178
C	1.5592246112	-0.9704257476	-0.5628346864
C	2.8928660856	-0.2473346006	-0.5703992309
C	-5.0899349532	-1.8574318556	0.1015088482
C	-6.096013909	-1.6669020808	-1.0420416645
C	-4.9102187217	-3.3310369171	0.4746923564
H	-4.5364974325	-3.9105912891	-0.3786732861
H	-4.2159242607	-3.4489479052	1.312048452
H	-5.8730973772	-3.7602564382	0.765130178
H	-5.7765950269	-2.2160034179	-1.9344243764
H	-7.0784479387	-2.0467392571	-0.7447373611
H	-6.2133923844	-0.6142462364	-1.3244471436
H	-5.4280753249	-1.3159836212	0.9928652693
C	-3.8854017596	2.2903088139	0.7722678458
C	-3.819293324	3.2717547549	-0.4059087145
C	-4.916028665	2.7142837962	1.8217717933
H	-5.9231178134	2.7611474303	1.3888659823
H	-4.929055993	2.0233303568	2.6700372914
H	-4.6743538586	3.7126666874	2.1967876788
H	-3.5288061696	4.2652900289	-0.0504772022
H	-4.7963907892	3.3592559173	-0.8933943523
H	-3.094426667	2.9629135407	-1.1680346844
H	-2.9057097993	2.2235061465	1.2593532408
H	-5.2013965786	0.7013834315	0.2351872942
H	-1.8150092359	1.2481503702	-0.3580875859
H	-1.0837581519	-1.5131249903	0.2510147959
H	-1.0467714741	-1.122084621	-1.4839318095
H	-3.1319749349	-1.9158938627	-0.7388515088
H	0.4595030997	0.3994127606	0.7135376134
H	0.4738619108	0.8254899681	-1.0038472219
H	1.5742489334	-1.7728976597	0.1835268427
H	1.4215200299	-1.447632386	-1.5433657709
N	2.9716082946	0.8364845282	-1.3601837385
C	4.1344801639	1.493816163	-1.4211108064
C	5.2735835175	1.1210175928	-0.7091094944
C	5.1869936328	-0.0047896684	0.1189132769

C	3.9719567346	-0.7018732055	0.189463763
H	4.1600190275	2.3638224652	-2.0735948734
H	6.1958996602	1.685053641	-0.791116388
C	6.3161264241	-0.4416180442	0.8893871949
H	3.8817138605	-1.5782096394	0.8227102445
N	7.2250557023	-0.7991204884	1.5194390505

DIG:15_oc

C	-5.0325517881	-1.6302911871	-0.2800633544
N	-3.8198661387	-1.0099228136	-0.846003032
C	-3.2461170547	0.1590489399	-0.332682448
N	-1.9878243219	0.4086752968	-0.2415429951
C	-1.022105688	-0.637279687	-0.5186568455
C	0.3590567176	-0.233200587	0.0074341531
C	1.4440066678	-1.2828376766	-0.2942930581
C	2.7830153247	-0.9157902227	0.3035409584
N	-4.1824671228	1.1030229179	0.0851871147
C	-3.7477014621	2.4450664447	0.4924194408
H	-3.1168823315	-1.7008818799	-1.0802450425
H	-5.0265901874	1.1069104584	-0.4778542936
C	-5.4487770463	-2.7858107068	-1.1946651208
H	-5.8309214033	-0.8802392829	-0.3039384787
C	-4.8449327444	-2.0847839125	1.1748842644
H	-2.8552874543	2.2881501151	1.1040820734
C	-3.3625624883	3.3277798806	-0.7034742051
C	-4.8491616015	3.079712386	1.3467443915
H	-0.9455116393	-0.8276371422	-1.6053676193
H	-1.3000488792	-1.6052687363	-0.0569910625
H	0.634917134	0.7320503115	-0.4351988091
H	0.2981589791	-0.0782025439	1.0906015499
H	1.544242415	-1.4141978	-1.3795399739
H	1.1362841467	-2.2491227282	0.1256816185
H	-4.5384231996	4.0674519944	1.7048370688
H	-5.7722359878	3.2165320013	0.7664905611
H	-5.0833530496	2.4525793501	2.2130772801
H	-3.0087576216	4.3095249189	-0.3659804551
H	-2.5636211072	2.8511550573	-1.277213685
H	-4.2253206744	3.4922880708	-1.3634205428
H	-5.7739807221	-2.5077423434	1.5759610537
H	-4.0651671897	-2.8537630408	1.2428645676
H	-4.5525086814	-1.2394006936	1.8048421891
H	-6.3778743977	-3.2442513531	-0.8399987131
H	-5.5996622396	-2.4374019325	-2.221441443
H	-4.6792617503	-3.5693574209	-1.2089674188
C	3.8190248042	-0.4217140514	-0.4862971534
C	5.0341801047	-0.067600719	0.1148502925
C	5.1634780639	-0.2243350787	1.4983826781
C	4.0622556064	-0.728569089	2.1946289591
N	2.8996907781	-1.0711869178	1.6395499073
H	3.7066736177	-0.3055601361	-1.5595631062
O	6.0018015975	0.4043686161	-0.7130893522
H	6.0734672459	0.0267877031	2.0301028842
H	4.133942002	-0.8648984642	3.2734607854
C	7.2498020365	0.7768744642	-0.1435135531
H	7.8650200234	1.1240677754	-0.975235087
H	7.1316560749	1.5884518121	0.5856260594
H	7.7407836329	-0.0767913672	0.3408869974

DIG:15_ocH⁺

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C -3.3398427404	-0.0381457163	-0.0265838219
N -2.0389096792	0.2625078759	-0.171765531
N -4.2161040029	0.9112931093	0.3438307317
C -0.9539530179	-0.7066452823	-0.3950261647
C 0.3994112601	-0.0125253272	-0.2429610411
C 1.5778481578	-0.9552309742	-0.5297662622
C 2.8969796607	-0.2057684307	-0.584833994
C -5.0863466494	-1.8613109471	0.0945130882
C -6.0568408141	-1.670040537	-1.0793609982
C -4.9209414472	-3.3349100421	0.4744187965
H -4.5194828679	-3.9151140356	-0.3658276118
H -4.2541786117	-3.452580007	1.3338836953
H -5.893169009	-3.7632352342	0.733351929
H -5.7109388555	-2.2202880243	-1.961131126
H -7.0487891034	-2.047654361	-0.8120981126
H -6.1628963287	-0.617285877	-1.3657326042
H -5.4515818473	-1.3190991881	0.9747390097
C -3.8916664528	2.2890698606	0.7834432814
C -3.7691264486	3.2503491001	-0.407112787
C -4.9612741423	2.7392990431	1.7815514578
H -5.9489881093	2.7855096133	1.305976365
H -5.0147754445	2.0636109624	2.6404581814
H -4.7276138431	3.7424639341	2.1487739509
H -3.4862997591	4.2476136429	-0.0559155582
H -4.7243799831	3.3360549148	-0.9365206627
H -3.0153172607	2.9247944772	-1.1333752594
H -2.9334468888	2.2242978657	1.3121007524
H -5.1977440099	0.6959583065	0.2349512609
H -1.7938046671	1.2385340332	-0.2634772543
H -1.0596637547	-1.5172169511	0.3360216732
H -1.038130352	-1.1391927501	-1.40275546
H -3.1000260156	-1.926402875	-0.6762450101
H 0.4861492616	0.3964522192	0.7716704413
H 0.4703755105	0.8273448467	-0.9445467713
H 1.6284446275	-1.7510871718	0.2222737703
H 1.4162765955	-1.4428121894	-1.5020878423
N 2.9095431106	0.8956417871	-1.3614422916
C 4.0641326203	1.5600495289	-1.453382408
C 5.2451844663	1.1941980434	-0.806304749
C 5.2187603869	0.0516678761	0.0020456068
C 4.0110630734	-0.6574565334	0.1114572177
H 4.0562010746	2.4458519305	-2.0864940807
H 6.1403097293	1.7897472375	-0.9377189627
O 6.2642964263	-0.4384149809	0.6996349979
H 3.9762296357	-1.546290921	0.7331732186
C 7.5178228014	0.2400977914	0.6198664805
H 8.2008376682	-0.3288658691	1.251123853
H 7.8957580687	0.2543509412	-0.4090996132
H 7.4378481044	1.2660836177	0.9981389273

DIG:16_oc

C 2.3886805635	2.3354173691	0.1987941258
N 1.8702311008	1.0476623398	-0.3016619996

C	2.5160769159	-0.172932011	-0.0668689669
N	1.9490627508	-1.2942882868	0.2042123969
C	0.5269154355	-1.3426963896	0.4864957997
C	0.1742472964	-2.656131124	1.192915052
C	-1.3317344319	-2.8014372644	1.4760150541
C	-1.6501375416	-4.0567925825	2.2585268861
N	3.9041048666	-0.0933405316	-0.1707367771
C	4.7212541906	-1.31133566	-0.1095355512
H	0.8680946647	0.9703721783	-0.1728630139
H	4.2144994754	0.5640215393	-0.8787550866
C	1.5388685441	3.4603021688	-0.3989553114
H	3.4104753756	2.4481120518	-0.1792552339
C	2.435571924	2.4006709744	1.7323658644
H	4.2937025251	-1.9086364307	0.7001396879
C	4.6496089622	-2.1349477538	-1.4037390635
C	6.1589791257	-0.9208366926	0.246331129
H	-0.0616251952	-1.2719788382	-0.446911843
H	0.1893191505	-0.5036400752	1.1259004375
H	0.5237719918	-3.4922151195	0.5742815756
H	0.7250760054	-2.7121584721	2.1387565988
H	-1.8900332508	-2.7961109136	0.5303255088
H	-1.6724748962	-1.9388207467	2.0627348286
H	6.7869259726	-1.8128912722	0.3483708705
H	6.6053704156	-0.2933181193	-0.5375388662
H	6.1917326429	-0.3620871135	1.1872798752
H	5.2399128199	-3.0549874709	-1.3142655972
H	3.6124829257	-2.4083774978	-1.613816421
H	5.0469829459	-1.564356247	-2.2542924395
H	2.8588434888	3.3539636523	2.0714320245
H	1.4271488417	2.3082578529	2.1550044957
H	3.0527399441	1.5901141768	2.1315485113
H	1.9224824667	4.4390351706	-0.0919455769
H	1.5382848289	3.4114457907	-1.4925828093
H	0.4984866385	3.391431622	-0.0536046666
C	-2.1764764291	-5.1813036234	1.6227772405
C	-2.4322323429	-6.3608601534	2.3573778339
C	-2.143252338	-6.3051609671	3.7389868129
C	-1.6222705933	-5.1313891238	4.2695227214
N	-1.3687084265	-4.0170498949	3.5746048423
H	-2.3849544864	-5.130088886	0.5607245875
N	-2.9320560029	-7.5003075033	1.7600788058
H	-2.320713752	-7.1496083264	4.3935230248
H	-1.3992971152	-5.0867061909	5.3356224183
C	-3.336197185	-8.6261393571	2.5860984171
C	-3.3583471032	-7.4591326107	0.3711445018
H	-3.6770125103	-8.4575309191	0.0655479561
H	-4.1959744026	-6.764148941	0.2045937551
H	-2.5326593685	-7.158574782	-0.2847251583
H	-3.6695492326	-9.4412375414	1.9410375751
H	-2.4953747297	-8.9981693962	3.1838140961
H	-4.157685462	-8.373306057	3.2741310711

DIG:16_och⁺

N	-1.6359575664	0.8444506761	-0.0923555025
C	-2.5059791395	-0.1657630307	-0.262241463
N	-2.0475013514	-1.376827127	-0.6157573687
N	-3.8266417025	0.0452539112	-0.1265595894

C	-0.6569832826	-1.7009284321	-0.9756456553
C	-0.5976511589	-3.1060291089	-1.5739228391
C	0.8351544627	-3.561256682	-1.8856827946
C	0.8866062111	-5.0389352528	-2.2404141184
C	-1.963059052	2.2750589543	0.1046633688
C	-2.2119743766	2.5997507172	1.5842860145
C	-0.8294465581	3.1153368857	-0.4888471613
H	0.1138405567	2.9344837974	0.0415041085
H	-0.6842250602	2.8952541354	-1.5507093409
H	-1.0632941636	4.1787490726	-0.3876269393
H	-1.3054749544	2.4302161455	2.17535944
H	-2.4975216339	3.6504741213	1.6959549105
H	-3.0099880125	1.9857520722	2.0175663631
H	-2.8719137454	2.4653432084	-0.4784737197
C	-4.9135451707	-0.896976985	-0.4828548767
C	-5.2405800388	-1.8488268296	0.6760305243
C	-6.1318005119	-0.0810242757	-0.9226235151
H	-6.5099418114	0.5376291695	-0.0990517015
H	-5.8917898862	0.5688590431	-1.7695288807
H	-6.9397492332	-0.7533264589	-1.2244311671
H	-6.0130256645	-2.5612420297	0.3699310385
H	-5.617379176	-1.291577789	1.5407079794
H	-4.3667966298	-2.4226707132	1.0052667206
H	-4.5530835493	-1.4684248197	-1.3460291413
H	-4.1084756853	0.8961184073	0.340721014
H	-2.6740376884	-2.1625527973	-0.5091212601
H	-0.3037539491	-0.952600752	-1.6952574754
H	-0.0168856472	-1.6492934794	-0.082779519
H	-0.660347291	0.5912255705	-0.0059885684
H	-1.2081347478	-3.139053397	-2.4852902795
H	-1.0207533418	-3.831414779	-0.8685315384
H	1.2668123289	-2.9615244745	-2.6958147238
H	1.4625105941	-3.3956904302	-0.9973713067
N	0.2022676234	-5.8530186707	-1.4185897204
C	0.2634143409	-7.1625420511	-1.6989130249
C	0.9699466098	-7.7170701544	-2.7556012997
C	1.6895887672	-6.8655490432	-3.6278387806
C	1.6232367977	-5.4806017906	-3.3342903202
H	-0.2913209699	-7.8180701509	-1.0290787555
H	0.9567788315	-8.790747239	-2.89486029
N	2.4034854152	-7.349031935	-4.6917109125
H	2.1456608987	-4.7566900141	-3.9484033556
C	3.1387503096	-6.4365798756	-5.5549374772
C	2.4504722085	-8.7827122602	-4.9469975937
H	3.0645613083	-8.9691142048	-5.8286220584
H	2.8911905028	-9.3307890585	-4.1037385013
H	1.449813396	-9.1920716774	-5.1380908316
H	3.6366085932	-7.0079312644	-6.3390227444
H	2.4714489179	-5.7102001267	-6.0380600086
H	3.9072450761	-5.8814387275	-4.9999423619

DIG:17_oc

C	-5.0160376054	-1.7369014151	-0.3858335834
N	-3.8540408808	-0.9966400885	-0.9133743015
C	-3.3636205154	0.1730238541	-0.3185194953
N	-2.1263043806	0.4948496847	-0.1833336456
C	-1.0896300563	-0.4726544962	-0.4915985494

C	0.2521226748	-0.0169847994	0.0908359906
C	1.4071390012	-0.9782150434	-0.2418973604
C	2.7117311871	-0.5552694314	0.3975931039
N	-4.3674493179	1.029580814	0.1311324507
C	-4.0276716531	2.3639704166	0.640032528
H	-3.1022627336	-1.6204758728	-1.1828974793
H	-5.1934133332	1.0220599153	-0.4582729399
C	-5.3884794485	-2.8276119719	-1.3938695035
H	-5.8534638809	-1.0338286204	-0.3240458075
C	-4.7669940565	-2.3086093836	1.0177075809
H	-3.1440941036	2.2200221125	1.2675514133
C	-3.6651484315	3.3480860189	-0.4815540498
C	-5.1888352464	2.871454897	1.50050083
H	-0.9767779872	-0.5955203206	-1.584961271
H	-1.3189250083	-1.4802229766	-0.0926855251
H	0.4770436872	0.9873107612	-0.2898028375
H	0.159574712	0.0720890517	1.1791715769
H	1.5297199459	-1.0481827033	-1.3310973066
H	1.1565314671	-1.9819070886	0.1244982041
H	-4.9487158944	3.8481671853	1.9350565893
H	-6.1027087258	2.9939220651	0.9026583925
H	-5.4074577415	2.1720073928	2.3138928096
H	-3.3823312932	4.323895199	-0.0682920114
H	-2.822710783	2.9594409474	-1.05928345
H	-4.517870388	3.5053689907	-1.1561941615
H	-5.6587419462	-2.8232803324	1.3956350254
H	-3.9406981963	-3.0304389687	1.001275707
H	-4.5109645042	-1.5073899788	1.7176254283
H	-6.2800733259	-3.3712460411	-1.0638564435
H	-5.5855797893	-2.3971228709	-2.3808711458
H	-4.5758695502	-3.5593350025	-1.496881693
C	3.7054416338	0.0705692573	-0.3538585488
C	4.9053658945	0.4874593188	0.2644556699
C	5.0193073019	0.2286807679	1.6483675752
C	3.9668014396	-0.403447928	2.298245432
N	2.8275720147	-0.7985334481	1.7175108436
H	3.550629517	0.2218414958	-1.4166262127
N	5.9046189741	1.1043034902	-0.4417460236
H	5.9011199074	0.5202731459	2.2075991988
H	4.0491101491	-0.6062400303	3.3662263183
C	7.1974824205	1.4701469702	0.1355554168
C	8.0426950651	1.8578010524	-1.0867091132
C	7.0009995355	2.4055612308	-2.0752136084
C	5.7840739249	1.4961689731	-1.8460959175
H	7.0965346116	2.3123774184	0.8389420278
H	7.6319833865	0.6295861705	0.6904423521
H	8.5258560859	0.9659031508	-1.5032022008
H	8.8270379691	2.5793918258	-0.8397753627
H	7.3418227843	2.3928670696	-3.114690286
H	6.7457294727	3.440513905	-1.8183431242
H	5.8079995446	0.6158069211	-2.5080683401
H	4.8366564693	2.0180303431	-2.0287841659

DIG:17_ocH⁺

N	-3.7816058495	-1.2977706612	-0.2255149223
C	-3.3247345207	-0.0499400439	-0.0248788033
N	-2.0247068234	0.2160044728	-0.2268278839

N -4.1515441015	0.9123050326	0.4198715212
C -0.9785938466	-0.7751722656	-0.5296726114
C 0.3975613415	-0.1232348428	-0.4009406829
C 1.5419231187	-1.0645653364	-0.8020745731
C 2.8669082483	-0.324816232	-0.8992113137
C -5.1162763116	-1.8248794148	0.1393529882
C -6.1452626413	-1.5784052155	-0.9728799627
C -4.9728322167	-3.3114638079	0.4754590959
H -4.6430753344	-3.883329304	-0.4008849527
H -4.2574514181	-3.4688735858	1.2882434342
H -5.9396084081	-3.7171326477	0.7863662075
H -5.8638207677	-2.1138689453	-1.8860848508
H -7.1307326636	-1.9374090501	-0.6598590022
H -6.2387238921	-0.5161229839	-1.2267904248
H -5.4168072023	-1.2950003683	1.0510422876
C -3.7626614839	2.2619897512	0.892478646
C -3.6811421817	3.2660745669	-0.2656137441
C -4.7593746172	2.6999428575	1.9685147888
H -5.7708523023	2.7934550022	1.5536968628
H -4.7842905467	1.9906932877	2.801305906
H -4.4751424022	3.6801359586	2.3613522424
H -3.3471795282	4.2401256153	0.1052863248
H -4.6629064939	3.3999120001	-0.7329493304
H -2.9818514784	2.9468406971	-1.0468763747
H -2.7777719743	2.1502798258	1.3605171133
H -5.1435401692	0.7310394108	0.3504211634
H -1.7536751043	1.186407455	-0.3061261111
H -1.0839298519	-1.6114757086	0.1718795913
H -1.113354653	-1.1627973552	-1.5500835551
H -3.1791477308	-1.9216433705	-0.7463287251
H 0.5408998161	0.2228444804	0.6305501188
H 0.4585260059	0.7564100864	-1.0532128988
H 1.6248103243	-1.8989234546	-0.0954543259
H 1.3149710237	-1.5018014112	-1.7857626531
N 2.826994284	0.846577159	-1.5582469967
C 3.9933166679	1.4982721721	-1.6785321162
C 5.2077635459	1.0515249044	-1.1810547617
C 5.255004538	-0.1793707659	-0.4833616327
C 4.0232491829	-0.8672297393	-0.3502263309
H 3.9545469838	2.4446955896	-2.2161959321
H 6.1019723692	1.6426218615	-1.3395888297
N 6.4147982232	-0.6727884919	0.0332565666
H 3.9735555671	-1.8113443527	0.1806952005
C 7.6935712326	0.0459893442	-0.0049482647
C 8.5960399489	-0.7713169466	0.9305339374
C 8.0477340859	-2.2004507134	0.792202497
C 6.5313590017	-1.988245979	0.6704604316
H 8.0947818504	0.0769944929	-1.0292154412
H 7.5696573644	1.0806582349	0.335279076
H 8.4795679433	-0.4193872033	1.9621238085
H 9.653345863	-0.687314082	0.6652030772
H 8.3102737339	-2.8472658524	1.6338229734
H 8.4326254104	-2.6663774681	-0.1222408552
H 6.0423503935	-1.9908641364	1.6569371634
H 6.0514454469	-2.7621845234	0.059515839

S11. Cartesian coordinated for the hydrogen bonded TRIS series of bases and their conjugated acids.

TRIS:1

C	-0.1370253264	-2.7499700602	-2.0614450577
N	-0.1195278993	-2.7496008149	-0.6002224325
C	1.2629497245	-2.8160270853	-0.1052522759
C	1.4177518353	-2.6570390112	1.4117219199
C	0.7802653388	-1.3893446624	2.0101524402
N	1.223074951	-0.1523211411	1.3838884077
C	0.3737707244	0.781514903	0.7924076888
N	0.5559691795	2.060526261	0.7384076096
C	1.5474754199	2.6975490369	1.5810672269
C	2.8178693025	3.1251973503	0.8229619267
C	3.6609722689	1.9724704883	0.2685370072
N	4.0944720332	0.9869694796	1.2742563789
C	4.7469593696	-0.1457130111	0.6239423712
C	-0.9624226106	-3.8221788557	-0.0772919557
N	-0.7563332266	0.227157464	0.2160064218
C	-1.6980976079	1.0764627723	-0.4939171126
C	-2.9753661091	0.3008277559	-0.830512782
C	-3.9813802277	1.1671588577	-1.5951538266
N	-5.2737022287	0.514536683	-1.8193616229
C	-6.2786508174	1.4768207238	-2.2508781378
C	-5.1899210015	-0.5934059623	-2.7608686026
C	4.9687595424	1.5635726376	2.2926892985
H	-1.2531368997	1.4937069864	-1.4129716915
H	1.0091052824	-1.368156677	3.086913158
H	-0.3075237017	-1.4369207112	1.9242656993
H	1.0156150978	-3.531181031	1.9412391364
H	2.4963525286	-2.6535342249	1.6208451867
H	1.7459562081	-3.763801145	-0.4165714455
H	1.8108055507	-2.0020160094	-0.5928892476
H	-0.6485292964	-0.724752289	-0.1377124552
H	1.0957662373	3.6147995287	1.9871783336
H	1.8356551868	2.0890375041	2.4560053369
H	3.4252237304	3.7687391907	1.4738521313
H	2.5186292702	3.7454486257	-0.0313784012
H	4.5368383713	2.3860944862	-0.2702446958
H	3.0600989346	1.4295371355	-0.4703579531
H	2.1378312269	0.2055142099	1.6568144074
H	-1.9227084696	1.9362874963	0.1447034421
H	5.0258255703	-0.8948578804	1.3735498152
H	4.05417763	-0.6094148474	-0.0858282195
H	5.6626198928	0.1434278924	0.0730609213
H	5.2607452782	0.7840673063	3.0046320832
H	5.8916855292	2.0004104319	1.8648292348
H	4.4450948778	2.345726714	2.8476892708
H	-1.9761697189	-3.7143924443	-0.4764838501
H	-0.5902415604	-4.8285465659	-0.3492574326
H	-1.0253553248	-3.7637044764	1.0124594512
H	-1.1668270725	-2.6426229115	-2.4189215128
H	0.4464432392	-1.9033868748	-2.4379046089
H	0.2813496085	-3.6778157316	-2.4961570383

H -2.7095846483	-0.5856533557	-1.4228439432
H -3.4439979926	-0.0620160784	0.0920669959
H -4.1737855614	2.0721096393	-1.004939971
H -3.5304157988	1.5082740144	-2.5510484453
H -6.1785491392	-1.0519706581	-2.8731321509
H -4.8411295895	-0.2836041198	-3.7676189702
H -4.5084060871	-1.3636880562	-2.3886289204
H -7.248607272	0.976840199	-2.351357774
H -6.3808887884	2.2685937528	-1.5008213797
H -6.0410909484	1.9551701889	-3.2228186075

TRIS:1H⁺

C -2.1517900628	3.1830679344	1.4858611918
N -1.1840498089	3.2782677887	0.3843763376
C 0.1902671073	3.246327244	0.9199759306
C 1.2917496256	3.2232990119	-0.1467570438
C 1.1406144018	2.1575092475	-1.2426710524
N 1.0896893609	0.7742034645	-0.7618981278
C -0.0107403681	-0.0008360578	-0.750581585
N 0.1104936934	-1.340721398	-0.7524648111
C 1.285962742	-2.0795850469	-1.2209218435
C 2.1381224368	-2.716812286	-0.1120792155
C 2.6930497754	-1.7540249164	0.9445143834
N 3.410323654	-0.586083292	0.39867035
C 3.7881036922	0.3211997173	1.4910792983
C -1.4493056346	4.4836664515	-0.4137206104
N -1.2312562567	0.566211455	-0.7327136823
C -2.4681124526	-0.0770395401	-1.1838674715
C -3.4264252896	-0.5110082019	-0.0631860232
C -2.8593632314	-1.5024446729	0.9595435077
N -2.2223513907	-2.6965804762	0.3728316291
C -1.6377647965	-3.5221480966	1.4387794492
C -3.1564710036	-3.4995468625	-0.4291841698
C 4.6026564632	-0.967900883	-0.3708032637
H 1.9958927038	2.2328269716	-1.9242048403
H 0.2448867513	2.3421292262	-1.8410288306
H 1.3696767303	4.1970030461	-0.645159081
H 2.2471128369	3.0789546674	0.3732107945
H 0.3684881706	4.1033153604	1.5934458865
H 0.2690684963	2.3416928831	1.5357060187
H -1.2818110715	1.5631036657	-0.4428367633
H 0.926308901	-2.8735448096	-1.8854123682
H 1.8886368104	-1.4052021103	-1.8347595612
H 2.9508717669	-3.2687284265	-0.5995155498
H 1.5420601304	-3.4715216037	0.4161754323
H 3.3405922531	-2.3236413466	1.6346146397
H 1.8620088587	-1.3639943142	1.5453840619
H 1.9828635615	0.3287265995	-0.472531008
H -2.9881938686	0.6398555489	-1.8294384198
H -0.7218017508	-1.8928857649	-0.4632814995
H -2.1979038534	-0.9282714722	-1.814535059
H -4.3246282212	-0.92017317	-0.5408632205
H -3.7619650088	0.3740958268	0.4916334058
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H -2.093088831	-0.9981043625	1.5612788897
H -2.6364071808	-4.3824648945	-0.8117063162
H -4.0256636957	-3.8385422944	0.1589587609

H	-3.5213101005	-2.9270798034	-1.2857468993
H	-1.1296715696	-4.3859180111	0.9987994803
H	-0.9047761469	-2.9353815968	2.0024939072
H	-2.3975524707	-3.893782054	2.1461260578
H	5.1017573383	-0.0652516401	-0.7347656521
H	5.323796212	-1.5407483298	0.2360284988
H	4.3254476901	-1.5719371399	-1.2382212128
H	4.2888900734	1.2036828525	1.0807132749
H	2.8914139394	0.6470642542	2.0286134304
H	4.4699276199	-0.1544418142	2.2154912806
H	-2.4835033646	4.4609905651	-0.7692808836
H	-1.3045611983	5.4088796764	0.1689505129
H	-0.7942533335	4.5211270536	-1.2876641359
H	-3.1687710026	3.1683553419	1.0814896984
H	-1.9853572459	2.2570183199	2.0461124687
H	-2.0740249468	4.029242455	2.1886711452

TRIS:2

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N	1.3482624464	0.6110090041	1.1621739105
N	0.6356506648	-1.6460304423	0.7909142604
N	-0.9016167872	0.0581631811	1.1950945926
C	-1.2784092028	1.4451005326	1.414243305
H	-1.5700147063	-0.5138348547	0.6868340837
C	2.7398051492	0.2341344706	1.3099956808
H	1.5842327881	-1.8951229604	0.5312832794
C	-0.2365618523	-2.7278096568	1.2265395805
C	-1.2805120708	2.3062785323	0.1412495806
H	-0.5718067458	1.8613688931	2.1372067199
H	-2.275505814	1.4489029761	1.8752007033
H	3.1834689549	0.8909535809	2.0718880756
H	2.8820240019	-0.7950734194	1.6800069472
C	3.5682265323	0.4189318694	0.0241260923
H	0.3173240701	-3.4085960637	1.8892923573
H	-1.04228178	-2.2969752088	1.8237422496
C	-0.8296935447	-3.5524216931	0.068314138
H	4.626486011	0.2310626364	0.2496538859
C	3.144757768	-0.467790561	-1.1375865417
H	3.4821348291	1.4619017468	-0.3064627573
H	3.7856977374	-0.2817548642	-2.0146115636
O	3.2589016643	-1.8401853192	-0.7532662058
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C	2.9855796527	-2.725257318	-1.8202610179
H	3.1131074606	-3.7431256093	-1.4408606846
H	1.9564510427	-2.6061448268	-2.1958036195
H	3.6802520586	-2.5684803818	-2.6601356954
H	-0.2826549018	2.2709935119	-0.3064395311
C	-1.6569045326	3.7546682298	0.4221231838
H	-1.9908125766	1.8961145403	-0.5899176134
H	-2.6410042245	3.8130401247	0.9233209103
O	-1.69652154	4.462749861	-0.8056489072
H	-0.9213178579	4.2160439054	1.1043901127
C	-2.0111741323	5.8259187189	-0.6372030547
H	-2.0143339753	6.2842073036	-1.6302810119
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H	-1.268299103	6.3439236721	-0.0081223266
H	-1.5069367477	-4.3078914225	0.4876177599

C	-1.5713129086	-2.7306434357	-0.9776174432
H	-0.026553507	-4.0958255568	-0.4484483124
H	-1.983442321	-3.3939249491	-1.7551373653
O	-2.6308890828	-2.0107366959	-0.3525815923
H	-0.8816796037	-2.0255366507	-1.4674052764
C	-3.456833977	-1.3366373744	-1.2854359228
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TRIS:2H⁺

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N	-1.263763291	0.466985284	0.7995093554
C	-1.6827644037	1.8003810484	1.248894879
H	-1.9996991691	-0.196821293	0.5329091201
H	0.8269074819	1.8326093425	0.5307889032
C	2.3974790924	0.5569708283	1.2436029159
H	1.1704008254	-1.6295590617	0.5338012824
C	-0.7166538761	-2.3516461328	1.2542032862
C	-2.0693687582	2.7710512609	0.1230008434
H	-0.8812505122	2.2263701509	1.8561958396
H	-2.5438569454	1.6621005737	1.9112727143
H	2.7109183966	1.3706480873	1.9062064533
H	2.3650122502	-0.3508561679	1.8499494636
C	3.4295017167	0.4059353433	0.1158404151
H	-0.1677334811	-3.0239583006	1.9220989299
H	-1.4890339456	-1.868164086	1.8561581228
C	-1.3589472356	-3.1785939319	0.1306104944
H	4.3983263413	0.2071065286	0.5889853163
C	3.1296512084	-0.6951412464	-0.8959957412
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H	3.9882401728	-0.8187413974	-1.5698412437
O	2.8829661191	-1.9171189365	-0.1979493067
H	2.2562920037	-0.4398144317	-1.518255481
C	2.9452481371	-3.0673319518	-1.0384233795
H	2.7601680463	-3.9372983331	-0.4046413868
H	2.1903940162	-3.0253486979	-1.8373350498
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C	-0.9658612714	3.064963634	-0.8878246949
H	-2.9394809887	2.3852719202	-0.4233413274
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C	1.1799030319	4.0935462113	-1.0265574071
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H	-2.0151632223	-3.9165352504	0.6069373389
C	-2.162128441	-2.3759557453	-0.887536463
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H	-1.5045613032	-1.7503000442	-1.513104042
C	-4.1229728101	-1.0296707045	-1.040311265

H -4.7858297055	-0.4324829779	-0.4103955467
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TRIS:3

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H -1.6169871734	-0.3712450531	0.7140864167
C 2.7173959524	0.1630662707	1.4044163522
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S -1.4569611221	4.8418714603	-1.1438512939
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C -1.8783289753	6.498310844	-0.4995210858
H -1.8924608584	7.1822421807	-1.3523783847
H -2.8668451793	6.5029310835	-0.0290274849
H -1.1297402318	6.8478963402	0.2185638471
H -1.4425172384	-4.4589978793	1.0951032224
C -1.5446629785	-3.2292693007	-0.6897397108
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S -3.1191898808	-2.3787182055	-0.2513441429
H -0.9055852721	-2.5205027306	-1.2266737125
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TRIS:3H⁺

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C	-1.5790729846	1.8920453267	1.4866465062
H	-2.0080317416	-0.0383192282	0.7015722145
H	0.9740188219	1.7527113396	0.7002171098
C	2.4268555048	0.4196747451	1.5003266315
H	1.0348567245	-1.7235907138	0.7043344547
C	-0.8505301189	-2.3165221393	1.4945032615
C	-2.10234987	2.8558145148	0.4111935987
H	-0.7100051879	2.3061067524	2.0029604699
H	-2.358988468	1.7533914674	2.2439703511
H	2.687257903	1.1637959044	2.2615224767
H	2.3488326909	-0.541158203	2.0142593412
C	3.5336977268	0.3958267799	0.435461582
H	-0.339347842	-2.9212895075	2.2520623021
H	-1.6421399313	-1.7696005767	2.0120832829
C	-1.4254452791	-3.2535414494	0.4212372957
H	4.4784204598	0.1876107176	0.951643759
C	3.3415768554	-0.5991775824	-0.7129366804
H	3.6326289515	1.3986102553	0.0003205061
H	4.1958002269	-0.5367556979	-1.3941510854
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H	2.4367112834	-0.3636815002	-1.2856181613
C	3.1092100669	-3.2342730821	-1.6721525014
H	3.0155719475	-4.2949754515	-1.4275891235
H	2.2355890373	-2.9188685626	-2.2493531799
H	4.017741981	-3.0879408449	-2.2619207381
H	-2.3986422249	3.7815680278	0.9186684391
C	-1.1342102439	3.1791019612	-0.7308662677
H	-3.0164068682	2.4372874336	-0.0291596668
H	-1.6118839281	3.8776960607	-1.4247192278
S	0.4103747063	3.9595999178	-0.0976284376
H	-0.8751201591	2.2727768177	-1.2909991403
C	1.2580868387	4.3184920815	-1.6772896786
H	2.2185227322	4.7754887583	-1.4275006562
H	1.4321893963	3.406535224	-2.2551801226
H	0.6739460924	5.0280316984	-2.2689590756
H	-2.0780385346	-3.9726076609	0.9304038435
C	-2.1914475364	-2.5784452605	-0.7206624329
H	-0.6064733121	-3.8360581224	-0.020003208
H	-2.5591077257	-3.3418084768	-1.4132872735
S	-3.6378411431	-1.6296973685	-0.0858328416
H	-1.5361370391	-1.9018862659	-1.2819031619
C	-4.3795339542	-1.0794466352	-1.663852674
H	-5.2577149716	-0.4804980279	-1.4114660786
H	-3.682221143	-0.4694284739	-2.2449006218
H	-4.6996118544	-1.9422576995	-2.2535002682

TRIS:4

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C	0.5623295508	-3.4460270759	-0.3495560244
C	0.4942725499	-2.4466626115	-1.521963716
N	-0.4476725993	-1.3783301918	-1.2659517939
C	-0.062954959	-0.138978536	-1.2082873633
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C	1.7859474738	1.5335184677	-1.6487489551
C	2.7863218713	2.2125296182	-0.6951605051
C	2.216306458	2.5745173882	0.6891807837
P	0.8893961732	3.8466112064	0.713249981
N	-1.006536891	0.8661926028	-1.2548840742
C	-2.4222796505	0.5616042232	-1.3360911411
C	-3.0424016122	0.1183176309	0.0006722741
C	-4.5538607341	-0.1292764159	-0.1137137306
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H	1.5117525957	-2.1118767421	-1.7763470571
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H	-0.4568477758	-3.8025322669	-0.1556277769
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H	1.9480813618	-0.4023081267	-0.8743936801
H	-2.9320501364	1.4629787804	-1.7010412135
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H	-2.5252809051	-0.7943143519	0.3158009601
H	-2.8601519478	0.8841590174	0.7637809417
H	-5.0660641038	0.7915923391	-0.4257156013
H	-4.7696520869	-0.8888498309	-0.8786747244
H	2.3121455737	1.3219488501	-2.5942801048
H	-0.7719548324	1.7495970669	-0.8015832866
H	0.9627945014	2.2074394578	-1.886086163
H	3.1961911901	3.1030490311	-1.1909100772
H	3.6295736016	1.5291300689	-0.5344307146
H	3.021038564	2.9150844885	1.3544311478
H	1.785069413	1.6709235281	1.1365986461
C	-4.7595655175	-2.3782950764	1.7348018343
O	-5.0565614807	0.2625093966	2.6359353209
O	-0.3262430008	3.5020815066	-0.1166589668
C	1.6784565312	5.4203703526	0.2003737838
O	3.3607194072	-1.4414269321	-0.0030787386
C	3.7694615335	-4.0839080242	0.808175583
H	4.845206798	-3.9263756318	0.933582052
H	3.4266627	-4.8219567874	1.5410860715
H	3.5958753837	-4.473658048	-0.1988370474
H	-5.2450899318	-2.7822809686	2.6287310525
H	-4.9917808261	-3.020410467	0.878298122
H	-3.6781858234	-2.3842036657	1.8989477861
H	0.9463718914	6.229433465	0.2846648358
H	2.5512249437	5.6604732634	0.8169739974
H	1.9893463462	5.3502379908	-0.8460973624
C	0.5089358786	4.0759245429	2.4914609851
H	1.3992769519	4.3411997891	3.0715318846
H	-0.2395133222	4.8668603662	2.6006780195
H	0.0845678829	3.1489950382	2.8895011554
C	-7.110304695	-0.8283659578	1.0659778006
H	-7.6433936058	-1.22449205	1.9360772572
H	-7.5239353131	0.1576260819	0.8320594231
H	-7.2735382786	-1.4951799215	0.2122329715
C	3.230716088	-1.9874812736	2.7369759083
H	4.2973711588	-1.7739556133	2.8575242711
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TRIS:4H⁺

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C	-1.9321636669	1.519046151	1.3200759263
C	2.2816140753	0.9137800427	1.3200759263
C	-0.3494506217	-2.4328254737	1.3200759263
H	-2.5165530529	1.243224809	2.2074514942
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H	0.1816123604	-2.8010108567	2.2074514942
H	-1.1514707935	2.207337645	1.6450581889
H	2.4873455576	-0.1064655652	1.6450581889
H	-1.3358749774	-2.1008713598	1.6450581889
C	-2.8849607053	2.1839189948	0.3130914301
C	3.3338093674	1.4064900608	0.3130914301
C	-0.4488488754	-3.5904083355	0.3130914301
H	-3.4087834512	2.9940028128	0.8355528358
H	4.297273906	1.4550919568	0.8355528358
H	-0.8884906681	-4.4490940496	0.8355528358
C	-2.2436346466	2.7160018651	-0.9830472198
C	3.4739436207	0.5850439667	-0.9830472198
C	-1.2303091874	-3.3010451117	-0.9830472198
H	-3.6535024768	1.4525714887	0.0351333952
H	3.0847147339	2.4377405117	0.0351333952
H	0.5687875295	-3.8903112805	0.0351333952
H	-3.0281207587	3.0931229925	-1.6513921637
H	4.1927831534	1.075868305	-1.6513921637
H	-1.164662608	-4.1689905774	-1.6513921637
P	-0.9795125061	4.0377637893	-0.7767833976
P	3.9865619545	-1.1705988826	-0.7767833976
P	-3.0070496617	-2.8671641867	-0.7767833976
H	-1.7439804824	1.8965804969	-1.5157460779
H	2.5144768174	0.5620414514	-1.5157460779
H	-0.7704965483	-2.4586212284	-1.5157460779
H	-1.9707379904	-0.4421462961	0.5133743897
H	0.602458756	1.9277826104	0.5133743897
H	1.368279021	-1.4856355942	0.5133743897
O	0.2412256463	3.5643080077	-0.0046437559
O	2.966168144	-1.9910612431	-0.0046437559
O	-3.2073940036	-1.5732460446	-0.0046437559
C	-1.8107771828	5.4600043411	0.0117298529
C	5.6338907411	-1.1618228312	0.0117298529
C	-3.8231137716	-4.2981807899	0.0117298529
H	-1.1091920961	6.2983289652	0.0622855661
H	6.0091086188	-2.1885756513	0.0622855661
H	-4.899916736	-4.1097525939	0.0622855661
H	-2.6979902785	5.7713535277	-0.5492687883
H	6.3471335939	-0.5491483451	-0.5492687883
H	-3.6491435287	-5.2222044626	-0.5492687883
H	-2.1051874188	5.2021000653	1.0331068166
H	5.5577442044	-0.7779039498	1.0331068166
H	-3.452556999	-4.4241953954	1.0331068166
C	-3.6801301325	-2.7982784313	-2.4739169218
C	-0.5833154566	4.5862256981	-2.4739169218
C	4.2634453758	-1.7879465468	-2.4739169218
H	-3.5552855822	-3.7511241871	-2.9982522959
H	-1.4709263622	4.9545300239	-2.9982522959

H	5.0262117311	-1.2034051168	-2.9982522959
H	-4.7462462741	-2.555681315	-2.4270353433
H	0.1598378798	5.3882108019	-2.4270353433
H	4.586408181	-2.8325287669	-2.4270353433
H	-0.1551736787	3.7529687527	-3.0395794237
H	-3.1725793389	-2.0108683025	-3.0395794237
H	3.3277528042	-1.7420997302	-3.0395794237

TRIS:5

S	-3.170406997	-2.8359399261	-1.0567174305
C	-1.3363048656	-2.982718194	-0.9013060663
C	-0.8949698352	-3.5375121413	0.4559882747
C	-0.9465075342	-2.5238827834	1.6178362503
N	-0.0108547093	-1.4359048154	1.4268221289
C	-0.4214274406	-0.2147995285	1.2677265203
N	-1.7187011786	0.1810526872	0.9619115353
C	-2.3487838038	1.4323040736	1.3575136545
C	-3.1277644052	2.0642628002	0.1868220551
C	-2.2847730037	2.3595706671	-1.0573062706
S	-1.1640809419	3.8109356636	-0.8459642361
N	0.4831503699	0.8222029159	1.37520019
C	1.8896919006	0.5622406571	1.6142225634
C	2.6501035738	0.1037788134	0.3563948511
C	4.138491104	-0.1047949673	0.6237808981
S	4.9954606745	-0.62359975	-0.9295451771
H	-0.6476895186	-3.0749993886	2.5226882694
H	-1.9877415147	-2.2102067009	1.784930198
H	-1.4858268868	-4.4292137454	0.7086400966
H	0.1459501701	-3.8657653899	0.3448159807
H	-1.0424698785	-3.6522324503	-1.7193654235
H	-0.8944621494	-1.9950513394	-1.0752105902
H	-2.3727135562	-0.5622271246	0.7212452187
H	2.335017602	1.4866854558	2.0035789149
H	1.9645706034	-0.2065300403	2.3886791268
H	2.1918522416	-0.8283262939	0.0079768731
H	2.5384045268	0.853964953	-0.4355962678
H	4.6159017004	0.8200988311	0.9716161553
H	4.3161731131	-0.897184233	1.3622629448
H	-3.0591041983	1.2629186263	2.1816810845
H	0.2760454271	1.6850591496	0.8725720883
H	-1.5872046588	2.1178624587	1.728551687
H	-3.6337996606	2.9752301818	0.5342193483
H	-3.9155132561	1.3635727707	-0.1189662807
H	-2.9205066262	2.6082884682	-1.9158996257
H	-1.6647088413	1.4912010442	-1.3062460284
O	4.8409308351	0.4983644267	-1.9368934548
O	-0.1128091662	3.4604563135	0.2015990776
C	-0.3402154567	3.6757300814	-2.4772558759
O	-3.664614688	-1.7093815843	-0.1517541211
C	-3.1770105318	-2.1655336298	-2.7634973539
H	-4.2164600265	-1.939269918	-3.0124822012
H	-2.5793825958	-1.2500778875	-2.7985629945
H	-2.7832296418	-2.9129220979	-3.458526285
H	0.425718535	4.4539426233	-2.5116935638
H	0.1321964884	2.6934331004	-2.5684243974
H	-1.0691429953	3.8366948817	-3.2771810954
C	6.702275248	-0.5248643952	-0.2557514549

H	7.3866526994	-0.7873013741	-1.0662478927
H	6.9025367454	0.4981955603	0.0762069217
H	6.8171430044	-1.2324285058	0.5713191799

TRIS:5H⁺

C	-0.0000001194	-0.0000000647	0.6506543876
N	-0.2214372666	1.327123419	0.6280241682
N	1.260041105	-0.4717916117	0.6280241682
N	-1.0386041967	-0.8553320013	0.6280241682
C	0.6538581653	2.3641164485	1.1840601904
C	1.7204556961	-1.7483162063	1.1840601904
C	-2.3743142197	-0.6158004362	1.1840601904
H	0.132186351	2.825908523	2.0309675566
H	2.3812152711	-1.5274311999	2.0309675566
H	-2.5134019803	-1.2984775171	2.0309675566
H	1.560368543	1.8989103273	1.5723228835
H	0.8643201884	-2.3007741616	1.5723228835
H	-2.4246890896	0.4018636402	1.5723228835
C	0.9828039587	3.4707548613	0.1684691951
C	2.5143597777	-2.5865108262	0.1684691951
C	-3.4971640946	-0.8842442291	0.1684691951
H	1.5023069426	4.2773759959	0.7005570619
H	2.9531626796	-3.4397241749	0.7005570619
H	-4.4554699804	-0.837652015	0.7005570619
C	1.8016001857	3.0462111521	-1.0554336655
C	1.7372960271	-3.0833373048	-1.0554336655
C	-3.538896571	0.0371259586	-1.0554336655
H	0.0400788757	3.8986254508	-0.1950584907
H	3.3562691193	-1.9840222504	-0.1950584907
H	-3.3963483532	-1.9146033945	-0.1950584907
H	1.8949275464	3.8815890649	-1.7585896303
H	2.414090841	-3.5818501263	-1.7585896303
H	-4.3090187455	-0.2997391326	-1.7585896303
S	3.5241457976	2.548200168	-0.6193336857
S	0.4447330575	-4.3261000718	-0.6193336857
S	-3.9688792133	1.7778997098	-0.6193336857
H	1.3434688937	2.1980296763	-1.5776864845
H	1.231814968	-2.2624932297	-1.5776864845
H	-2.57528422	0.0644633594	-1.5776864845
H	-1.16943393	1.6444840772	0.3740724707
H	2.0088818289	0.1905172524	0.3740724707
H	-0.8394482571	-1.8350015236	0.3740724707
O	3.4357371265	1.1740797145	0.0559654293
O	-0.7010858275	-3.5624756899	0.0559654293
O	-2.7346516571	2.3883957814	0.0559654293
C	4.1156123631	2.2480377707	-2.3221885828
C	-0.1109484866	-4.6882439443	-2.3221885828
C	-4.0046642347	2.4402059796	-2.3221885828
H	5.1215607188	1.8309258958	-2.2361410517
H	-0.9751521443	-5.3508648378	-2.2361410517
H	-4.1464089327	3.519938748	-2.2361410517
H	3.4586389372	1.5343467443	-2.8270259942
H	-0.4005363329	-3.7624427547	-2.8270259942
H	-3.0581029625	2.2280958163	-2.8270259942
H	4.1559792313	3.1962413301	-2.8660165157
H	0.6900364498	-5.1973044574	-2.8660165157
H	-4.8460160393	2.0010629332	-2.8660165157

TRIS:6

S	-2.3348051707	-3.2149897053	-0.9311244269
C	-0.5378265328	-3.1373386232	-0.6364752373
C	-0.1581820227	-3.5442705214	0.7907573984
C	-0.4816451691	-2.4957811637	1.8700909469
N	0.2734756831	-1.2770398624	1.6675163443
C	-0.3049124146	-0.1258400266	1.552428718
N	-1.6558073535	0.1089973278	1.2984652677
C	-2.4413958505	1.1699612135	1.9191255974
C	-3.546016388	1.6721464017	0.9756765257
C	-3.0561023352	2.1413502732	-0.3984905989
S	-2.1137924353	3.6979795969	-0.3075638571
N	0.4515922334	1.0291405782	1.6501418291
C	1.891323869	0.9501203876	1.812504287
C	2.6313119375	0.5992316334	0.5080279781
C	4.1391001546	0.4708304348	0.7289987182
S	4.9775053619	0.0620488192	-0.8354221014
H	-0.1739057593	-2.9336205397	2.8317971752
H	-1.5720218612	-2.3605765493	1.9398145881
H	-0.6356600499	-4.4999337005	1.0353841119
H	0.9259060745	-3.7069683479	0.7873139565
H	-0.0959774068	-3.8195081179	-1.3703117032
H	-0.2189249283	-2.1139319346	-0.8562905567
H	-2.1848081155	-0.7176557959	1.0407686058
H	2.2388116535	1.9175914354	2.1963244582
H	2.0984636574	0.1872034357	2.5679933457
H	2.239987722	-0.3509080904	0.135472841
H	2.4406750694	1.3711338013	-0.2466362534
H	4.5859268239	1.4049187798	1.0877851068
H	4.3742878344	-0.3349893154	1.4329446854
H	-2.9212517766	0.822598213	2.8481358688
H	0.1088457887	1.8264769102	1.1207560373
H	-1.7724318317	1.9845548869	2.1989166617
H	-4.1052724901	2.4778135988	1.4640407895
H	-4.2562692214	0.8566979371	0.7878542608
H	-3.9022668625	2.3465959764	-1.062230267
H	-2.400236364	1.3952010012	-0.8554764478
O	4.8664964301	1.2225849857	-1.7362240118
O	-0.7454219296	3.4095365796	0.1774774176
O	-2.9363551739	4.6991312478	0.3905572641
O	-2.9828610775	-2.0151562448	-0.3491794617
O	-2.8192481425	-4.5527273908	-0.5544065621
C	6.7176355899	-0.0950575452	-0.3571204699
H	7.2627404499	-0.3345546313	-1.273249928
H	7.0720082605	0.8535544091	0.0517450015
H	6.8271070964	-0.9053959156	0.366642012
O	4.515111882	-1.2654324879	-1.2768471123
C	-2.4752385777	-3.0550368195	-2.7289861304
C	-1.9537137986	4.2018076432	-2.0376670017
H	-3.5450999642	-3.0482177528	-2.9501776205
H	-2.0175549023	-2.1164685282	-3.0489224917
H	-1.9970214144	-3.9110685088	-3.2089742951
H	-1.3542376072	5.1151851052	-2.0312047574
H	-1.4365526498	3.4194229972	-2.5972506632
H	-2.9429079948	4.4028725093	-2.4537768433

TRIS:6H⁺

C	0.0037533052	0.0054917636	0.9136384738
N	-1.3194715681	0.2505685781	0.8964408637
N	0.8764192454	1.0296494457	0.8901656317
N	0.453788543	-1.26219391	0.8902169125
C	-2.0025953405	1.3959435342	1.510569593
C	2.2167600971	1.0522515047	1.4887893237
C	-0.1980256238	-2.4337630822	1.4886772374
H	-2.5164767344	1.045215926	2.4142906898
H	2.1819517215	1.6889186148	2.3815907133
H	0.3680163227	-2.7196002228	2.383983118
H	-1.2605333607	2.1266355667	1.8350638199
H	2.476395411	0.0487851904	1.8292899763
H	-1.1982389069	-2.1573797405	1.825408949
C	-3.052610621	2.0367569223	0.5930783803
C	3.2901097319	1.6212526308	0.5502634586
C	-0.2365989048	-3.6499577542	0.5528375996
H	-3.5791544938	2.7989094038	1.176254453
H	4.2153757873	1.7158228922	1.1274092345
H	-0.6267773045	-4.4954063485	1.1282122214
C	-2.541319966	2.6677361438	-0.7072080841
C	3.580235939	0.8298080357	-0.7302329738
C	-1.0524286392	-3.5078446386	-0.7376364179
H	-3.7944364807	1.2793585506	0.3119672217
H	2.9987212753	2.6334520994	0.2443778544
H	0.787936543	-3.9082006828	0.2585675038
H	-3.3799787137	3.0896824206	-1.2701551246
H	4.360108034	1.3338682192	-1.3098728017
H	-1.0026959645	-4.4382986218	-1.3122207477
S	-1.3807636537	4.0423073834	-0.3781014012
S	4.2005067329	-0.8488480538	-0.3543872253
S	-2.8194154276	-3.1981303829	-0.3841175047
H	-2.0080705812	1.955979994	-1.3437509165
H	2.6958346637	0.7014892129	-1.3609056681
H	-0.7113409054	-2.6821604607	-1.3687277062
H	-1.9225910989	-0.517576815	0.5848827136
H	0.5094941932	1.9340539919	0.5767153043
H	1.421741185	-1.3990139579	0.5814910767
O	-0.0123961112	3.4589211022	-0.3049172625
O	3.0155195018	-1.7457003221	-0.2566235688
O	-2.9985668784	-1.7231008978	-0.2844271833
O	-1.8900612665	4.8188478606	0.7594274945
O	5.1270329218	-0.7595422891	0.7812845297
O	-3.2243575787	-4.0469366926	0.7435278333
C	5.1111338325	-1.3525610497	-1.8261450737
C	-3.6937537587	-3.7254996904	-1.8696854901
C	-1.4286265515	5.0623959961	-1.8635104761
H	5.4291852294	-2.3827392546	-1.6480504497
H	4.4536467015	-1.3052737904	-2.6968103414
H	5.9823588201	-0.7055926766	-1.9460715789
H	-0.6891935205	5.8526473298	-1.7121788808
H	-1.161428921	4.4562246383	-2.7316911738
H	-2.4253731383	5.4954316819	-1.9683886552
H	-4.7461864165	-3.4823846257	-1.7041164865
H	-3.310865471	-3.1773066616	-2.7331238244
H	-3.5716948368	-4.8033930112	-1.9927581646

TRIS:7

C	0.3926228347	-0.1910536003	-0.976193662
N	0.5078821878	-1.4776529743	-1.0836570361
N	1.4388935368	0.690057163	-0.7283231247
N	-0.8402616211	0.4014321329	-1.2020430973
C	1.8332457673	-2.050828151	-0.9877936509
C	1.296922246	2.1245629095	-0.5773444392
C	-2.0139017185	-0.426716742	-1.4341661271
H	2.2837863319	0.2896401051	-0.3363914894
H	-1.02998094	1.2898361025	-0.7526252997
C	2.2585298234	-2.3289284839	0.4727420904
C	0.8508326048	2.5747064623	0.8319434544
C	-2.6110612036	-1.0424189567	-0.1597808936
H	1.8340175491	-3.0084789296	-1.5281237951
H	2.6014908694	-1.4274721349	-1.478386361
H	2.2658887706	2.5830929148	-0.812061859
H	0.5919189094	2.4841049394	-1.3327400463
H	-2.7624095445	0.2011186114	-1.9360116748
H	-1.7196075554	-1.2203949625	-2.1261035827
C	3.7494231322	-2.6379817292	0.6212104775
C	0.3744737715	4.0285760675	0.8754170426
C	-3.8215411333	-1.9255666668	-0.4610633023
H	3.9689360886	-3.071625587	1.6094070862
H	4.0775197345	-3.4016275777	-0.1006552136
H	2.0156573386	-1.4614760663	1.0963062293
H	1.6649503261	-3.1639282008	0.8619033892
H	1.6841693933	2.4379479872	1.531430274
H	0.0400555041	1.9253469625	1.1786553007
H	0.299713769	4.3862825281	1.9130654261
H	1.0972043573	4.7053980344	0.3943357674
H	-1.8347417165	-1.6338795116	0.3348573788
H	-2.9058159368	-0.2496653826	0.5384142133
H	-3.5446900398	-2.7596632405	-1.1233565668
H	-4.5877875995	-1.3633796866	-1.020733477
C	4.6540512424	-1.4209146794	0.4707133592
C	-0.9897842835	4.2466333213	0.2280455812
C	-4.5043345561	-2.4987486099	0.7752145272
O	4.216713089	-0.2863989662	0.3534001976
O	-1.6525118801	3.3237530362	-0.2169309906
O	-4.2103795432	-2.1485226777	1.9027875009
C	6.1502770044	-1.6769477587	0.479684154
H	6.4377410884	-2.2003488722	-0.4415312753
H	6.4373529917	-2.3241957519	1.3165236071
H	6.6916277968	-0.7303493106	0.5351652061
C	-1.497889874	5.6749127717	0.1668455666
H	-0.8462624797	6.276359762	-0.4798920585
H	-1.4777660549	6.1401944275	1.1597099677
H	-2.5148023685	5.6915094892	-0.2297953419
C	-5.5835681637	-3.5428114327	0.5264672499
H	-6.3002157757	-3.2005614154	-0.2299368657
H	-5.1272054971	-4.4633243158	0.139672143
H	-6.1054545736	-3.7675493538	1.4590920404

TRIS:7H⁺

C	-0.0000000117	0.0000000409	0.389090521
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H	-0.257548118	-3.22946491	0.9743158568
H	-1.0031940348	2.2970459599	1.2937623312
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C	-1.6353525298	2.6284718837	-0.7739541895
C	3.0939996363	0.1020209444	-0.7739541895
C	-1.4586471416	-2.7304927052	-0.7739541895
H	-0.792545089	2.2918613821	-1.3873554352
H	2.3810826703	-0.4595664591	-1.3873554352
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C	-1.5147246413	4.1399482043	-0.5572420084
C	4.342662583	-0.7581840318	-0.5572420084
C	-2.8279379767	-3.3817640497	-0.5572420084
H	-2.5435639883	2.407248477	-1.3443840265
H	3.3565202755	0.9991668428	-1.3443840265
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H	-1.74487896	4.6830457355	-1.4839779064
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H	-3.1831970761	-3.8526323021	-1.4839779064
C	-0.1319170692	4.5833170825	-0.0922545201
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C	-3.9033104745	-2.4059020029	-0.0922545201
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H	5.027302345	-0.3002068927	0.1722541969
H	-2.773638021	-4.2036680457	0.1722541969
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O	-3.649862553	-1.2274072019	0.1296921673
C	0.100370047	6.0655749567	0.0739487788
C	5.2027569245	-3.1197104376	0.0739487788
C	-5.3031270067	-2.9458643963	0.0739487788
H	-0.6420796231	6.4978307476	0.7556592607
H	5.9483262555	-2.6928580576	0.7556592607
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H	-5.9642720183	-2.1671404016	0.4576343853
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TRIS:8

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H -2.4521669875	2.4692876963	0.9477516564
H 2.6061510193	0.1633802854	2.155206032
H -1.954956389	-3.109627087	1.7910419928
H -0.7790337207	2.4168344557	1.4824651275
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C -1.0236583442	2.3937386059	-0.6822717126
C 2.463102949	-1.0738185445	0.3736146301
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H -1.330751312	4.5188219944	-0.3519256618
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H 5.8339452093	-4.8591587874	0.9794965797
H 7.1319284337	-3.6423303266	-1.6311683051
C 6.0648603506	-3.9028102288	-1.6074916092
H 7.0540748537	-3.5734644496	0.8803946483
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H 5.9803118109	-4.9987962515	-1.6080830416
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H -7.484791857	-3.2250917487	0.337296367
H -7.719826676	-0.7435682864	0.6455939201
C -7.0094681318	-0.5999121552	-0.1787856624
H -7.3622087218	-3.0144052534	-1.4216431088
H -6.0708027688	-3.8430644019	-0.5337153654
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H -7.5816313438	-0.4681587792	-1.1073307659
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TRIS:8H⁺

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H	-2.0290865015	-0.2689940488	0.1702521908
H	0.7815875829	1.891737698	0.1702521908
H	1.2474991242	-1.6227433342	0.1702521908
C	-1.6798289167	1.8119647113	0.4589084617
C	2.4091219409	0.548792377	0.4589084617
C	-0.7292928187	-2.3607567733	0.4589084617
H	-2.6909252857	1.8088378449	0.876392022
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H	-0.2210366884	-3.2348284814	0.876392022
H	-1.0299236403	2.2930985353	1.1951727448
H	2.5008434168	-0.2546090144	1.1951727448
H	-1.4709195711	-2.0384892058	1.1951727448
C	-1.6561419241	2.5881623516	-0.8746802181
C	3.0694853194	0.1401800196	-0.8746802181
C	-1.4133431898	-2.7283420561	-0.8746802181
H	-0.7996287524	2.2644783929	-1.4736651765
H	2.3609102025	-0.4397401664	-1.4736651765
H	-1.5612812447	-1.8247379114	-1.4736651765
C	-1.5802533139	4.1065588754	-0.6794496346
C	4.3465109769	-0.6847397066	-0.6794496346
C	-2.7662574576	-3.4218188537	-0.6794496346
H	-2.554901948	2.3410208475	-1.4503657594
H	3.3048345105	1.0420997842	-1.4503657594
H	-0.749932357	-3.3831203167	-1.4503657594
H	-1.8099517097	4.6080236403	-1.6272548553
H	4.8956414003	-0.7365474431	-1.6272548553
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C	-0.1957860284	4.5572541983	-0.194322421
C	4.0445909332	-2.109071208	-0.194322421
C	-3.8488046993	-2.4481826752	-0.194322421
H	-2.3480682152	4.4383352535	0.0324906295
H	5.0177451994	-0.1856806857	0.0324906295
H	-2.6696767788	-4.2526542527	0.0324906295
O	0.7021177032	3.7235698696	0.0141847522
O	2.87364726	-2.4698364854	0.0141847522
O	-3.5757647577	-1.2537330691	0.0141847522
N	0.019610045	5.8842604707	-0.0057575535
N	5.0861140394	-2.9591128157	-0.0057575535
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C	6.488024816	-2.6439900187	-0.2551139876
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H	5.1682532917	-5.0387887276	-0.338649712
C	4.8336143449	-4.3311520452	0.4295165306
H	6.8750930166	-3.2491823784	-1.0847516186
H	6.626811773	-1.5928948048	-0.4988718485
H	5.3840027152	-4.5363021615	1.3550096997
H	3.7667130303	-4.4566846011	0.6004196266

C	-5.5337749197	-4.2967990849	-0.2551139876
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H	-6.9478456764	-1.9564440631	-0.338649712
C	-6.1676948594	-2.0204565753	0.4295165306
H	-6.2514209777	-4.3294137997	-1.0847516186
H	-4.6928932412	-4.9425397223	-0.4988718485
H	-6.620554257	-2.3945318278	1.3550096997
H	-5.7429585846	-1.0337266556	0.6004196266
C	-0.9542496908	6.9407894186	-0.2551139876
H	-1.0544284154	7.5683687737	0.638163589
H	1.7795925902	6.9952331058	-0.338649712
C	1.33408072	6.3516089356	0.4295165306
H	-0.6236718334	7.5785964932	-1.0847516186
H	-1.9339183263	6.5354348421	-0.4988718485
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H	1.9762457598	5.4904115718	0.6004196266

TRIS:9

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N	1.0232587611	0.5959732339	1.0412180224
N	0.1737450735	-1.5548598021	0.913780779
H	-2.077549028	-0.2623785256	0.6155222696
H	0.9096492736	1.5419877879	0.691324713
C	-1.5375582044	1.7456314548	0.8581304264
C	2.3836931853	0.086282289	0.9747893405
C	-0.9723906033	-2.4379535839	0.9208853348
H	-2.5438005612	1.9376698885	1.2524671837
H	3.0370747004	0.8369627188	1.4402293907
H	-0.6625567631	-3.4019692948	1.3512784985
H	-0.8372061399	2.2514131444	1.5289165976
H	2.4229541676	-0.821127866	1.5837092471
H	-1.7922040472	-2.0706113666	1.5624692023
C	-1.4307032232	2.3365878235	-0.5654110083
C	2.8669894272	-0.2207378243	-0.4509570706
C	-1.5239776516	-2.7087215903	-0.4982770941
H	-0.5496015195	1.9209556146	-1.0641085661
H	2.1865029251	-0.9480921413	-0.9019517787
H	-1.5817062588	-1.7671946199	-1.05384501
C	-1.3322094505	3.8650109368	-0.574751058
C	4.293932824	-0.7699124496	-0.4652486948
C	-2.9070943859	-3.365801182	-0.495455201
H	-2.3047242011	2.021768394	-1.1483343643
H	2.8188566288	0.6867109389	-1.0649972117
H	-0.8144257434	-3.3463896081	-1.0381420515
H	-1.5287417222	4.2582513213	-1.5818974136
H	4.3404404914	-1.7075024995	0.1086992926
H	-3.1293523381	-3.8153132905	-1.4742637153
C	0.0414590171	4.3628779421	-0.1199893867
C	4.8210948449	-1.0292152892	-1.8759561693
C	-4.0285650794	-2.3810658409	-0.1613993974
H	-2.1064273219	4.3067665778	0.0701331252
H	4.9800901464	-0.0785176806	0.048308251
H	-2.9354898724	-4.1981177129	0.2233894704
O	0.9477323515	3.5960001763	0.2215043881
O	4.1444255172	-0.8462884271	-2.8853956691
O	-3.8277405174	-1.181794658	0.0634868058

N	0.2352348157	5.7095064674	-0.1173855719
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C	7.0414864965	-1.7316723437	-0.8631458566
C	8.2052628866	-2.4732025241	-1.5408043226
C	8.2096753231	-1.8931399127	-2.9656161167
C	6.7167774905	-1.7262268611	-3.283722826
H	7.3851444957	-0.7880680875	-0.411731425
H	6.5746496364	-2.3246850628	-0.0694681219
H	7.9906768304	-3.5482628733	-1.5735576485
H	9.1525163838	-2.3366473308	-1.0100108608
H	8.7238622539	-2.5330353689	-3.689088522
H	8.7075386525	-0.9155635432	-2.9712295491
H	6.2909715498	-2.631646806	-3.7379851905
H	6.4988429807	-0.8944067336	-3.959413714
C	-5.6977952136	-4.2664605055	-0.4129070154
C	-7.1810170636	-4.2907486788	-0.0093352285
C	-7.6506063633	-2.8554576013	-0.2998125955
C	-6.4449278266	-1.9979583457	0.1100805513
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H	-5.0964802986	-4.9783380858	0.1617815025
H	-7.2709033693	-4.5073122157	1.0619138213
H	-7.7463497602	-5.0531835746	-0.5534286775
H	-8.5609063971	-2.5833923098	0.2424299152
H	-7.8511162361	-2.7349312067	-1.3714119969
H	-6.4819399896	-1.7173577637	1.1712328619
H	-6.3414939544	-1.0750906777	-0.4666393846
C	-0.7312337756	6.7385403918	-0.5228226555
C	-0.0575872042	8.0489963145	-0.085053155
C	1.4426528841	7.7361917826	-0.2165270236
C	1.5431533843	6.2768155386	0.2490250694
H	-0.8918659627	6.7200065494	-1.6109816516
H	-1.7031337826	6.5867938514	-0.0416921311
H	-0.3080076836	8.2635632804	0.9607605383
H	-0.38008136	8.9024884831	-0.688681187
H	2.074341725	8.4072297529	0.3726724132
H	1.7534262189	7.8187731447	-1.265072132
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TRIS:9H⁺

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H	1.1705577703	-1.6834541995	-0.2489964119
C	-1.5917506875	1.8885115248	0.0374635507
C	2.4313744133	0.4342403601	0.0374635507
C	-0.8396239097	-2.3227525975	0.0374635507
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H	2.9731170566	1.287602403	0.4556417703
H	-0.3714620236	-3.2185965104	0.4556417703
H	-0.9191002535	2.3353716604	0.7751340281
H	2.4820414257	-0.3717220715	0.7751340281
H	-1.5629413562	-1.9636503016	0.7751340281

C	-1.5321232954	2.6717555044	-1.2913460463
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H	2.3446210608	-0.5493198791	-1.8959027695
H	-1.6480353867	-1.7558418707	-1.8959027695
C	-1.3655867505	4.1797836818	-1.0793722282
C	4.3025923398	-0.9072594333	-1.0793722282
C	-2.9370057732	-3.2725249612	-1.0793722282
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H	-1.5728808695	4.7168588924	-2.0137806659
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C	0.0409865724	4.5483370659	-0.6008939339
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C	-3.9594690279	-2.2386734232	-0.6008939339
H	-2.1039708403	4.5530314839	-0.3555085461
H	4.9950264632	-0.4544239548	-0.3555085461
H	-2.8910558068	-4.0986082417	-0.3555085461
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O	2.7368584671	-2.6287093293	-0.3742940312
O	-3.6449581781	-1.0558347038	-0.3742940312
N	0.3133400548	5.8582216884	-0.4400729074
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C	5.9694997542	-5.3113644952	-0.2697211031
C	4.6386574912	-4.588543074	-0.0205340334
H	6.556029834	-2.8922854429	-1.7561274662
H	6.6856858667	-2.0349586707	-0.20901499
H	7.1996568643	-4.0445250371	1.0009044434
H	7.9812816537	-4.4306337664	-0.5390560755
H	6.1100280512	-6.1631722496	0.4008561828
H	6.0071468005	-5.6864977764	-1.2991668117
H	4.3520755664	-4.6032835962	1.038507917
H	3.8006833833	-4.9908372404	-0.5950385322
C	-5.7444812403	-4.018784395	-0.6787717393
C	-7.153568138	-3.9763465038	-0.0681775342
C	-7.584526345	-2.5140565968	-0.2697211031
C	-6.2931235002	-1.7229240993	-0.0205340334
H	-5.7828074718	-4.2315460721	-1.7561274662
H	-5.105168724	-4.7724948763	-0.20901499
H	-7.1024897468	-4.2128236339	1.0009044434
H	-7.8276821096	-4.6966761931	-0.5390560755
H	-8.3924776479	-2.2098537947	0.4008561828
H	-7.9282248194	-2.3590932547	-1.2991668117
H	-6.1625982046	-1.467366611	1.038507917
H	-6.2225334142	-0.7960701509	-0.5950385322
C	-0.6081286445	6.9842584738	-0.6787717393
C	0.1331670962	8.1833445777	-0.0681775342
C	1.6150264069	7.8254203794	-0.2697211031
C	1.6544658251	6.3114664606	-0.0205340334
H	-0.7732225461	7.1238308024	-1.7561274662
H	-1.5805173266	6.8074528344	-0.20901499
H	-0.0971673014	8.2573479583	1.0009044434

H	-0.153599728	9.1273092468	-0.5390560755
H	2.2824494128	8.3730253317	0.4008561828
H	1.921077835	8.0455903184	-1.2991668117
H	1.8105224542	6.0706494946	1.038507917
H	2.421849847	5.7869066786	-0.5950385322

TRIS:10

C	0.1896382792	-0.0031665371	1.3359510103
N	1.5344525467	0.2463882904	1.0828584861
N	-0.140888022	-1.3438962255	1.3693460424
N	-0.7371262481	0.8891652132	1.5198908576
C	2.6470381271	-0.5890876771	1.5158794122
C	-1.5057582929	-1.7614474435	1.6345614629
C	-0.4114706167	2.2735215169	1.7947588068
H	3.1528659685	-0.1355958618	2.3838302071
H	-1.4764815723	-2.8082906228	1.9647816536
H	-0.9885944785	2.5852173758	2.6792166732
H	2.2566556241	-1.5527517633	1.8475167852
H	-1.878437867	-1.1584233179	2.4686295746
H	0.6466980574	2.4501892302	2.0478101209
C	3.6871398221	-0.7809473968	0.3992269573
C	-2.457752987	-1.6050495701	0.4384219822
C	-0.8209677834	3.2118124091	0.6427461527
H	4.5468022232	-1.3303687082	0.8083295213
H	-2.3347094302	-0.5879437158	0.05586087
H	-0.7934424478	4.2536841718	0.9936837959
C	3.1366857177	-1.4994017483	-0.8532635135
C	-3.9315882484	-1.8528177669	0.826065972
C	0.04810891	3.0679803071	-0.6289770002
H	4.0564007487	0.2053541179	0.090607363
H	-2.1725008959	-2.2893336862	-0.3705246008
H	-1.8613505442	2.9881192617	0.3760708174
H	3.8622909941	-1.4142336522	-1.6709669602
H	-4.1109282035	-2.9214986831	0.981174649
H	-0.4558207645	3.5458385068	-1.4778780553
C	2.7805513049	-2.9386555079	-0.6322697493
C	-4.9095358433	-1.3848578777	-0.2077536321
C	1.4284210164	3.6342418265	-0.478565018
H	2.2321613664	-0.9740149593	-1.1748728104
H	-4.1382922969	-1.3553273092	1.7848033159
H	0.1334879826	2.0045545168	-0.8753420186
H	1.7945253057	1.2116223267	0.885999379
H	0.4111330781	-1.9784096655	0.7895345515
N	1.626195441	-3.3719921435	-0.1473429244
N	-5.5419467314	-2.1560109715	-1.0754579304
N	2.4635756592	3.0045159468	0.0591009083
C	1.7277978818	-4.7422912175	-0.0798193287
C	-6.3081133116	-1.3049281242	-1.8387020552
C	3.5070507026	3.9014092094	0.0472280177
N	3.6308103586	-3.9890489176	-0.8743468186
N	-5.2316411618	-0.058630672	-0.3881472131
N	1.7707742103	4.915677603	-0.832253606
C	2.9559269423	-5.1468074982	-0.5287269769
C	-6.1381124832	-0.0074775452	-1.4318856928
C	3.1036158687	5.0880125545	-0.5026576314
C	4.9651214983	-3.9242784601	-1.4500257234
C	-4.8127556433	1.0714158908	0.427919027

C	0.9182580763	5.9068471002	-1.4709652811
H	3.409264433	-6.1207968895	-0.6389439069
H	-6.5585361712	0.9287349901	-1.769873437
H	3.6184941063	6.0179579646	-0.6933722329
H	0.9131781904	-5.3522702142	0.2856913455
H	-6.934504516	-1.6756795937	-2.6396426168
H	4.4825928404	3.6406216439	0.4345687433
H	1.4346526778	6.8687014182	-1.4682811473
H	0.6956896185	5.6313333709	-2.5076673572
H	-0.0218797053	6.0166560237	-0.9235765056
H	5.4566656497	-4.8892176667	-1.3106426382
H	4.9266213179	-3.7017992644	-2.5222766562
H	5.5622695883	-3.1574279023	-0.9496707864
H	-4.859905351	1.9826173748	-0.1745375382
H	-5.4658092024	1.1961352355	1.30053859
H	-3.7840193145	0.9387483794	0.7717493113

TRIS:10H⁺

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N	1.3176354724	-0.2756113651	0.8877901167
N	-0.8975035658	-1.0032997635	0.8877901167
C	0.4833757687	2.423719476	0.955501374
C	1.8573153676	-1.6304750874	0.955501374
C	-2.3406899156	-0.7932444016	0.955501374
H	-0.0986388334	3.2576755393	1.3593860445
H	2.8705498051	-1.5434136882	1.3593860445
H	-2.771909751	-1.714261864	1.3593860445
H	1.274662658	2.210808526	1.6794150261
H	1.2772856315	-2.2092941602	1.6794150261
H	-2.5519470687	-0.0015143788	1.6794150261
C	1.0840428414	2.8116053539	-0.4113432909
C	1.8929008553	-2.3446109705	-0.4113432909
C	-2.9769424759	-0.4669943964	-0.4113432909
H	1.3446356314	1.9055918479	-0.9679995953
H	0.9779737479	-2.1172841937	-0.9679995953
H	-2.3226081586	0.2116923328	-0.9679995953
C	2.3345671497	3.6940195283	-0.2891514912
C	2.0318317929	-3.8688038767	-0.2891514912
C	-4.3663977218	0.1747843354	-0.2891514912
H	0.324499868	3.3362266501	-1.0012119516
H	2.7270077119	-1.9491381084	-1.0012119516
H	-3.0515063591	-1.3870885547	-1.0012119516
H	2.5751816097	4.1143123733	-1.2753208718
H	2.2755088437	-4.2873285341	-1.2753208718
H	-4.8506892326	0.1730161478	-1.2753208718
C	3.5247812702	2.9407598759	0.2370862903
C	0.784382738	-4.5229297148	0.2370862903
C	-4.3091627874	1.5821698259	0.2370862903
H	2.1235977761	4.5601845786	0.3565797799
H	2.8874374171	-4.1191815649	0.3565797799
H	-5.0110339724	-0.4410030267	0.3565797799
H	-1.4197112346	1.5004011741	0.7601938995
H	2.0092417641	0.4793057541	0.7601938995
H	-0.5895293087	-1.9797069412	0.7601938995
N	3.5417526761	1.6661067645	0.6077648558
N	-0.3279849404	-3.9003008278	0.6077648558

N	-3.2137665149	2.2341940503	0.6077648558
C	4.8345883601	1.4030308453	1.0084061922
C	-1.2022332116	-4.8883914134	1.0084061922
C	-3.6323539277	3.4853605551	1.0084061922
N	4.7605911602	3.5062907183	0.3867488408
N	0.6562418691	-5.875937895	0.3867488408
N	-5.4168318086	2.3696471637	0.3867488408
C	5.6030733304	2.5264310691	0.8774373211
C	-0.6135825643	-6.115619032	0.8774373211
C	-4.9894895453	3.5891879499	0.8774373211
C	5.1320224326	4.8784264963	0.064995607
C	1.6588306741	-6.8836747016	0.064995607
C	-6.7908518859	2.0052481924	0.064995607
H	6.6447969067	2.723306475	1.0813500166
H	-0.9639452496	-7.1162158158	1.0813500166
H	-5.6808504363	4.3929093278	1.0813500166
H	5.1317654082	0.4282411957	1.3686538042
H	-2.1950143355	-4.6583594617	1.3686538042
H	-2.9367498518	4.230118253	1.3686538042
H	1.2798550581	-7.8633904245	0.3589604139
H	1.8693590517	-6.8959857845	-1.009110891
H	2.5881264672	-6.6910126121	0.6091677563
H	-7.4498227824	2.8233085647	0.3589604139
H	-6.9067777852	1.8290808106	-1.009110891
H	-7.0886495186	1.1041233831	0.6091677563
H	6.1699689451	5.0400818468	0.3589604139
H	5.0374199544	5.0669049609	-1.009110891
H	4.5005242721	5.586889216	0.6091677563

TRIS:11

C	0.2828990998	0.3718904839	0.9932890153
N	-1.0724809958	0.6951465869	1.0166978931
N	1.1227379842	1.4664114709	1.1171739069
N	0.791715649	-0.8104219068	0.8550628728
C	-1.6607065201	1.7734042898	1.8022678256
C	2.5648743604	1.3007384541	1.0569169208
C	-0.0134944055	-2.0066194154	0.9890864367
H	-2.0984159346	1.3802884767	2.7358054995
H	3.0203733664	2.1650544278	1.561705837
H	0.5219075869	-2.69477968	1.6621033676
H	-0.8713043325	2.4663773469	2.0954483972
H	2.8177335135	0.4054792981	1.6322826283
H	-1.0012154573	-1.8422445685	1.4503470135
C	-2.7644619032	2.5122354081	1.0281352324
C	3.1351750054	1.1752994357	-0.3640692304
C	-0.1898751824	-2.745584076	-0.3519058296
H	-3.2272814053	3.2522002939	1.6960312522
H	2.662796831	0.3155199709	-0.850753264
H	-0.5737503557	-3.7583819369	-0.1634850286
C	-2.2973690868	3.2027358912	-0.2713102516
C	4.6654769709	0.9994015987	-0.3627107976
C	-1.1091182965	-2.0399109116	-1.3744545519
H	-3.54756821	1.7886952367	0.763715792
H	2.8778845121	2.0684722348	-0.9482778612
H	0.805477861	-2.8532868096	-0.801286804
H	-3.1812776635	3.5369694349	-0.8288549229
H	5.1242615457	1.8298486384	0.1923933581

H	-0.9563048157	-2.4906571593	-2.3632938747
C	-1.3832083404	4.3765417128	-0.0754246051
C	5.2612922044	0.9555701906	-1.7385183915
C	-2.5725071716	-2.1125839609	-1.0465597389
H	-1.7911113556	2.4545138425	-0.8921242023
H	4.925492119	0.0781740012	0.1754468356
H	-0.8011179507	-0.9902132546	-1.4576521423
H	-1.7148980347	-0.0677807643	0.814059374
H	0.7688254336	2.347628101	0.7444823443
N	-0.0479263981	4.2241526313	0.2553627132
N	5.3713089562	2.0931166783	-2.5183829778
N	-3.1470531863	-1.3606223958	-0.0354083748
C	0.4427026901	5.4422431341	0.3494096076
C	5.8991494539	1.6900973191	-3.6530720618
C	-4.41934186	-1.6992670254	-0.0110539131
C	-1.6731301972	5.71764067	-0.1764755694
C	5.7359672253	-0.131526132	-2.4353175935
C	-3.5382278025	-2.9050824974	-1.6226564626
N	-0.4986369782	6.3946716715	0.0974870721
N	6.144648666	0.3459733164	-3.6677311178
N	-4.7190826809	-2.6358879346	-0.9542704933
H	-2.5856851493	6.2427319548	-0.4192011463
H	5.816658455	-1.1776867807	-2.1770782419
H	-3.4959082447	-3.6211862057	-2.4305410894
C	-0.3027516064	7.8330960395	0.0954824312
C	6.7236611654	-0.4238870072	-4.7511581877
C	-6.0195266403	-3.2247995344	-1.2153534116
H	0.7335067244	8.0495766419	0.3646395777
H	6.9292512714	0.2451101043	-5.5903841489
H	-6.7433306991	-2.8142802101	-0.50752523
H	-0.5023047664	8.2520094148	-0.8964449533
H	7.6635010891	-0.8935661046	-4.4404130346
H	-6.3543728827	-2.9951571153	-2.2325240356
H	-0.9624200927	8.3149357148	0.824641058
H	6.0331899246	-1.2047458311	-5.0882283293
H	-5.9851519947	-4.3120682296	-1.0898700044
H	1.467202695	5.6963868649	0.5888226875
H	6.1343455126	2.3182564453	-4.5036864141
H	-5.1701722752	-1.3019879793	0.6600473375

TRIS:11H⁺

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N	-0.9584713602	0.9446504375	-0.9341322146
N	-0.3388555965	-1.3023857654	-0.9341322146
C	1.8582365324	1.6517689082	-1.3319345413
C	-2.3595921019	0.7833955892	-1.3319345413
C	0.5013555695	-2.4351644974	-1.3319345413
H	2.5722005502	1.4643849158	-2.1442945513
H	-2.5542948131	1.4953985622	-2.1442945513
H	-0.0179057371	-2.959783478	-2.1442945513
H	1.0665984881	2.2799273091	-1.7430080578
H	-2.5077742125	-0.2162622682	-1.7430080578
H	1.4411757244	-2.0636650409	-1.7430080578
C	2.5938394543	2.3652158279	-0.1866125901
C	-3.3452567195	1.0637229468	-0.1866125901
C	0.7514172652	-3.4289387747	-0.1866125901

H	3.1282197605	3.2225211285	-0.6154279178
H	-4.3548950418	1.0978572169	-0.6154279178
H	1.2266752813	-4.3203783455	-0.6154279178
C	1.7075690485	2.8483176414	0.9813018919
C	-3.3204999597	0.054639354	0.9813018919
C	1.6129309113	-2.9029569954	0.9813018919
H	3.3561267199	1.6836114015	0.2118622198
H	-3.1361136037	2.064685297	0.2118622198
H	-0.2200131162	-3.7482966985	0.2118622198
H	2.3609488675	3.198845784	1.7881193325
H	-3.9507561455	0.4452188043	1.7881193325
H	1.589807278	-3.6440645883	1.7881193325
C	0.7525279028	3.9480390364	0.6209003982
C	-3.795366052	-1.3223112373	0.6209003982
C	3.0428381492	-2.6257277991	0.6209003982
H	1.1491887898	1.9948977011	1.3882201841
H	-2.302226482	-0.0022221648	1.3882201841
H	1.1530376922	-1.9926755363	1.3882201841
H	2.0016669983	-0.3524560836	-0.6801508621
H	-0.6955975771	1.9097225122	-0.6801508621
H	-1.3060694212	-1.5572664287	-0.6801508621
N	-0.3704776171	3.7170400512	-0.1551629103
N	-3.0338123026	-2.1793630536	-0.1551629103
N	3.4042899198	-1.5376769976	-0.1551629103
C	-0.9630294258	4.8899731638	-0.2945617311
C	-3.7533262708	-3.2789945292	-0.2945617311
C	4.7163556966	-1.6109786346	-0.2945617311
C	0.8121542079	5.2837273104	0.9387060851
C	-4.9819191814	-1.9385174794	0.9387060851
C	4.1697649735	-3.345209831	0.9387060851
N	-0.2879392653	5.8760702171	0.3499379877
N	-4.9448564498	-3.187397827	0.3499379877
N	5.2327957151	-2.6886723901	0.3499379877
H	1.5195769202	5.8549426715	1.5217214597
H	-5.8303175513	-1.6114791198	1.5217214597
H	4.3107406311	-4.2434635517	1.5217214597
C	-0.6563224626	7.2840153505	0.4191216083
C	-5.9799811037	-4.2103996009	0.4191216083
C	6.6363035664	-3.0736157495	0.4191216083
H	-1.5715667542	7.4392397297	-0.1553014753
H	-5.6567872136	-5.0806365977	-0.1553014753
H	7.2283539679	-2.3586031319	-0.1553014753
H	-0.8341365458	7.5822087154	1.456373816
H	-6.1493170914	-4.5134877966	1.456373816
H	6.9834536372	-3.0687209188	1.456373816
H	0.1366775691	7.907071533	-0.0042443785
H	-6.9160636017	-3.8351695195	-0.0042443785
H	6.7793860325	-4.0719020135	-0.0042443785
H	-1.8748466423	5.0798572902	-0.844885575
H	-3.4618621397	-4.1635934655	-0.844885575
H	5.336708782	-0.9162638247	-0.844885575

TRIS:12

C	0.1591620756	-0.5348658064	-1.4276014767
N	-1.1809213116	-0.1947526839	-1.3352792111
N	0.5166378847	-1.7671979549	-1.2619255262
N	1.0004745192	0.54547685	-1.6823950917

C	-2.1760537462	-1.2041979907	-1.015114045
C	1.8466652731	-2.2268702438	-1.6042052613
C	0.6550272169	1.7128425336	-2.4836024881
H	-3.1512846622	-0.8320729742	-1.3596296217
H	-1.9353270875	-2.1000524768	-1.594351559
C	-2.2576831135	-1.564661546	0.4763949861
H	-1.2740504263	-1.9253957567	0.7952701056
C	-3.3304332849	-2.6350943074	0.7569647609
H	-2.4898977796	-0.6668013668	1.0641165551
H	-4.3025549952	-2.279004372	0.3936161011
C	-3.4605676854	-2.9461424807	2.2294521849
H	-3.0856110512	-3.5504155611	0.2028077848
H	1.131315318	1.6524066307	-3.4761338208
H	-0.4224167578	1.7133524322	-2.6562597105
C	1.1023486829	3.0242322389	-1.8158492982
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C	0.4311061661	3.3202002202	-0.4553289641
H	2.1873446068	2.9773163117	-1.6526545326
H	0.9974783668	4.1105529472	0.0514874802
C	-1.0150018272	3.7462491692	-0.5578820198
H	0.4979306618	2.4192482921	0.1637847932
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H	1.7383821086	-3.1587479774	-2.179980317
C	2.6831435773	-2.5706559063	-0.3565971286
H	2.4124636452	-1.536533501	-2.2514292311
H	3.557248107	-3.1682189873	-0.6519870158
C	3.1553663994	-1.3519761997	0.4733723018
H	2.0632523791	-3.2036125724	0.2899669084
H	3.4484311718	-1.6936771166	1.473278764
C	4.3216482613	-0.6153584094	-0.1438095559
H	2.3124519439	-0.6638068725	0.6030274766
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C	-1.3743826308	5.1019505121	-0.5664650785
C	-2.7161741819	5.4565799776	-0.6763809569
H	-0.604388593	5.8637821283	-0.4819870005
H	-3.0108367823	6.5027903799	-0.6796255241
C	-3.6728789048	4.4468627272	-0.7758045649
C	-3.2310300889	3.1256521873	-0.7623436083
H	-4.7315363977	4.6723731095	-0.8586905076
H	-3.9414924211	2.3043655758	-0.8365609622
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TRIS:12H⁺

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H	0.3005100952	7.3999323028	0.9772693962
H	-6.5587844327	-3.4397167251	0.9772693962
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H	1.7569989241	5.5212298704	1.7407743638
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TRIS:13

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N	1.4547860533	-2.3855153898	-0.5299110485
N	1.8720495426	-0.0419569958	-0.8619836146
C	-1.2553265056	-1.9142900664	-0.3054533486
C	2.7942842608	-2.8044154634	-0.8883552665
C	1.5061016874	1.1063090838	-1.68464405
H	-0.9878166165	-2.7660652632	-0.9370213715
H	-2.2387569093	-1.5486760498	-0.6323738551
C	-1.3301378401	-2.3687842565	1.1605656777
H	-0.3343500168	-2.709634334	1.4625006693
C	-2.3590820018	-3.4990573039	1.3606561866
H	-1.6034047572	-1.5206896189	1.8020554885
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H	-2.0664077259	-4.3709701362	0.7631043748
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C	1.9115958909	2.4358111305	-1.0277596928
H	1.7233166181	3.2558133934	-1.7341415405
C	1.2175966717	2.7293721001	0.3224592019
H	2.9947870222	2.4209509773	-0.8487337863
H	1.7507914242	3.5450628164	0.8237884219
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H	1.3008967077	1.8397265681	0.9551468613
H	-0.5157350077	0.05443803	-0.1791738374
H	2.7039132075	-3.7111194461	-1.5046301587
C	3.633158935	-3.1878302769	0.3451551601
H	3.3471251233	-2.0760445544	-1.5048355024
H	4.5181911287	-3.7560795687	0.0274890325
C	4.0787066355	-1.9966154545	1.22981422
H	3.025445601	-3.8589803728	0.9631882042
H	4.3752842914	-2.373452967	2.2151588781
C	5.2320363248	-1.2181515087	0.6451671277
H	3.2248882133	-1.3271307214	1.3815743038
N	-1.1422816217	2.1111247061	0.1377438489
C	-0.6284723418	4.4531569801	0.1232221952
C	-1.9801729914	4.7343425183	-0.0054676063
H	0.0940469861	5.2585200139	0.171378251
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C	-2.9271007275	3.7193677717	-0.0628382512
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C	5.9721218757	0.3628163762	-0.8778369711
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C	7.5703424567	-0.7378204197	0.4696177022
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H	5.6983600918	1.0787924547	-1.6495509415
H	8.1079674686	0.7589183867	-0.9904325465
N	8.9685674228	-0.9654972934	0.9000686802
H	6.7723791092	-2.1815816936	1.8433195791
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C	-2.0035714109	-5.3115014675	4.6705462113
C	-1.8541921259	-5.0342032307	3.3189249241
H	-3.9663473671	-2.7044966811	5.4807065573
H	-2.8808306078	-4.7113902337	6.5487995677
N	-1.344399341	-6.5054956992	5.2430897962
H	-1.2602295914	-5.6845801321	2.6888471882
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O	-1.5556959301	7.0134758451	-0.0272948281
O	9.1604441633	-1.7954417034	1.7845608457
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TRIS:13H⁺

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C	-0.0684499097	2.4873673097	1.1795421149
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H	2.8851175955	-0.8281142906	1.9478297298
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C	2.9984866394	-1.7583719631	0.0066900088
C	-3.0220380462	-1.717579468	0.0066900088
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H	-3.996000465	-2.0131319872	0.4162560404
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C	2.1769912275	-2.4669651043	-1.0948253072
C	-3.2249500014	-0.6518470016	-1.0948253072
H	-0.9666533574	3.5557507474	-0.458681886
H	3.5626972183	-0.9407288565	-0.458681886
H	-2.5960436341	-2.6150217157	-0.458681886
H	0.8574197718	3.7562837256	-1.9639532573
H	2.8243273071	-2.6206890138	-1.9639532573
H	-3.6817468522	-1.1355945365	-1.9639532573
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C	1.6077982342	-3.7996757684	-0.665570433

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H	-1.6329626475	1.2051602497	0.5554048732
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N	3.0244478111	2.3298023096	0.1107805038
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C	4.2910993959	2.4636263715	0.5326669922
C	-0.011986612	-4.9480141196	0.5326669922
C	-4.2791125571	2.4843879234	0.5326669922
C	5.0995477168	3.5504752237	0.2101364986
C	0.5250279436	-6.1915753293	0.2101364986
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C	-6.1875917749	1.6564025748	-0.59010732
C	3.2209307332	4.4239646062	-1.0407106761
C	2.2208004306	-5.0013899887	-1.0407106761
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H	-3.779731258	3.2209744343	1.1568577091
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H	-6.2098878689	3.482761712	0.5578879627
N	5.332870006	5.7176920386	-0.9743317917
N	2.2852316163	-7.4772467665	-0.9743317917
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H	2.7969898722	5.1994187725	-1.6670614285
H	3.1043338686	-5.0219735166	-1.6670614285
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O	4.7842186538	6.5566220495	-1.680642904
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O	-8.2365312072	2.7307470206	-0.5542737392

TRIS:14

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N	-1.6919274992	0.5182027875	0.9394571224
C	1.8472993891	0.2250345217	1.9308255914
C	-1.5329487821	-2.2451929683	1.8313311548
C	-2.089148222	1.881477464	1.2736950821
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H	1.6750550933	-0.4722661803	2.7553560739
C	2.6295800175	-0.4849348863	0.814782862
H	2.0104752506	-1.3025752898	0.4310240342
C	3.9799111996	-1.0348350579	1.3156765622
H	2.8140589611	0.211854822	-0.0135153702
H	4.5730842859	-0.2164529453	1.7415360389
C	4.7822483247	-1.6688151059	0.2058518978

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H	-3.020239382	3.6126774677	0.3748351153
C	-1.6110572237	2.829851991	-1.0968434772
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H	-2.1505078872	3.1279989077	-2.0031516266
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H	0.5768178476	1.5311259949	0.8753891371
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H	-2.4970660082	-1.7234927806	1.9504965059
H	-2.316830401	-4.0789601509	0.9703868264
C	-2.0718463575	-2.6821343306	-0.6800683946
H	-0.6397973089	-3.7167156033	0.555414398
H	-1.8033173319	-3.3863083444	-1.4758791023
C	-3.5532927266	-2.4031426149	-0.7636806957
H	-1.5150983102	-1.7568028442	-0.8655477252
N	0.5332348344	3.4568596207	-0.1018823472
C	-0.6790134784	5.1810268759	-1.2417689726
C	0.3248153116	6.1085751923	-0.9402776542
H	-1.5506504655	5.485729508	-1.8114245533
C	0.2106600122	7.4709862606	-1.3785227315
C	1.4426985387	5.6849272707	-0.2082811778
C	1.4887765944	4.3508677614	0.1831666929
H	2.2431470566	6.3721703162	0.0414646542
H	2.3372727538	3.9776967973	0.7523439026
N	-4.0163018806	-1.2752077503	-0.1896439913
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C	-6.2662102133	-1.8625180115	-0.8202260756
C	-5.7924682416	-3.0360796825	-1.4234145871
C	-4.4201309012	-3.3076301863	-1.3921190861
H	-2.4675255597	-0.1039984094	0.7238514281
H	-5.6544537172	-0.1036086395	0.2589030149
H	-7.3220060023	-1.6161086509	-0.8242993109
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C	6.2266545629	-2.716065001	-1.8981586096
C	5.5046216977	-3.5864516785	-1.0701480776
C	4.7719614225	-3.0537685734	-0.0023197891
H	6.7194596722	-0.6449543936	-2.2233025376
H	6.8087978872	-3.0909344447	-2.7327209887
C	5.5167335383	-5.0018894358	-1.310562041
H	4.2055235224	-3.7066398027	0.6535356592
N	0.1166805087	8.5743740305	-1.7323974409
N	-7.4363403696	-4.6767127362	-2.5883391547
N	5.5258312578	-6.1478949995	-1.5071244025

TRIS:14H⁺

C	0.000000046	0.0000000268	0.8577476346
N	-0.6339810229	1.1868887192	0.8514187084
N	1.3448663394	-0.0444006082	0.8514187084
N	-0.7108851786	-1.1424880305	0.8514187084

C	-0.0682937529	2.4914774133	1.2111684961
C	2.1918296551	-1.1865945017	1.2111684961
C	-2.1235357643	-1.3048828312	1.2111684961
H	-0.7219839647	2.9298124917	1.9747911936
H	2.8982840742	-0.8396497112	1.9747911936
H	-2.1762999716	-2.0901627	1.9747911936
H	0.9060832744	2.3450512521	1.6805062025
H	1.577832366	-1.9572166796	1.6805062025
H	-2.4839155025	-0.3878344921	1.6805062025
C	0.0171718908	3.4599503559	0.0205778623
C	2.9878190043	-1.7448463915	0.0205778623
C	-3.0049907572	-1.7151038839	0.0205778623
H	0.2509086897	4.4581782678	0.4113116345
H	3.7354413354	-2.4463823531	0.4113116345
H	-3.9863498871	-2.0117958342	0.4113116345
C	1.0350368752	3.0837424662	-1.0804614425
C	2.1530809226	-2.4382393808	-1.0804614425
C	-3.1881176598	-0.6455030049	-1.0804614425
H	-0.9762106343	3.5309960672	-0.4393135571
H	3.5460376578	-0.9200747448	-0.4393135571
H	-2.5698268855	-2.610921242	-0.4393135571
H	0.8365437713	3.7035873263	-1.9607224538
H	2.7891288698	-2.5762617404	-1.9607224538
H	-3.6256725032	-1.1273255054	-1.9607224538
C	2.4763014178	3.2682267303	-0.663569946
C	1.5922167106	-3.7786532203	-0.663569946
C	-4.0685179904	0.5104265705	-0.663569946
H	0.876364546	2.0428942962	-1.387768968
H	1.3310161305	-1.7804010279	-1.387768968
H	-2.2073805385	-0.2624931878	-1.387768968
H	-1.634530525	1.2027317408	0.6070405448
H	1.8588615497	0.8141791675	0.6070405448
H	-0.2243308868	-2.0169108279	0.6070405448
N	3.0162913871	2.322878287	0.1322245089
N	0.5035259587	-3.7736240299	0.1322245089
N	-3.5198172078	1.4507458233	0.1322245089
C	4.2841687779	2.4719004439	0.5453514519
C	-0.0013557632	-4.9461491376	0.5453514519
C	-4.2828128768	2.4742487742	0.5453514519
C	5.0862152821	3.55202168	0.1953352833
C	0.5330334144	-6.1808024034	0.1953352833
C	-5.6192485585	2.6287808038	0.1953352833
C	4.5312550403	4.5365395709	-0.6336081229
C	1.6631310393	-6.1924516813	-0.6336081229
C	-6.1943859416	1.6559121909	-0.6336081229
C	3.2072301377	4.3896484506	-1.066296647
C	2.1979320488	-4.9723669203	-1.066296647
C	-5.4051620486	0.5827185501	-1.066296647
H	4.6773308043	1.6868276963	1.1866592067
H	-0.8778297196	-4.8941010665	1.1866592067
H	-3.7995009468	3.2072734507	1.1866592067
H	6.1074382742	3.6287572139	0.5505988657
H	0.08887684	-7.1035752244	0.5505988657
H	-6.1963149763	3.474818091	0.5505988657
C	5.3036258057	5.6767327243	-1.0361426101
C	2.2643818926	-7.4314409621	-1.0361426101
C	-7.5680075604	1.7547083182	-1.0361426101
H	2.7579838379	5.1380542245	-1.7101944656

H	3.0706936112	-4.9575110991	-1.7101944656
H	-5.8286773112	-0.1805430449	-1.7101944656
N	2.7539307203	-8.433366359	-1.3631662616
N	-8.6804748207	1.8317092955	-1.3631662616
N	5.9265442383	6.601657144	-1.3631662616

TRIS:15

C	-0.4468678692	-0.0215903562	1.7347580533
N	0.6408862181	0.8315940537	1.834768711
N	-0.2992914711	-1.2764526959	2.0142223002
N	-1.6175346189	0.6007722862	1.3104978074
C	1.9496777839	0.3126253261	2.1949828786
C	-1.4350549709	-2.1569789044	2.1934907873
C	-1.9953575924	1.9786238682	1.5940004132
H	2.5433817338	1.1488074813	2.591445671
H	1.8068903583	-0.4105637291	3.0026073698
C	2.7064191769	-0.3531451721	1.0352226019
H	2.0937657105	-1.177180351	0.6541749842
C	4.0883404246	-0.8796953753	1.4681246672
H	2.8413369365	0.3673713276	0.2181744613
H	4.6689221575	-0.0564338487	1.9040886322
C	4.8749033314	-1.4488589394	0.3107312048
H	3.962385648	-1.6429242186	2.2463040698
H	-2.7782439058	2.0094227721	2.3701348337
H	-1.1312455079	2.5032047872	2.0047843206
C	-2.5318259358	2.7013198306	0.346364272
H	-2.9065887709	3.6912730548	0.6417356725
C	-1.5189548033	2.8467405082	-0.8118394823
H	-3.3957022519	2.1392278371	-0.0332784158
H	-2.0639231801	3.1219301725	-1.7223418077
C	-0.4335182824	3.8692163672	-0.56586485
H	-1.0558336784	1.8698396879	-0.9884214222
H	0.6483503448	1.6247930334	1.1929600214
H	-1.2630319561	-2.7362198827	3.1138441205
C	-1.5710893889	-3.1778213417	1.0475476719
H	-2.3952785283	-1.6358784269	2.3407158145
H	-2.245449635	-3.9893777494	1.3556695655
C	-2.0614563649	-2.5947043678	-0.2997067095
H	-0.5820255824	-3.6235150372	0.8860221782
H	-1.8334283148	-3.3081687474	-1.1004224267
C	-3.5432283416	-2.297114352	-0.3267460903
H	-1.5005303473	-1.6782153859	-0.5143529658
N	0.6254832992	3.4792211491	0.1776349056
C	-0.5370898931	5.1607511514	-1.0793519038
C	0.478915988	6.0916998458	-0.8279564105
H	-1.3903255345	5.4602950345	-1.6794360653
O	0.311378428	7.3257843601	-1.3634522934
C	1.5772479495	5.6889431065	-0.0596662306
C	1.5865538387	4.3768298665	0.411361428
H	2.4021123417	6.3521037927	0.1703704224
H	2.4262267268	4.0296931061	1.0110506529
N	-3.9589390833	-1.1426246118	0.2425468531
C	-5.2702175557	-0.8896641883	0.2528617867
C	-6.24529481	-1.728261187	-0.2848088184
C	-5.8140267988	-2.9220665352	-0.8750568274
C	-4.4418749596	-3.2009764276	-0.8915920493
H	-2.397168009	-0.0166184693	1.0902299318

H	-5.5712341633	0.0474682301	0.7191056732
H	-7.2897668884	-1.4450880814	-0.2374974268
O	-6.6244484757	-3.8477096915	-1.4449438194
H	-4.0967704743	-4.1229861426	-1.3481389013
N	5.4556839369	-0.5516891758	-0.515358788
C	6.1265746306	-1.0311512945	-1.5628733479
C	6.27342851	-2.3864971771	-1.8675694504
C	5.6695650115	-3.3084655759	-1.006575925
C	4.960247756	-2.8240733775	0.0996415325
H	6.5887518559	-0.2887429795	-2.2134836548
H	6.839492465	-2.6889839648	-2.740555951
O	5.7140895186	-4.6589956128	-1.1514255572
H	4.4863406115	-3.5290308408	0.7751869746
C	6.4194460323	-5.1911525867	-2.2640231041
H	6.3222312654	-6.2754905152	-2.1878963599
H	5.985805533	-4.8527056646	-3.2137741102
H	7.4822131567	-4.918407874	-2.23423117
C	-8.0263989731	-3.6064454016	-1.4491938356
H	-8.4742841391	-4.4675467148	-1.947445839
H	-8.4226082573	-3.5291274673	-0.4289500061
H	-8.2739361562	-2.6939184425	-2.0059074917
C	1.3254058154	8.2999350342	-1.1445949954
H	0.9881203974	9.2001890419	-1.6604449911
H	1.4483668433	8.5165577796	-0.0761045246
H	2.2865977342	7.9777049893	-1.5640212263

TRIS:15H⁺

C	-0.0000001795	-0.0000000147	1.141852066
N	-0.633502157	1.1871376531	1.138572338
N	1.3448421873	-0.0449400426	1.138572338
N	-0.7113405687	-1.1421976544	1.138572338
C	-0.0566394904	2.4930793421	1.4678857278
C	2.1873895326	-1.1974886109	1.4678857278
C	-2.1307505806	-1.2955907751	1.4678857278
H	-0.7033889611	2.9513008251	2.2263250572
H	2.9075957128	-0.8664978809	2.2263250572
H	-2.2042072901	-2.0848029881	2.2263250572
H	0.9212932546	2.3517602765	1.9310634337
H	1.5760372593	-1.9737436785	1.9310634337
H	-2.4973310523	-0.378016642	1.9310634337
C	0.0265280052	3.4372940948	0.2573796332
C	2.9635197472	-1.7416211512	0.2573796332
C	-2.9900482908	-1.6956729875	0.2573796332
H	0.2727932782	4.4411994009	0.6259995685
H	3.7097946089	-2.4568457868	0.6259995685
H	-3.9825884255	-1.9843536581	0.6259995685
C	1.0336713277	3.0329331337	-0.8423711927
C	2.1097612214	-2.4116523732	-0.8423711927
C	-3.1434330875	-0.6212808045	-0.8423711927
H	-0.9713340415	3.5051199763	-0.1937747833
H	3.521189707	-0.9113602101	-0.1937747833
H	-2.5498562039	-2.5937598102	-0.1937747833
H	0.8357642949	3.6406462501	-1.7314156746
H	2.7350097348	-2.5441164135	-1.7314156746
H	-3.5707745682	-1.0965298806	-1.7314156746
C	2.4804792937	3.2082902205	-0.4379803031
C	1.5382209303	-3.7523033695	-0.4379803031

C	-4.0187007624	0.5440131051	-0.4379803031
H	0.8596920443	1.9889124388	-1.1310075106
H	1.2926024192	-1.7389715466	-1.1310075106
H	-2.152295002	-0.2499409361	-1.1310075106
H	-1.6347306505	1.2103448571	0.8835273376
H	1.8655544623	0.8105456656	0.8835273376
H	-0.2308243503	-2.0208905667	0.8835273376
N	3.0056282039	2.269848674	0.3851086824
N	0.4629322559	-3.7378748933	0.3851086824
N	-3.4685609983	1.4680261754	0.3851086824
C	4.2762508052	2.4272791153	0.7784064974
C	-0.0360402832	-4.9169815653	0.7784064974
C	-4.2402110605	2.489702406	0.7784064974
C	5.0946491994	3.4854183641	0.3962660055
C	0.4711359899	-6.1548049895	0.3962660055
C	-5.5657857278	2.6693865814	0.3962660055
C	4.5507599052	4.4549131821	-0.4580401778
C	1.5826877782	-6.1685304529	-0.4580401778
C	-6.1334482219	1.7136172268	-0.4580401778
C	3.218303761	4.3020388021	-0.8739294865
C	2.1165227537	-4.9381523926	-0.8739294865
C	-5.3348270531	0.6361135465	-0.8739294865
H	4.6712557439	1.6592788505	1.440596868
H	-0.898650492	-4.8750657444	1.440596868
H	-3.7726057903	3.21578685	1.440596868
H	6.1142585123	3.5366091878	0.7573718546
H	0.0056638872	-7.0634079683	0.7573718546
H	-6.119922938	3.5267987365	0.7573718546
O	5.2011831443	5.5357928094	-0.9241005378
O	2.1935453744	-7.2722533148	-0.9241005378
O	-7.3947290571	1.7364604614	-0.9241005378
H	2.7868861991	5.044418639	-1.5370909305
H	2.9751513326	-4.9357237428	-1.5370909305
H	-5.7620380702	-0.1086949401	-1.5370909305
C	1.6908733429	-8.554086352	-0.5404786946
C	-8.253493015	2.8127037291	-0.5404786946
C	6.5626191337	5.741382579	-0.5404786946
H	2.3336102237	-9.2809362651	-1.0370843552
H	-9.2043319449	2.6195022188	-1.0370843552
H	6.8707211827	6.6614340023	-1.0370843552
H	1.7506671362	-8.6926005084	0.545141743
H	-8.4033466898	2.8301778632	0.545141743
H	6.6526790152	5.8624226012	0.545141743
H	0.6564076123	-8.6885896527	-0.8766941203
H	-7.852743425	3.7758289814	-0.8766941203
H	7.1963352742	4.9127606273	-0.8766941203

TRIS:16

C	-0.7272979566	-0.1176842207	1.9708003796
N	0.5648009824	0.36424716	2.1174043338
N	-0.9868745093	-1.3445069673	2.2867062081
N	-1.626351979	0.8164081542	1.4626673899
C	1.6290750533	-0.5183833831	2.5642619813
C	-2.3460967595	-1.8316162673	2.3975865622
C	-1.5793806623	2.2515382461	1.7053017234
H	1.2356927287	-1.121762184	3.3871710619
H	2.436463846	0.1124914254	2.9641775437

C	2.1884490135	-1.4471489218	1.4739558951
H	1.3779347504	-2.0846620757	1.1085787672
C	3.3385393259	-2.3307672534	1.9941559028
H	2.5442865936	-0.8430450765	0.626905544
H	4.1410471797	-1.6970215535	2.3964758004
C	3.8965773558	-3.2440927199	0.9255795083
H	2.9653324039	-2.9512096	2.8178946602
H	-2.3516799102	2.5431542858	2.4368827582
H	-0.6162362899	2.5027314155	2.1522718236
C	-1.8092360949	3.0611029019	0.4175764914
H	-1.8944978089	4.1261530734	0.6757356239
C	-0.7276797889	2.8702556282	-0.669682446
H	-2.7754446522	2.7613125323	-0.0096295248
H	-1.1088235086	3.2674657822	-1.6182530634
C	0.5923970997	3.5363717927	-0.3512791941
H	-0.5631470889	1.7960269587	-0.8058285086
H	0.848339558	1.0942035051	1.4632499472
H	-2.4128203272	-2.4181316781	3.3268615559
C	-2.7198627196	-2.7835217063	1.2449031667
H	-3.1062908716	-1.0377801592	2.4846244569
H	-3.6312490646	-3.3395136042	1.5080187583
C	-2.9196573512	-2.1058170203	-0.1322576214
H	-1.9094654231	-3.516578278	1.1506599223
H	-2.8630836336	-2.8712216354	-0.9157078409
C	-4.2370293621	-1.3739926044	-0.2629761019
H	-2.0934884805	-1.4073869682	-0.3067049432
N	1.4493866233	2.8546299195	0.4354956198
C	0.8755378363	4.8108833109	-0.8430825363
C	2.0976348452	5.447146653	-0.5312137434
H	0.1387330497	5.2994805487	-1.4694317664
N	2.4135004433	6.6969106077	-1.0139389188
C	2.981110065	4.7214676393	0.3011311838
C	2.6055069531	3.4605011777	0.7389570681
H	3.939496147	5.1243580741	0.6041755308
H	3.2815589027	2.8961364468	1.3798272397
N	-4.3253949336	-0.1502956987	0.3000155181
C	-5.5091179115	0.4717103593	0.2178145515
C	-6.6366740346	-0.0423327273	-0.4044286608
C	-6.5593780976	-1.3176582046	-1.0105265876
C	-5.3139570279	-1.9766411009	-0.9139498287
H	-2.5483182069	0.4600981196	1.2125415829
H	-5.5614868988	1.454947589	0.6841251751
H	-7.549400823	0.540239146	-0.4137301941
N	-7.6336272138	-1.8806669111	-1.6622223033
H	-5.1729986803	-2.9622041223	-1.3409324401
N	3.1752163087	-4.3465869964	0.6477378266
C	3.6505378713	-5.14104214	-0.3169196045
C	4.8136622223	-4.91345542	-1.0428811172
C	5.5733553342	-3.7555187263	-0.7667426348
C	5.0811086985	-2.9214506085	0.2605198622
H	3.0633772896	-6.0354290788	-0.5267378694
H	5.1156871949	-5.628446358	-1.798483619
N	6.7287559135	-3.4551085025	-1.4640679614
H	5.6113890867	-2.0218381575	0.5501651892
C	-7.5417069937	-3.240056774	-2.1705636173
C	-8.9259395856	-1.2153998792	-1.6340797421
H	-9.6381801528	-1.7920372767	-2.2267411007
H	-9.3264702407	-1.1198756386	-0.6137059138

H	-8.8648698329	-0.2105477095	-2.070582657
H	-8.4745066479	-3.4967776472	-2.6755787287
H	-6.728422281	-3.3359156892	-2.9005305166
H	-7.3698992075	-3.9756105343	-1.3707944792
C	3.6339122763	7.3544270239	-0.5748608599
C	1.4290633995	7.4513227376	-1.7728218322
H	3.7241808297	8.3168895215	-1.0812634463
H	3.6446741432	7.5354060354	0.5102883111
H	4.5196712359	6.7587188423	-0.8289123364
H	1.8693752431	8.3991500973	-2.0868603962
H	1.1231231942	6.9090567746	-2.6761911236
H	0.5256475245	7.6707001212	-1.1845576289
C	7.5697501605	-2.3555574628	-1.0221789029
C	7.2859015663	-4.4348275017	-2.3812228452
H	8.4071246759	-2.2462735961	-1.7143380086
H	7.0132142097	-1.4108671696	-1.0223695535
H	7.976232301	-2.51022186	-0.0103088107
H	8.1656637628	-4.0091490988	-2.8680058932
H	7.5871319571	-5.3670957657	-1.877917496
H	6.5644778565	-4.6919863732	-3.1659155061

TRIS:16H⁺

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N	-0.6493553555	1.1785927497	0.9009623577
N	1.3453690321	-0.0269379394	0.9009623577
N	-0.6960133635	-1.1516545881	0.9009623577
C	-0.0904802527	2.4868635559	1.248463913
C	2.198927234	-1.1650733791	1.248463913
C	-2.1084466681	-1.3217899546	1.248463913
H	-0.7447378892	2.9273391876	2.0113787972
H	2.907519139	-0.8187074611	2.0113787972
H	-2.1627809367	-2.1086315043	2.0113787972
H	0.8890795484	2.3520070581	1.7097310438
H	1.5923581804	-1.9459688024	1.7097310438
H	-2.4814374157	-0.4060380334	1.7097310438
C	-0.0155239331	3.4488465466	0.0517957621
C	2.9945507821	-1.7109789513	0.0517957621
C	-2.9790265358	-1.737867373	0.0517957621
H	0.221355684	4.4494282443	0.4358865864
H	3.7426401423	-2.4164135662	0.4358865864
H	-3.9639955131	-2.0330144558	0.4358865864
C	0.9970086497	3.0705537371	-1.0522821708
C	2.1606733076	-2.3987114854	-1.0522821708
C	-3.1576816441	-0.6718420294	-1.0522821708
H	-1.0138901679	3.5135057134	-0.399196757
H	3.5497303805	-0.8786980132	-0.399196757
H	-2.5358398995	-2.634807478	-0.399196757
H	0.794646089	3.6904799532	-1.9322243427
H	2.7987264395	-2.5334234752	-1.9322243427
H	-3.5933722154	-1.1570562558	-1.9322243427
C	2.4437439863	3.2462039969	-0.6430807511
C	1.5894232265	-3.7394461694	-0.6430807511
C	-4.0331668996	0.4932423947	-0.6430807511
H	0.8288446499	2.0300052038	-1.3566883132
H	1.3436138438	-1.7328029231	-1.3566883132
H	-2.1724581806	-0.2972020586	-1.3566883132
H	-1.653490045	1.1904122503	0.6474903587

H	1.8576723646	0.8367584602	0.6474903587
H	-0.2041820065	-2.0271704883	0.6474903587
N	2.9628278864	2.3014418675	0.1719105648
N	0.5116932718	-3.7166049489	0.1719105648
N	-3.4745208451	1.4151633037	0.1719105648
C	4.2374292943	2.4718231126	0.5640164249
C	0.0219470545	-4.9056327704	0.5640164249
C	-4.2593760357	2.43380988	0.5640164249
C	5.0436344849	3.5310911689	0.1888988717
C	0.5361975053	-6.1334609743	0.1888988717
C	-5.5798316771	2.6023700276	0.1888988717
C	4.5176711758	4.5285919367	-0.6699518218
C	1.6630401651	-6.1767137711	-0.6699518218
C	-6.1807110278	1.6481220566	-0.6699518218
C	3.1719872964	4.3484308648	-1.0761266314
C	2.1798580397	-4.9212368101	-1.0761266314
C	-5.351845023	0.5728061675	-1.0761266314
H	4.6396251319	1.7041170614	1.2226936098
H	-0.8440038073	-4.8700915575	1.2226936098
H	-3.7956210115	3.1659747182	1.2226936098
H	6.0605867232	3.5763812927	0.556891361
H	0.066943784	-7.036812509	0.556891361
H	-6.127530194	3.4604314385	0.556891361
N	5.2626691176	5.5961222308	-1.0832764169
N	2.2150495482	-7.3556660615	-1.0832764169
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H	3.0388581146	-4.8629405124	-1.7330167708
H	-5.7308589857	-0.2002578681	-1.7330167708
C	4.6807889797	6.5974159058	-1.9682577764
C	3.3731353763	-7.3523899176	-1.9682577764
C	-8.0539240429	0.754974234	-1.9682577764
C	6.6458582453	5.73661227	-0.6438505236
C	1.6451229273	-8.6237880039	-0.6438505236
C	-8.2909808594	2.8871759561	-0.6438505236
H	7.0684589222	6.6426663101	-1.0785847628
H	2.2184884047	-9.4427979458	-1.0785847628
H	-9.2869470138	2.8001318579	-1.0785847628
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H	1.6815921069	-8.7262494941	0.448453725
H	-8.3979497027	2.9068234652	0.448453725
H	7.2603386103	4.8864200826	-0.9671837596
H	0.6015947124	-8.7308475164	-0.9671837596
H	-7.8619330095	3.844427656	-0.9671837596
H	5.4291520069	7.3594158184	-2.1869281435
H	3.6588651447	-8.3814912667	-2.1869281435
H	-9.0880168385	1.0220756705	-2.1869281435
H	4.3576207539	6.1561514429	-2.9201183873
H	3.1525732546	-6.8518857929	-2.9201183873
H	-7.5101936954	0.6957345722	-2.9201183873
H	4.2339981752	-6.8521535305	-1.5056285365
H	3.8171401612	7.0928267652	-1.5056285365
H	-8.0511380232	-0.2406730125	-1.5056285365

TRIS:17

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N	-1.0383504485	-0.3178999201	1.6338711195
C	-0.4579393688	-3.0153971881	1.7541397936
C	2.6198813922	-0.0005759713	2.038419803
C	-1.4522316642	1.0554135225	1.8333038579
H	0.0116075041	-3.9169489918	2.1730471263
H	2.7692390699	0.6469041541	2.9188584334
H	-2.2486377243	1.0552301014	2.594124514
H	-1.2129914973	-2.6692643092	2.4661309874
H	2.6882871546	-1.0299060021	2.3933488161
H	-0.6613028951	1.7158670315	2.2243494583
C	-1.137109929	-3.3597311423	0.4191101703
C	3.7396833448	0.3027701501	1.0281461014
C	-2.058689465	1.6766305042	0.5595820309
H	-1.585533154	-2.4441868293	0.019116451
H	4.7084960851	0.2464776138	1.5444128579
H	-2.6037244093	2.5949547443	0.8215911426
C	-2.2161185258	-4.4472760405	0.5834381858
C	3.7583179022	-0.6081265385	-0.2200127722
C	-1.0454401119	1.9925740636	-0.5669833645
H	-0.3869374599	-3.7069849604	-0.3031926469
H	3.6239430495	1.340415973	0.6871367259
H	-2.795187043	0.9644572041	0.1668814006
H	-1.7603173918	-5.350620551	1.0081560003
H	4.410501005	-0.1538847477	-0.9756766268
H	-1.5903034093	2.1191322923	-1.5105105664
C	-2.8691537924	-4.821775098	-0.7277974958
C	4.226122411	-2.0215514797	0.0476866011
C	-0.2229752258	3.2364864936	-0.311491585
H	-2.9774934415	-4.0969345897	1.2927616579
H	2.746067975	-0.6401329129	-0.6374990091
H	-0.379353938	1.1317816637	-0.6937122864
H	1.4213644087	-2.2584285782	1.1801669867
H	1.0722640037	1.1914328771	1.2791708197
N	-2.1962660946	-5.6959648487	-1.5022377255
N	3.3145297417	-2.8842685427	0.5416988865
N	0.8233457055	3.1236153423	0.5344498067
C	-2.7550826739	-6.0021170197	-2.6792335032
C	3.7333359133	-4.1321574474	0.7974762953
C	1.5224350022	4.2380975137	0.7913405967
C	-3.9584512248	-5.4936158117	-3.1517879974
C	5.0238092101	-4.5935778907	0.5893343631
C	1.2546371644	5.4861945674	0.2506121175
C	-4.66886059	-4.5759109897	-2.3464431854
C	5.9910026137	-3.7007283974	0.073349155
C	0.1652407511	5.6203806469	-0.6406667529
C	-4.0846368805	-4.2495221301	-1.1036482129
C	5.5498684121	-2.3858426005	-0.1954680409
C	-0.5736335819	4.4469391663	-0.90861087
H	-2.2038680363	-6.714243223	-3.2941487592
H	2.9796396721	-4.8128367215	1.1905691966
H	2.3620468148	4.12331246	1.4760357268
H	-4.3394436565	-5.8147763394	-4.1147855503
H	5.2665356983	-5.6268914092	0.8084346622
H	1.885889017	6.3297883909	0.5048425479
N	-5.8633476868	-4.0339725868	-2.7472254242
N	7.2824122985	-4.0899216483	-0.1564606449
N	-0.1536285884	6.8210849122	-1.2142082285

H	-4.5645595114	-3.543187154	-0.4350149174
H	6.236319452	-1.6435863918	-0.5877164238
H	-1.4303944833	4.4753670348	-1.5725495348
C	-6.6757067638	-3.1534461072	-1.9086958438
C	8.2900149517	-3.2339585272	-0.7842338674
C	-1.2080998669	6.9892663383	-2.2151740885
C	-6.4560216566	-4.2636118057	-4.0634581513
C	7.8052633932	-5.41224604	0.1907111691
C	0.5191637346	8.0793481394	-0.8888690295
C	-7.5871821148	-3.2266788565	-4.1381709123
C	9.3236977874	-5.2575569836	0.0190997997
C	-0.3701427606	9.1467954506	-1.5444468407
H	-5.7138250726	-4.1244719016	-4.8594440458
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H	-6.8450898909	-5.2908955314	-4.1527503485
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H	1.5418582968	8.0996442031	-1.2977503824
C	-8.0066454772	-3.0556576892	-2.6693378673
C	9.4474460477	-4.1975536934	-1.0867764885
C	-0.9760164176	8.4102652264	-2.7497204581
H	-6.8025083629	-3.5744961961	-0.9038212859
H	7.8946719132	-2.7631579898	-1.6925557117
H	-1.1256063879	6.2307645317	-3.002972574
H	-2.2062910892	6.886456242	-1.760974023
H	-6.2031173408	-2.1649918321	-1.7933340635
H	8.6039836672	-2.4267984167	-0.1036095208
H	-1.1625745922	9.4492692955	-0.849673588
H	-7.198346393	-2.2797658319	-4.5314036127
H	9.7676641039	-4.8857154981	0.9501569735
H	0.1914063236	10.0433361692	-1.822820803
H	-8.406471176	-3.5482434984	-4.7881797106
H	9.8131623914	-6.2032541384	-0.2312661152
H	-0.2562191095	8.383792165	-3.5764018737
H	-8.6692692441	-3.8760215584	-2.3685523843
H	9.2996295311	-4.6594018296	-2.0701339435
H	-1.8958144132	8.8715567168	-3.1208976112
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C	-2.3910538961	-0.6902880246	1.5480392908
C	1.7933340226	-1.7255693369	1.5480392908
C	0.5977199797	2.4158575561	1.5480392908
H	-2.6583089259	-1.4245192223	2.3187513804
H	2.5628244069	-1.5899033831	2.3187513804
H	0.0954846252	3.0144228001	2.3187513804
H	-2.5001409509	0.297721956	1.9979805504
H	0.9922358075	-2.3140464878	1.9979805504
H	1.5079052495	2.0163247265	1.9979805504
C	-3.3412692657	-0.8651493971	0.3526123065
C	2.4198760982	-2.4610492998	0.3526123065
C	0.9213932738	3.3261988916	0.3526123065

H	-4.3701864811	-0.8732130307	0.734778679
H	2.9413180173	-3.3480859299	0.734778679
H	1.42886857	4.2212991552	0.734778679
C	-3.2166260843	0.1965279942	-0.7623936844
C	1.4381149159	-2.8839438339	-0.7623936844
C	1.7785112746	2.6874160344	-0.7623936844
H	-3.160515772	-1.8543618143	-0.0867695884
H	3.1861824343	-1.8099059737	-0.0867695884
H	-0.0256665562	3.6642679828	-0.0867695884
H	-3.7680468062	-0.1588424545	-1.6396597225
H	2.0215851132	-3.1838029628	-1.6396597225
H	1.7464617992	3.342645612	-1.6396597225
C	-3.7367878922	1.5627462755	-0.3693748974
C	0.5150160812	-4.0175263143	-0.3693748974
C	3.2217719172	2.4547802335	-0.3693748974
H	-2.1657210901	0.2810447229	-1.0658710893
H	0.8394687847	-2.0160917763	-1.0658710893
H	1.3262524116	1.7350472481	-1.0658710893
H	-0.7555865247	-1.8899705789	0.9357437804
H	2.0145559054	0.290628231	0.9357437804
H	-1.2589692745	1.5993425426	0.9357437804
N	-2.9431005328	2.3062751217	0.4344247736
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N	3.4688431068	1.3956623944	0.4344247736
C	-3.4162830799	3.5066891048	0.8144509235
C	-1.3287401987	-4.7119324195	0.8144509235
C	4.7450233848	1.2052435093	0.8144509235
C	-4.6409934084	4.0267686779	0.438934727
C	-1.1667871567	-6.0326024628	0.438934727
C	5.8077806714	2.0058339795	0.438934727
C	-5.4836952802	3.2613379749	-0.4057629708
C	-0.0825537872	-6.37968834	-0.4057629708
C	5.5662491735	3.1183505598	-0.4057629708
C	-4.9849319562	1.9948599465	-0.8007273312
C	0.7648666967	-5.3145076168	-0.8007273312
C	4.2200653657	3.3196478649	-0.8007273312
H	-2.7643839273	4.0922695564	1.4605371896
H	-2.161817322	-4.4401614184	1.4605371896
H	4.9262013555	0.3478920567	1.4605371896
H	-4.9315786229	5.0120239674	0.7827873369
H	-1.8747506594	-6.7768842853	0.7827873369
H	6.8063293885	1.7648605125	0.7827873369
N	-6.6963147071	3.7165106032	-0.8155249365
N	0.1295648671	-7.657433883	-0.8155249365
N	6.5667499462	3.9409234745	-0.8155249365
H	-5.5750136143	1.3477090135	-1.4392891403
H	1.6203566739	-5.5019578565	-1.4392891403
H	3.9546570466	4.1542490377	-1.4392891403
C	-7.5661972218	2.9983976955	-1.7554614182
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C	7.9577478414	3.8247378935	-0.357301143
C	-8.742516113	4.8980800582	-0.8525754345
C	0.1293964057	-10.0202810093	-0.8525754345
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H	-7.2270404261	5.0657987281	0.7334404759

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H	8.4368429091	2.9359896163	-0.7943187922
C	-8.6388644614	4.0345931037	-2.1194550311
C	0.8253722182	-9.4987725686	-2.1194550311
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H	5.8313981774	5.879138823	-1.2774958515
H	-8.0071825525	2.1105696164	-1.2774958515
H	2.1757844813	-7.9897082447	-1.2774958515
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H	-9.1730310306	5.8857250675	-1.0376856489
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H	8.1691505583	4.8639197994	-2.9648443119
H	-8.2968532781	4.6427320778	-2.9648443119
H	0.127702826	-9.5066516825	-2.9648443119
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H	1.7025225697	-10.0861455965	-2.4036341453

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C	-0.0025445192	0.037385866	0.2512287883
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N	-0.03610317	1.322663453	0.2694078124
C	1.2092709538	2.0656453745	0.2434769899
C	-2.4575407956	0.0235662255	0.2513139531
C	1.218075496	-2.0880032438	-0.2828348034
C	0.932292101	3.5622855654	0.0696989633
H	1.7846335618	1.920310371	1.1770602213
H	1.8772817876	1.7376110907	-0.5791454419
C	-3.6285433435	-0.9235164075	-0.015441764
H	-2.5711638551	0.5090822348	1.2340817638
H	-2.4389382211	0.8320572051	-0.4846311366
C	2.6641111407	-2.5878783734	-0.2962127395
H	0.6109643268	-2.7945903678	0.299679879
H	0.8075559166	-2.0881061926	-1.3043317664
C	2.2038214073	4.4141557492	0.052991908
H	0.367426917	3.7028329093	-0.8607568258
H	0.2688675257	3.88423333	0.8821809984
C	-4.9830196951	-0.2130247416	0.0661899868
H	-3.5000679191	-1.3798723742	-1.0053259276
H	-3.6077444034	-1.7492958048	0.7122934955
C	2.7953609139	-3.9937470487	-0.8886578563
H	3.2810346515	-1.8863755301	-0.8765960657
H	3.054285976	-2.5740144184	0.7298698886
H	1.9693409119	5.4774857782	-0.0703691436
H	2.7697821152	4.3064741391	0.9871919557
H	2.869907959	4.1251308716	-0.770262613
H	-5.8080647942	-0.9086732755	-0.1222281098
H	-5.140266676	0.2313991537	1.0564081744

H	-5.0510475614	0.5939305533	-0.6731970641
H	3.8395629253	-4.3238299257	-0.8903009798
H	2.2165247191	-4.7239570032	-0.310477423
H	2.4336420514	-4.0254794859	-1.9232434478
H	-1.1730395307	-1.5613348525	0.6663746025
H	1.9922615868	-0.2194888123	0.2087000257

TRIS:18H⁺

N	0.0162467398	-0.1425342269	-1.3404768472
C	-0.0006793129	-0.1495303098	0.0014599453
N	1.1534338916	-0.1357381065	0.6865189592
N	-1.1711603548	-0.1354051188	0.6577533874
C	1.2719751958	-0.0557912855	2.1500535435
C	1.2251567743	-0.0599477781	-2.1737888856
C	-2.4972388846	-0.0632374074	0.026365209
H	2.0070837733	-0.2758592403	0.1643765096
H	-0.862268042	-0.2831714631	-1.819477692
H	-1.146231055	-0.269196298	1.6590113309
C	2.7422517091	0.064575368	2.5590988128
H	0.7129465424	0.8204806375	2.5017810763
H	0.8321152288	-0.9527362813	2.6091759543
C	0.8459482992	0.0690553096	-3.6511706655
H	1.8094856481	0.8142665237	-1.8601297823
H	1.8421836769	-0.957980232	-2.0261616878
C	-3.5884033096	0.0797509056	1.090338465
H	-2.5184334708	0.8015677881	-0.6487263226
H	-2.676033385	-0.9698846026	-0.5693626896
C	2.9071754556	0.1501088815	4.0793488216
H	3.2927839856	-0.8047994705	2.1749924527
H	3.1713138057	0.9563927874	2.0847640377
C	2.081010366	0.1601781788	-4.552284995
H	0.2380612999	-0.7982436904	-3.9421678502
H	0.2210835655	0.9619719634	-3.7808778511
C	-4.9862930473	0.1492980374	0.4680956646
H	-3.5320989805	-0.7741489141	1.7790049189
H	-3.3946165409	0.9853142848	1.6791885319
H	3.9653875994	0.2306387779	4.3430343192
H	2.394889381	1.0280307759	4.4883680888
H	2.5073459255	-0.7406781253	4.5766138621
H	1.7810958769	0.2530262156	-5.5997930929
H	2.69373992	1.033732483	-4.3033849532
H	2.7088682278	-0.7334388699	-4.4639899189
H	-5.7454850958	0.2481890517	1.2488855813
H	-5.0833135777	1.0113028043	-0.2012342569
H	-5.2149657186	-0.7557941412	-0.1055545558

S12. Cartesian coordinated for the „open chain“ TRIS series of bases and their conjugated acids.

TRIS:1_oc

C	6.656409429	-3.0703174697	-0.2501961168
N	5.2277901653	-3.3043300425	-0.0975676407
C	4.48968943	-2.0404658253	-0.0426706596
C	2.971510434	-2.20329479	-0.1562296858
C	2.249995754	-0.8619126659	-0.3241609344
N	0.8158659446	-1.0701555861	-0.3972797041
C	0.0479984368	-0.0373656416	-0.3924981982
N	-1.3342040553	-0.1951305177	-0.2956965712
C	-1.8797135098	-1.549508146	-0.320414297
C	-3.3879358306	-1.5210070463	-0.0625515844
C	-3.9851889716	-2.9321192589	-0.0407630941
C	4.9673732496	-4.1606387962	1.0518272819
N	0.4847694583	1.2843590793	-0.3912154121
C	-0.3849558602	2.4497040232	-0.4421473607
C	0.4087918733	3.7234793247	-0.136663679
C	-0.4792974161	4.972557633	-0.1497565846
H	-1.0212646319	5.0036879509	-1.1038865989
H	2.5210912594	-0.1914365912	0.512629175
H	2.6373266121	-0.3725101897	-1.240903108
H	2.5580410525	-2.6952969313	0.7317509482
H	2.7396905139	-2.846498842	-1.0132970927
H	4.736458695	-1.4698142821	0.8787869943
H	4.8404460998	-1.4290494678	-0.8853244271
H	1.4014877506	1.4147153371	-0.7971483455
H	-1.3607396614	-2.1225931827	0.4527737066
H	-1.6592390552	-2.0552795962	-1.2738079961
H	-3.5698093473	-1.0010703659	0.8853591666
H	-3.8994271257	-0.9456732329	-0.8475677141
H	-1.1741474428	2.3150005531	0.3059973714
H	-1.8655500041	0.4593963031	-0.85907452
H	-0.8838722862	2.5596530141	-1.4232822089
H	0.8975813086	3.5944759083	0.8355321861
H	1.2030691614	3.8586570236	-0.8834648915
N	0.2745606251	6.2208894254	-0.0408168791
H	-1.2500290825	4.8886976862	0.6454807515
H	5.5293457539	-5.0949487295	0.9438227226
H	5.2606966313	-3.6959072283	2.0157871252
H	3.9056166858	-4.4150307149	1.1072633272
H	7.1785177589	-4.0282213162	-0.3542649271
H	6.8419565934	-2.4826321111	-1.1561942528
H	7.1086669152	-2.5291020683	0.6061804525
N	-5.4481755022	-2.948349253	0.0034839403
H	-3.6835288426	-3.4504443172	-0.9599520112
H	-3.5454240703	-3.507098569	0.8010418642
C	-0.5536884356	7.3684437999	-0.3891863659
C	0.8774797151	6.4027266066	1.2742224111
H	0.0525149836	8.280401389	-0.3606352583
H	-0.9420567284	7.2512866515	-1.4068021467
H	-1.41579853	7.5124426899	0.2926138191
H	1.4465894704	7.338311351	1.2862151687
H	0.1297779108	6.4466141232	2.0918039593
H	1.5739137383	5.5889349017	1.4944701639
C	-5.9684169863	-4.2752687948	-0.2992049757

C	-5.9789370763	-2.4666282898	1.2724397626
H	-7.0737486952	-2.4809834997	1.2378321224
H	-5.6563688442	-3.0797237174	2.1384815663
H	-5.666297311	-1.4343177029	1.4530946787
H	-7.0633326175	-4.2435147168	-0.3264135083
H	-5.613612173	-4.5975016537	-1.2842545707
H	-5.6694743077	-5.0449155712	0.4407266602

TRIS:1_och⁺

C	-0.0000006102	-0.0000007684	0.7146284894
N	-0.6439679338	1.1775483552	0.709856985
N	-0.6978044035	-1.1464673916	0.709856985
N	1.3417705068	-0.0310832687	0.709856985
C	-2.1029346887	1.3488505281	0.64010283
C	-0.1166730596	-2.4956207511	0.64010283
C	2.2196059178	1.1467679179	0.64010283
C	-2.4547328161	2.8356714228	0.5685578075
C	-1.2283986616	-3.5436973138	0.5685578075
C	3.6831296472	0.7080235858	0.5685578075
C	-3.972649381	3.0582207458	0.4805883108
C	-0.6621737464	-4.9695262813	0.4805883108
C	4.6348212969	1.9113032304	0.4805883108
N	-4.3122410109	4.4660011487	0.3236237918
N	-1.7115515233	-5.9675114611	0.3236237918
N	6.0237907037	1.5015080074	0.3236237918
C	-5.6563517255	4.6370829136	-0.2246338134
C	-1.1876573206	-7.2170863679	-0.2246338134
C	6.8440072155	2.5800011492	-0.2246338134
H	-0.0865812523	2.0166243039	0.7843590428
H	-1.7031588316	-1.0832943401	0.7843590428
H	1.7897382534	-0.9333322689	0.7843590428
H	-2.4797385693	0.8284043814	-0.2501527149
H	0.522448465	-2.5617194106	-0.2501527149
H	1.9572882738	1.7333127241	-0.2501527149
H	-2.5689647853	0.8960745692	1.5263617242
H	0.5084574713	-2.6728266742	1.5263617242
H	2.0605054835	1.7767497999	1.5263617242
H	-1.9874151196	3.2883153721	-0.31404839
H	-1.8540586688	-3.3653102916	-0.31404839
H	3.8414719579	0.0769926144	-0.31404839
H	-2.0468340131	3.3382129416	1.454337698
H	-1.8675617848	-3.4417173476	1.454337698
H	3.9143939674	0.1035021009	1.454337698
H	-4.3473372479	2.5246186551	-0.4016076131
H	-0.0127168469	-5.0272144472	-0.4016076131
H	4.3600522643	2.502593487	-0.4016076131
H	-4.4689332811	2.6003080012	1.3620037698
H	-0.0174677268	-5.1703643739	1.3620037698
H	4.4863991774	2.5700540677	1.3620037698
H	-6.452394109	4.2500783432	0.4391541397
H	-0.4544803395	-7.7129770094	0.4391541397
H	6.906872618	3.462896361	0.4391541397
H	-5.7325398632	4.1242709791	-1.1890462844
H	-0.7054550891	-7.0266612634	-1.1890462844
H	6.4379931218	2.9023879792	-1.1890462844
H	-5.8452063407	5.7016702427	-0.3927682166
H	-2.0151896846	-7.9129329269	-0.3927682166

H	7.8603941947	2.211260379	-0.3927682166
C	-2.4483002357	-6.2134355586	1.5602706597
C	-4.1568431705	5.2270062986	1.5602706597
C	6.6051415757	0.986426955	1.5602706597
H	-4.3914754308	6.2782514969	1.3690961363
H	-4.8182390849	4.8694072777	2.3730707014
H	-3.1230338945	5.1838516444	1.9174718215
H	7.6328627532	0.6640018538	1.3690961363
H	6.6261496965	1.7380121292	2.3730707014
H	6.050863911	0.1126991864	1.9174718215
H	-3.2413891529	-6.9422556557	1.3690961363
H	-1.8079124421	-6.607421712	2.3730707014
H	-2.9278318469	-5.2965531359	1.9174718215

TRIS:2_oc

C	2.0761422673	7.0317828601	0.0114834012
O	2.3522790734	5.6507782968	-0.0268949338
C	1.1867670577	4.8634174434	-0.19719623
C	1.5883462688	3.3954448543	-0.2243607584
C	0.3965124168	2.4508420804	-0.4075682873
N	0.8574115327	1.0758284693	-0.4425662348
C	-0.0066929929	0.1236106699	-0.4296650803
N	-1.3927139744	0.2663559177	-0.501335967
C	-2.3147726037	-0.7037254034	0.0937018489
C	-3.726303067	-0.1175717492	0.1522793916
C	-4.7428371157	-1.0954851466	0.7296089293
O	-6.0049814605	-0.4588338895	0.7491688272
C	-7.0264279928	-1.2840417863	1.2666913714
N	0.4189049314	-1.1995073588	-0.3338420346
C	1.849168284	-1.4782222119	-0.4251606857
C	2.1129646928	-2.9663665291	-0.1926172221
C	3.5969549909	-3.3065047402	-0.2530537571
O	3.744550255	-4.7009846636	-0.0578658452
C	5.0921774453	-5.1159067403	-0.0900626613
H	-4.784588612	-2.0139865726	0.1172446634
H	-0.3260119237	2.6284916182	0.4145515091
H	-0.1324869381	2.7201175061	-1.3407979694
H	2.1064481417	3.1439716674	0.7083651954
H	2.3033783035	3.229886366	-1.0382191291
H	0.4749084025	5.0577334443	0.6261539387
H	0.6734373725	5.1436504552	-1.1353117058
H	-1.6932616592	1.2257979953	-0.3926897379
H	2.3489117016	-0.8688710962	0.3329628236
H	2.26026779	-1.1552845621	-1.3947928362
H	1.7154533686	-3.2668547103	0.7838837175
H	1.5930092946	-3.5706380124	-0.9496398924
H	-1.981530585	-1.0054560567	1.0979694178
H	-0.1522442399	-1.8497943754	-0.8621514425
H	-2.3355598186	-1.6158720936	-0.5188426313
H	-3.7288955545	0.7902593915	0.7703703803
H	-4.0479586557	0.1757624742	-0.8543043903
H	-4.44971204	-1.4006743998	1.7498308021
H	3.0298328595	7.5503980073	0.143811575
H	1.6063132436	7.383050021	-0.9225361778
H	1.4087065947	7.2943222579	0.8494895017
H	4.0228904274	-3.009752597	-1.2280375354
H	4.1511694515	-2.749714665	0.5230935056

H	-7.9536240727	-0.7058498825	1.2376751704
H	-7.1565900581	-2.1987542682	0.665630637
H	-6.8232025622	-1.5818165881	2.3083099471
H	5.1016971969	-6.1978102363	0.0677356072
H	5.566546183	-4.8923732028	-1.0599262659
H	5.688053379	-4.6341802582	0.7025842501

TRIS:2_ocH⁺

C	-0.0000004771	-0.000000732	0.4917695695
N	-0.6465771413	1.1761242929	0.4842326476
N	-0.6952662947	-1.1480150611	0.4842326476
N	1.3418420046	-0.0281114278	0.4842326476
C	-2.1060943806	1.344480948	0.4222369583
C	-0.1113088152	-2.4961723952	0.4222369583
C	2.2174017645	1.1516892512	0.4222369583
C	-2.4510077841	2.8315744973	0.3477286708
C	-1.2267129049	-3.5384229394	0.3477286708
C	3.6777192577	0.706846246	0.3477286708
C	-3.9571660228	3.0836929441	0.2862864574
C	-0.6919747653	-4.9688534596	0.2862864574
C	4.6491393567	1.8851583194	0.2862864574
O	-4.1337779066	4.4769064631	0.2388171334
O	-1.8102271238	-5.8184105971	0.2388171334
O	5.944003599	1.3415019379	0.2388171334
C	-5.4972869832	4.8648596747	0.1765748786
C	-1.4644499222	-7.1932207016	0.1765748786
C	6.9617354741	2.3283588307	0.1765748786
H	-0.0938361602	2.0146392704	0.5941923558
H	-1.6978120571	-1.0885848186	0.5941923558
H	1.791646786	-0.9260566479	0.5941923558
H	-2.4858829462	0.8199854374	-0.4638397075
H	0.5328119039	-2.5628311858	-0.4638397075
H	1.9530696109	1.7428435523	-0.4638397075
H	-2.5673991454	0.8954941806	1.313239343
H	0.5081775138	-2.6711806567	1.313239343
H	2.0592202003	1.7756842801	1.313239343
H	-1.987255906	3.2780935448	-0.5399021616
H	-1.8452856825	-3.3600615557	-0.5399021616
H	3.8325401571	0.0819658147	-0.5399021616
H	-2.0526384615	3.3514224414	1.2279943007
H	-1.876099092	-3.453348958	1.2279943007
H	3.9287361221	0.1019243205	1.2279943007
H	-4.3932767456	2.5973193236	-0.6044804679
H	-0.0527074928	-5.1033496142	-0.6044804679
H	4.4459828071	2.5060280945	-0.6044804679
H	-4.4571108526	2.6503176808	1.1710738163
H	-0.066688363	-5.1851307511	1.1710738163
H	4.5237977842	2.5348108742	1.1710738163
H	-6.0550792565	4.5183181539	1.0595924504
H	-0.885440025	-7.5030122199	1.0595924504
H	6.9405178502	2.9846918699	1.0595924504
H	-5.9868575048	4.4726946304	-0.7275306956
H	-0.8800397705	-7.4211186881	-0.7275306956
H	6.866895844	2.9484218616	-0.7275306956
H	-5.5137761496	5.9560418839	0.1480090344
H	-2.4011968522	-7.7530918431	0.1480090344
H	7.9149715705	1.7970477632	0.1480090344

TRIS:3_oc

C	2.0673510136	7.5041806935	0.0734306428
S	2.8248434207	5.8424808933	0.0849451031
C	1.325372254	4.8188895244	-0.1966315206
C	1.6895504723	3.333504553	-0.2295688618
C	0.4665173348	2.434198067	-0.4512536701
N	0.8800320399	1.0452967291	-0.4941303308
C	-0.0121191424	0.1197891129	-0.481601726
N	-1.3942385954	0.3041127039	-0.5541982272
C	-2.3402443481	-0.6211039891	0.074887562
C	-3.7511663235	-0.0257501752	0.0495878553
C	-4.7818731575	-0.9676363303	0.6765695281
S	-6.4518398002	-0.2056668523	0.6198654386
C	-7.4120898388	-1.5198018995	1.4483290871
N	0.3730451163	-1.2160881297	-0.3886113936
C	1.7939301254	-1.5403103767	-0.4718521235
C	2.0116927331	-3.0301365561	-0.1919367057
C	3.4940645757	-3.407084568	-0.2505498566
S	3.7057342621	-5.206140355	0.0533882911
C	5.5229099708	-5.3274175449	-0.0822158854
H	-4.8061107593	-1.9214535787	0.1355812818
H	-0.2648887206	2.6318210836	0.3579649362
H	-0.0294320147	2.7346133476	-1.3924249927
H	2.1719571894	3.0419358723	0.7109051181
H	2.4136693909	3.1391124191	-1.0291726615
H	0.6054308633	5.0215392323	0.6066606814
H	0.8639247016	5.122664995	-1.1448254143
H	-1.6595447675	1.2749958672	-0.4502673654
H	2.3126995544	-0.9249753446	0.2678094231
H	2.2158656163	-1.2644789458	-1.4512447851
H	1.6012406192	-3.2767375009	0.7944708368
H	1.4587537325	-3.63240855	-0.92728773
H	-2.0448337794	-0.8590750556	1.1080979522
H	-0.2156431311	-1.8450901464	-0.9236232501
H	-2.3495736588	-1.5698024844	-0.4773019412
H	-3.7547551696	0.928299756	0.5946818108
H	-4.0301949426	0.1957214855	-0.9878890828
H	-4.522077219	-1.1777823712	1.7210232523
H	2.872043763	8.2261100593	0.2364219327
H	1.592667604	7.7193715659	-0.8892994449
H	1.3311849827	7.6121721481	0.8765154527
H	3.9128515447	-3.1607467981	-1.2338465312
H	4.058400242	-2.84857972	0.5058579872
H	-8.4515360125	-1.183259583	1.48118857
H	-7.3645564893	-2.4597246988	0.8896263873
H	-7.0622579281	-1.6819272867	2.472651529
H	5.7872511067	-6.3756191482	0.0804702136
H	5.8687273311	-5.0279033556	-1.076563628
H	6.0200692379	-4.7174457642	0.6784832554

TRIS:3_och⁺

C	-0.0000007006	-0.0000009096	0.8736693387
N	-0.6180033196	1.1916455789	0.858680033
N	-0.7229955224	-1.1310301216	0.858680033
N	1.3409967403	-0.0606181861	0.858680033

C	-2.0653872383	1.4011928554	0.6977155235
C	-0.1807768278	-2.4892750024	0.6977155235
C	2.2461619644	1.0880794182	0.6977155235
C	-2.3467593709	2.8781620492	0.407932211
C	-1.319183604	-3.471435014	0.407932211
C	3.6659408732	0.593270236	0.407932211
C	-3.8441211955	3.1597831991	0.2480330965
C	-0.8143937617	-4.9089989678	0.2480330965
C	4.6585128555	1.7492130399	0.2480330965
S	-4.0785162457	4.9466593193	-0.0936577812
S	-2.2446763501	-6.0054290959	-0.0936577812
S	6.3231904941	1.0587670477	-0.0936577812
C	-5.8997517658	5.0028366368	-0.2203268962
C	-1.3827095741	-7.6107539813	-0.2203268962
C	7.2824592383	2.6079146157	-0.2203268962
H	-0.0612164001	2.0059467128	1.0806720352
H	-1.7065944504	-1.0559890718	1.0806720352
H	1.7678087489	-0.9499603699	1.0806720352
H	-2.4124052459	0.7783060347	-0.1349043548
H	0.5321679864	-2.4783580023	-0.1349043548
H	1.8802351579	1.7000492387	-0.1349043548
H	-2.5954649749	1.0876972825	1.6082582243
H	0.3557571706	-2.7915880019	1.6082582243
H	2.2397057026	1.7038879906	1.6082582243
H	-1.8165448804	3.1727615104	-0.5057266521
H	-1.8394214665	-3.1595555265	-0.5057266521
H	3.6559642453	-0.0132087128	-0.5057266521
H	-1.9521089758	3.4910715994	1.2294988876
H	-2.0473040421	-3.4361125214	1.2294988876
H	3.9994109163	-0.0549618068	1.2294988876
H	-4.2579383029	2.5712556604	-0.5798142811
H	-0.0978054087	-4.973111326	-0.5798142811
H	4.3557416099	2.4018529368	-0.5798142811
H	-4.3845066292	2.887910248	1.16296311
H	-0.3087521627	-5.2410500057	1.16296311
H	4.6932566901	2.3531370288	1.16296311
H	-6.3729331679	4.7035410935	0.7192415359
H	-0.8869213293	-7.8708933244	0.7192415359
H	7.2598523955	3.1673495022	0.7192415359
H	-6.2603242551	4.3748192512	-1.0400285875
H	-0.6585443196	-7.6090102241	-1.0400285875
H	6.918866473	3.2341882441	-1.0400285875
H	-6.1640590901	6.041805012	-0.4316020027
H	-2.1503289186	-8.3591350262	-0.4316020027
H	8.3143859071	2.3173272853	-0.4316020027

TRIS:4_oc

C	2.2415617184	7.5609469836	0.1065843064
P	2.9037729159	5.8505393459	0.1977639892
C	1.4518659279	4.7918564459	-0.2062645518
C	1.7708496025	3.2902285669	-0.2238026527
C	0.5241426433	2.4246031978	-0.4429845903
N	0.896257875	1.023914784	-0.4830367341
C	-0.0210654547	0.1239358858	-0.4584741924
N	-1.3997822641	0.3445987196	-0.5339837182
C	-2.3640046936	-0.5146164706	0.160552373
C	-3.7775990604	0.0487144592	-0.0057878664

C	-4.8369166429	-0.8133067875	0.6949134252
P	-6.5174358105	-0.0521036771	0.6410955029
C	-7.5481233853	-1.1861750648	1.6481055747
N	0.3292559485	-1.2198875188	-0.3562629997
C	1.7420776122	-1.5809661605	-0.4123578963
C	1.9077376701	-3.0907812	-0.2234816004
C	3.3844517619	-3.5113661237	-0.2080412213
P	3.6142253657	-5.3243659087	0.0383852707
C	5.4334511913	-5.5292169824	0.1571652608
H	-4.8761652944	-1.8232813446	0.2644567804
H	-0.1997509722	2.6468575995	0.3656894172
H	0.0360915401	2.7376043846	-1.3847846188
H	2.2431928525	3.0011512964	0.721284597
H	2.4907675718	3.0574720917	-1.0181175097
H	0.6966046963	5.0068711086	0.5624021056
H	1.0279043241	5.1165218018	-1.1673504786
H	-1.6304565677	1.3271606048	-0.4512707675
H	2.2546785127	-1.0329156214	0.3834606591
H	2.206782683	-1.2547808799	-1.3565145899
H	1.4323957597	-3.4027408926	0.7126669777
H	1.3821371325	-3.6183222058	-1.0339095839
H	-2.1209568755	-0.6192648781	1.2295303221
H	-0.269458927	-1.8367000807	-0.8940071306
H	-2.3303107096	-1.5231608825	-0.2684797586
H	-3.8260866851	1.0645189933	0.4073109047
H	-3.9988013958	0.1322237498	-1.0775384357
H	-4.5827181357	-0.9269009473	1.757104573
H	3.0594069758	8.2726939187	0.2567500383
H	1.7608245263	7.7665783669	-0.8560623189
H	1.5112395373	7.7066085838	0.908611373
H	3.8929035811	-3.2052405977	-1.1328012723
H	3.9023119569	-3.0109151455	0.6207477025
H	-8.5924838035	-0.8617739174	1.6038931393
H	-7.4806613999	-2.2217493038	1.2971999998
H	-7.2198386014	-1.1395961755	2.6910614391
H	5.6751720427	-6.5955604681	0.2073562693
H	5.9540280074	-5.0843892895	-0.6979321124
H	5.7884473942	-5.0552523629	1.0774782534
O	2.8482135773	-5.8879399523	1.2019962891
O	-6.5401047746	1.3812335878	1.092023152
O	3.5691774781	5.5197354126	1.5041163005
C	3.1834744957	-6.0847045967	-1.5776253755
C	-7.1113962323	-0.306865399	-1.0773678287
C	4.0149598134	5.7263174576	-1.2595649413
H	4.8558811117	6.4139789313	-1.1258722371
H	4.4136743838	4.7100289298	-1.3278541483
H	3.4972235046	5.971367875	-2.1933974652
H	3.3746544149	-7.1610430793	-1.5253076981
H	2.1180437999	-5.9399028457	-1.780129642
H	3.7658844967	-5.6577722518	-2.4012797444
H	-8.1407311543	0.0572059087	-1.1536570987
H	-6.495179525	0.2745140498	-1.7697263664
H	-7.0832910379	-1.3617150288	-1.3713948497

TRIS:4_och⁺

C	0.0048362773	-0.0007069293	0.4798773294
N	-0.6002068031	1.1977552447	0.4573211405

N -0.7310455774	-1.1234890646	0.4706395618
N 1.3452423591	-0.0762560128	0.4603985636
C -2.0524532399	1.4207699722	0.3724519683
C -0.2027342722	-2.4943735513	0.3839170751
C 2.2648862797	1.0684823117	0.3616929156
C -2.3270617017	2.8999439588	0.0919694057
C -1.3497102704	-3.4649598692	0.0932199911
C 3.6832714796	0.5626672801	0.0896339937
C -3.8219236949	3.24619827	0.1226996942
C -0.9149685274	-4.9358843576	0.1388767356
C 4.7298901851	1.6849570804	0.1055996136
P -4.0439466176	5.0927183616	0.1504502777
P -2.4131417383	-6.0378707889	0.1176814853
P 6.4406658764	0.9561151417	0.1366261618
C -5.7779696942	5.3350339618	0.6736035686
C -1.7910141803	-7.6616502401	0.6800234282
C 7.5153439757	2.3432050999	0.6476977696
H -0.0358152461	2.0054521857	0.6857098078
H -1.7105764034	-1.0360588861	0.7073148552
H 1.7619142807	-0.9660460362	0.7007253298
H -2.4523548299	0.7920537409	-0.4317230064
H 0.5456961076	-2.5265710584	-0.4164303546
H 1.921662162	1.7189616387	-0.451195497
H -2.5337395485	1.122401954	1.3148890164
H 0.2903117178	-2.767372797	1.3278489128
H 2.2465021706	1.6465186201	1.2968358117
H -1.8928064924	3.1644786545	-0.8803421472
H -1.7824914963	-3.2228397101	-0.8855830942
H 3.6963531628	0.039321002	-0.8745853164
H -1.8251989526	3.5187832911	0.8471497153
H -2.145942255	-3.3298182494	0.8366917778
H 3.9682365842	-0.1699043543	0.8558291725
H -4.3659968073	2.7963125704	-0.7169444577
H -0.227114867	-5.1883570325	-0.6776516322
H 4.6093907173	2.3734639868	-0.7399646604
H -4.2732478724	2.8642259007	1.0477831815
H -0.3919794522	-5.1399015063	1.0824343887
H 4.6265664903	2.2751666933	1.0256536577
H -5.8949772572	4.9990044652	1.7083714149
H -1.4797687768	-7.5877221164	1.7264515037
H 7.2821190941	2.6216366489	1.6798884291
H -6.4786002775	4.7868597992	0.0343955435
H -0.9455304114	-8.0070541958	0.075229134
H 7.3887498314	3.2176117755	0.0001652776
H -6.0205265909	6.4014072063	0.632406678
H -2.5973954042	-8.3987183911	0.6157330838
H 8.5608506542	2.0220348511	0.6094147607
O -3.0073921215	5.7424236561	1.0236431372
O 6.4872650942	-0.2591086536	1.0197507192
O -3.5213844771	-5.447295601	0.9435821837
C 6.8733312045	0.6445277352	-1.6161561327
C -2.8224204686	-6.2756829918	-1.6522031574
C -4.0014477431	5.6165431735	-1.6046200417
H -3.6774074282	-6.9547692233	-1.7272986807
H -3.1120012276	-5.320476738	-2.1009649594
H -1.983051748	-6.6988300478	-2.2142401535
H -4.1703229104	6.6967382573	-1.6539284893
H -3.0150418911	5.4113988505	-2.0320274374

H	-4.7664345242	5.1101335912	-2.2028053601
H	7.894050297	0.2523327694	-1.6622637079
H	6.2041118338	-0.1116415506	-2.0380362064
H	6.8158512025	1.555655253	-2.2211176797

TRIS:5_oc

C	1.9640552571	7.4201572006	0.209261624
S	2.8422261529	5.8113745295	0.0751142026
C	1.3295421285	4.7926383184	-0.2288420966
C	1.6912982831	3.31007004	-0.2851801558
C	0.4632625317	2.4121439555	-0.4788798302
N	0.8781411844	1.0246128579	-0.5457425367
C	-0.0139297836	0.0990889646	-0.5414731607
N	-1.3967250931	0.2848741616	-0.6071459044
C	-2.3396931028	-0.6420108833	0.0247116727
C	-3.7565370294	-0.0671142304	-0.0488390361
C	-4.7875015628	-0.9880489966	0.6005658359
S	-6.4484687771	-0.167455743	0.576840497
C	-7.2795847044	-1.3869998692	1.6691616671
N	0.3734376347	-1.2368399218	-0.4702547377
C	1.7961725407	-1.5532995167	-0.5407027397
C	2.010140276	-3.0555585063	-0.3390007408
C	3.4931280905	-3.4221933952	-0.3349937319
S	3.6905732285	-5.2414532312	-0.0619053894
C	5.5166414173	-5.2070377202	0.1325465152
H	-4.8869060508	-1.9415115296	0.0672808146
H	-0.2436536019	2.6005976347	0.3529551496
H	-0.0610697768	2.7204992947	-1.402456513
H	2.1999753068	3.026848501	0.6425965614
H	2.3941959675	3.1198848872	-1.1057343673
H	0.6295716919	5.001633886	0.5899152374
H	0.8897599982	5.1460739399	-1.1706650997
H	-1.6589509643	1.2547228727	-0.4837972542
H	2.2982001626	-0.9818111658	0.2447172642
H	2.2393309469	-1.2206022367	-1.4926720251
H	1.5643855636	-3.3704852029	0.6107820969
H	1.4986399855	-3.6159629011	-1.136339198
H	-2.0673153462	-0.849248012	1.0709019732
H	-0.2096531819	-1.8593372966	-1.0185404262
H	-2.3179764156	-1.6038146386	-0.5030153441
H	-3.7940819429	0.9014207265	0.466496393
H	-4.0179282135	0.1149522709	-1.0993407565
H	-4.5310930359	-1.188604002	1.6476550498
H	2.7170078736	8.1780293792	0.4388941332
H	1.4747227351	7.6590356039	-0.7401495855
H	1.2345732729	7.3710651515	1.0231137024
H	3.980806401	-3.185108036	-1.2888689935
H	4.0217061839	-2.9040230257	0.4738390518
H	-8.3127072157	-1.0543279318	1.7948131939
H	-7.2630988463	-2.3766882477	1.2021990951
H	-6.7792415292	-1.4043567592	2.6417394683
H	5.8382881951	-6.2319769313	0.332420278
H	5.9818497632	-4.8451320284	-0.7896224021
H	5.7805650778	-4.5680242021	0.9802929854
O	3.0901825493	-5.5636875914	1.2899292497
O	-6.3117408712	1.1262350702	1.3510058972
O	3.3583976449	5.4602515061	1.4543134157

TRIS:5_ocH⁺

C	0.0021430975	-0.0037180557	0.4777925482
N	-0.6486266567	1.1704293229	0.4602036634
N	-0.6896755904	-1.1543104369	0.4667314349
N	1.3444871776	-0.026868436	0.4608649247
C	-2.105802772	1.3414889816	0.3449352548
C	-0.1101679744	-2.5020366592	0.3491207915
C	2.2193822979	1.1504067866	0.3403948606
C	-2.4190205238	2.8084887935	0.0451011418
C	-1.2257229615	-3.5074754061	0.0576039834
C	3.6492648601	0.6898337753	0.052422324
C	-3.9163860141	3.1111108443	0.0589450893
C	-0.737418763	-4.9548889072	0.0643575912
C	4.6548318736	1.8398115393	0.0584350597
S	-4.1052536688	4.9671650156	-0.0119932176
S	-2.248323819	-6.0471828186	-0.0283516606
S	6.3616283557	1.0846494796	-0.0046818085
C	-5.8389962607	5.0123436596	0.5807625129
C	-1.4270786924	-7.5716228173	0.5723266143
C	7.2576573878	2.5759893125	0.5720838445
H	-0.1163504278	1.999375029	0.6890589292
H	-1.6725169695	-1.1067143938	0.7004775995
H	1.7965510575	-0.9007559251	0.694860692
H	-2.4665945262	0.694015137	-0.4625191967
H	0.6248881006	-2.4919981188	-0.4637600527
H	1.8413593549	1.7791563031	-0.4740653572
H	-2.596205223	1.0345906564	1.2795756477
H	0.4077852755	-2.7716334207	1.2805192953
H	2.1925587485	1.7362112416	1.2702076541
H	-1.9840684141	3.0818530683	-0.9245452531
H	-1.6876476363	-3.2667631443	-0.9082929295
H	3.6746836475	0.1668266868	-0.9119608254
H	-1.9547520419	3.4488443389	0.8073499951
H	-2.0067315421	-3.4271105743	0.8255427674
H	3.9709053687	-0.023609973	0.8231580344
H	-4.4506189175	2.6766028136	-0.7929101739
H	-0.0868728206	-5.1921847195	-0.7845172979
H	4.5426785805	2.5114828431	-0.7994948908
H	-4.3761821571	2.7652798699	0.9919887596
H	-0.2156237983	-5.1874701935	0.9997786364
H	4.5812366093	2.4187783533	0.9863005827
H	-5.8917823641	4.5970511572	1.5910712739
H	-1.0498857577	-7.4083929429	1.585777139
H	6.9251516829	2.8351068379	1.5811980048
H	-6.4770644787	4.4542935144	-0.1115006072
H	-0.6189847986	-7.846830535	-0.1125398808
H	7.0839257038	3.400053077	-0.1268351558
H	-6.1437699803	6.0612615182	0.5985215271
H	-2.1839234797	-8.3593220003	0.5844770831
H	8.3206886666	2.3248235295	0.5887495615
O	-3.2119720314	5.5007988371	1.0880969942
O	6.3845533866	0.0563211061	1.1065179338
O	-3.1723749076	-5.5436049159	1.0601765577

TRIS:6_oc

C	2.1395795046	7.523859729	0.0846422331
S	2.7955929406	5.835455347	0.0726402483
C	1.3119845031	4.8099086117	-0.1852517393
C	1.6810156969	3.3258937404	-0.2244750585
C	0.4521533862	2.4343377796	-0.4460758253
N	0.868896203	1.0481390608	-0.494672269
C	-0.0185920015	0.1184762513	-0.4836021987
N	-1.4009338522	0.2938601638	-0.5524245928
C	-2.3388143238	-0.6411792093	0.0724567567
C	-3.7483952522	-0.0435004468	0.0570193348
C	-4.7704603873	-0.9914586986	0.6873547137
S	-6.4253840491	-0.2234803438	0.6551334328
C	-7.4797563256	-1.4561984454	1.4561470092
N	0.3752439836	-1.214989331	-0.3948097614
C	1.7993813372	-1.5239603471	-0.4647131609
C	2.0191794181	-3.013577164	-0.1870250859
C	3.5054921668	-3.3743262546	-0.2314134047
S	3.7225988719	-5.1626011994	0.0431476902
C	5.5146797248	-5.3929626839	-0.0616214117
H	-4.8450723572	-1.9347273681	0.1361428381
H	-0.2767790526	2.6291466787	0.3657560266
H	-0.0446889967	2.7385957677	-1.3853556261
H	2.166114889	3.0415370721	0.7148756319
H	2.4016136277	3.1457166856	-1.0284504512
H	0.626874869	5.0388818281	0.6387168605
H	0.8616763216	5.142145745	-1.1273226796
H	-1.6768196501	1.2624893114	-0.4563711152
H	2.3045748325	-0.9071660711	0.2831090106
H	2.2293665925	-1.2419434782	-1.4386869561
H	1.6098709223	-3.2725460165	0.7949366316
H	1.4908313003	-3.6223158659	-0.9321816147
H	-2.0372025722	-0.8869632895	1.1019189105
H	-0.2018273305	-1.8463703629	-0.9398717223
H	-2.3487227992	-1.5845158328	-0.4887563121
H	-3.7589385534	0.9028632189	0.6120543656
H	-4.0452063209	0.1767064954	-0.9742189994
H	-4.5361165757	-1.2026777768	1.7359205546
H	2.9987108983	8.1795033077	0.2452473041
H	1.6757333324	7.7437642363	-0.8791697084
H	1.4265768018	7.6342974348	0.9043490276
H	3.9495216189	-3.1462935395	-1.2063512109
H	4.0714399275	-2.8585016396	0.5513070977
H	-8.4860086343	-1.030401037	1.4647929062
H	-7.4693443191	-2.3802354193	0.8743865581
H	-7.1356593955	-1.6236876927	2.4788689019
H	5.6913384255	-6.4583350179	0.1046206337
H	5.8635671693	-5.1060833197	-1.0557765477
H	6.0054365197	-4.8063071769	0.7177854283
O	3.308631203	-5.4677050518	1.4227768842
O	-6.3841113849	0.967668037	1.5193446686
O	3.3228904079	5.5530341149	1.4181892619
O	3.109559267	-5.8723867634	-1.0926076925
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O	3.6603975877	5.7013069335	-1.1114696729

TRIS:6_och⁺

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N	-0.6600508321	1.1734605676	0.9484047101
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N	1.3361843305	-0.0182083128	0.9531573378
C	-2.1092593791	1.3456244168	0.7582302815
C	-0.1155083525	-2.4917772481	0.7622495291
C	2.2113224989	1.1501499277	0.7655088638
C	-2.3985485546	2.814949008	0.4444115796
C	-1.2395106156	-3.4826526954	0.45278138
C	3.6274763351	0.6658257279	0.4484073762
C	-3.8902448295	3.0942122692	0.2439713352
C	-0.7252915717	-4.9097914884	0.2480727174
C	4.6155027781	1.8184149044	0.2531864846
S	-4.0666109757	4.8885651665	-0.0965600723
S	-2.1826308268	-5.9730297619	-0.0880783401
S	6.2559158595	1.0755333344	-0.098825331
C	-5.8413722622	5.1246095979	-0.318156853
C	-1.4829278726	-7.6192794563	-0.3223710969
C	7.3458466914	2.4962201017	-0.3195082725
H	-0.1312593319	2.0037473061	1.1803473924
H	-1.6767495392	-1.1086977358	1.1822408446
H	1.7894809057	-0.8912994726	1.187839731
H	-2.4263664891	0.7046988975	-0.0724714796
H	0.5964259826	-2.4463167954	-0.0698436791
H	1.8145843665	1.7483197996	-0.0628559576
H	-2.649308802	1.0340649904	1.6633080143
H	0.4272957074	-2.7993601872	1.667066193
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H	-1.7705379076	-3.1649403396	-0.451284215
H	3.6111064512	0.0554017671	-0.4612414423
H	-2.0386772885	3.4457187219	1.2669799946
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H	4.3482798188	2.4518269902	-0.598530404
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H	-6.1850157503	4.5331811411	-1.1692392053
H	-0.8013408795	-7.6083157272	-1.1753722861
H	6.9976977274	3.0956021261	-1.1631518536
H	-5.9766449636	6.1895294069	-0.5239397781
H	-2.3311586501	-8.2765778011	-0.5300882819
H	8.3337755503	2.0824366209	-0.5372715966
O	-3.6456439035	5.5903392112	1.1254436061
O	6.6592129226	0.3540940737	1.1176884219
O	-2.9931894793	-5.9741809962	1.1391142985
O	6.1322737341	0.3714681908	-1.3839151568
O	-2.7524945009	-5.5170314295	-1.3646290352
O	-3.3931648897	5.1427129773	-1.3788913881

TRIS:7_oc

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C	-1.3500676445	4.6409679408	-1.7195515245
C	-1.8151222483	3.2283399535	-2.0860865487
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C	-1.3893628423	1.6213912517	-3.7641420858
N	-2.1509371936	0.6305859697	-3.1443633769
C	-1.8362305594	-0.7947650515	-3.2633439099
C	-2.6147227274	-1.5935618014	-2.2173205343
C	-2.3553285633	-3.0965295989	-2.3177791175
C	-3.0777361501	-3.9095786451	-1.2463748194
C	-2.9457568929	-5.4204011787	-1.3378181554
N	-0.745490109	1.1957411814	-4.9240844357
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C	2.0787691384	1.8867244887	-9.0042756905
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H	-2.343789832	-1.2519725933	-1.210383029
H	-3.6875609181	-1.397532517	-2.3289574083
H	-1.279324746	-3.3143858635	-2.2351101088
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H	2.3204912298	3.6624673929	-10.222081254
H	3.7487659834	3.2318262652	-9.2844245236
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O	-3.7252836094	-3.3750535677	-0.366413653
O	-0.624403724	7.1394799551	-0.6163342548

TRIS:7_och⁺

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N	0.7971866767	-1.0797024208	0.5461477769

C	-0.2129697246	2.4893383001	0.4088913682
C	-2.049345447	-1.4291063175	0.4088913682
C	2.2623149963	-1.0602320352	0.4088913682
H	-0.8117491514	2.6694268456	1.3133818269
H	-1.9059169891	-2.037708785	1.3133818269
H	2.717665965	-0.6317181132	1.3133818269
H	-0.8986887701	2.3928669083	-0.4417196292
H	-1.6229392483	-1.9747207348	-0.4417196292
H	2.521627843	-0.4181462261	-0.4417196292
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C	-3.5370541043	-1.1599253312	0.1831002729
C	2.7730517525	-2.4832160189	0.1831002729
H	1.4712549868	3.6990967343	1.0195853469
H	-3.9391393392	-0.5754041488	1.0195853469
H	2.4678841771	-3.1236926381	1.0195853469
C	0.062476072	4.9946315505	0.0412565896
C	-4.3567159442	-2.4432098854	0.0412565896
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H	1.3603432649	3.4479835893	-0.7152409684
H	-3.6662131155	-0.5458999451	-0.7152409684
H	2.3058696752	-2.9020836969	-0.7152409684
H	-0.6287335525	4.9991785375	-0.8135619937
H	-4.0150489382	-3.0440884731	-0.8135619937
H	4.6437823152	-1.955090117	-0.8135619937
C	1.0716302201	6.135916371	-0.1378465311
C	-5.8496746657	-2.1398991671	-0.1378465311
C	4.7780442702	-3.9960172565	-0.1378465311
H	-0.5555468919	5.2173150543	0.923327601
H	-4.2405540336	-3.0897752242	0.923327601
H	4.79610075	-2.1275398828	0.923327601
H	1.5259283932	1.30909552	0.737851452
H	-1.8966742758	0.6669450172	0.737851452
H	0.3707457072	-1.9760405898	0.737851452
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O	-6.2523212574	-0.9932784952	-0.1107863468
O	3.9863649357	-4.9180297696	-0.1107863468
C	0.5046278226	7.5235054412	-0.3467453957
C	-6.7678608518	-3.3247321824	-0.3467453957
C	6.2632328537	-4.1987733114	-0.3467453957
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H	6.5876322253	-3.7089080528	-1.2736005042
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H	-7.8028401645	-2.9836402538	-0.4052825944
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TRIS:8_oc

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H	-6.2475608836	5.5234062017	1.986835203
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H	-4.9133243635	5.1374929426	0.8856147158
H	-1.9925367761	-6.8238115566	0.8856147158
H	6.9058629889	1.6863169427	0.8856147158
H	-8.114906808	2.4413862612	1.0630344895
H	1.9431513235	-8.2484099452	1.0630344895
H	6.1717573338	5.8070220127	1.0630344895

TRIS:9_oc

N	-0.3548920736	6.7309473373	-0.995994566
C	0.5229762936	5.7430023758	-0.6423109371
C	-0.0458226496	4.3256218969	-0.5664792949
C	1.0304243145	3.2690417523	-0.3163096011
C	0.455040202	1.8528771462	-0.2160260341
N	1.5233012234	0.896204175	-0.002061584
C	1.2332788784	-0.3087133554	0.3417241239
N	-0.0443673998	-0.8639087065	0.4160053584
C	-0.3803479658	-1.9319561631	1.3613703925
C	-1.8977816185	-2.0443662303	1.51287939
C	-2.3016433504	-3.1545807496	2.4836279881
C	-3.8188251641	-3.2277863414	2.6715525999
N	-4.2839510886	-4.2338955301	3.4673315255
N	2.2491399272	-1.1961298956	0.689792196
C	3.6360499809	-0.7788321124	0.5105957834
C	4.5855977534	-1.8419278105	1.0630546747
C	6.0494715797	-1.4141249151	0.9522209981
C	7.0103327387	-2.491548422	1.4564359784
N	8.3414933946	-2.1891184496	1.4069013564
H	-1.9297901653	-4.1278348702	2.132704039
H	-0.2973491531	1.8343474068	0.5993217359
H	-0.1024008394	1.6264235826	-1.1444565156
H	1.5749693715	3.504522049	0.6036195775
H	1.773883004	3.2955437872	-1.1201316184
H	-0.5943249429	4.105431382	-1.4942006421
H	-0.8022673866	4.2960324235	0.2333212077
H	-0.7773968576	-0.1750769833	0.3108562656
H	3.7597714931	0.1713654418	1.038234639
H	3.8600900189	-0.5678434195	-0.5478366762
H	4.342087003	-2.0483175398	2.110885161
H	4.4525073402	-2.7918567711	0.5290229677
H	0.0906524893	-1.7551522383	2.3400289987
H	2.0722284352	-2.15214593	0.4017241686
H	0.0139498566	-2.8900898318	0.9931835704
H	-2.3091468045	-1.0927314366	1.8707373349
H	-2.3567991617	-2.2268753574	0.5346385748
H	-1.8277725988	-2.9920102369	3.4627648052
H	6.3012786929	-1.1676770361	-0.0899691053
H	6.2145949843	-0.4874275421	1.520285979
O	6.618003285	-3.5759538863	1.8836233678
O	-4.5832384724	-2.4247048032	2.1401440243
O	1.6997964906	5.9994863548	-0.3984460919

C	-3.4890889064	-5.2592002284	4.1538892045
C	-4.5028878751	-5.9138713065	5.1061088838
C	-5.8355696662	-5.7799784683	4.3493324301
C	-5.7292654159	-4.4008429168	3.6828862786
H	-3.087611735	-5.9936048611	3.4391318673
H	-2.6401112463	-4.8187737194	4.6875285654
H	-4.5451228193	-5.3512496801	6.0464013155
H	-4.2392777539	-6.948193048	5.3460766721
H	-6.7094671488	-5.8621414126	5.0021518284
H	-5.9148032679	-6.5633149673	3.585663235
H	-6.1095303475	-3.6003129233	4.3315558577
H	-6.2630292705	-4.3272744017	2.731472482
C	-1.7793351155	6.5779468249	-1.3108433423
C	-2.2922766998	8.0269797522	-1.344061763
C	-1.0664901409	8.8235293492	-1.8231644691
C	0.1068717924	8.1199003089	-1.1262890512
H	-1.9207917775	6.0875675688	-2.2862138597
H	-2.2945431376	5.9703753283	-0.5589594774
H	-2.5746951896	8.343607114	-0.3327400286
H	-3.1686922573	8.1439128167	-1.9887323293
H	-1.1228407397	9.8880440681	-1.5769828579
H	-0.9647018703	8.7372665954	-2.9119514079
H	0.3115600605	8.5477660394	-0.1352420048
H	1.0422814813	8.1541919656	-1.6915500173
C	8.9500743297	-0.950712781	0.9059808206
C	10.4184629163	-1.0763898324	1.342343546
C	10.6658630415	-2.5942797524	1.3164053533
C	9.3427551319	-3.1780872526	1.8325480188
H	8.8675561396	-0.8838020764	-0.1894432516
H	8.464454741	-0.0644095177	1.3280192653
H	10.5360655877	-0.6928348516	2.3629356267
H	11.0946133764	-0.5125552864	0.6927215211
H	11.523362657	-2.9003544645	1.9229598069
H	10.8486177346	-2.9277340042	0.2875021242
H	9.3366940527	-3.2762658971	2.9266370879
H	9.1013312799	-4.1608376291	1.4184429532

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C	-0.0183284582	-0.0057829449	-0.0312264947
N	0.4933029859	1.2345203893	-0.0485474986
N	-1.3482434538	-0.1838894195	-0.0398853685
N	0.8015280248	-1.0683058335	-0.041646124
C	-0.2802515393	2.481235111	-0.1568328238
C	-2.0372292003	-1.4799064565	-0.1404053531
C	2.2676749613	-1.0141869031	-0.1505120719
H	-0.8779035566	2.6302108569	0.7540822466
H	-1.8624549592	-2.0674067365	0.772543707
H	2.6923581593	-0.5554628279	0.7542585404
H	-0.9680102656	2.392800627	-1.0069905629
H	-1.6161371339	-2.0333499574	-0.988929415
H	2.5298171596	-0.3831537282	-1.0088944189
C	0.6806590088	3.6527555971	-0.3581446787
C	-3.5340039701	-1.2440673748	-0.3395450078
C	2.816411235	-2.4287586418	-0.3331119706
H	1.4009751501	3.6900897358	0.467039675
H	-3.9310480466	-0.6403530282	0.4844717333
H	2.5041103136	-3.0624722843	0.5047702208

C	-0.0335239348	5.0029341247	-0.4390886172
C	-4.3335731794	-2.5459187174	-0.4158866622
C	4.3428100424	-2.4626025023	-0.4261467098
H	1.2651679012	3.4953017533	-1.271164969
H	-3.6960967565	-0.6634590083	-1.2542763953
H	2.3871237008	-2.8762531907	-1.2362417206
H	-0.7194126252	5.0342870869	-1.2962473129
H	-4.0158402917	-3.1516420914	-1.2751152184
H	4.6952892184	-1.8929403484	-1.2964748615
C	1.0017324947	6.1332028791	-0.5512562743
C	-5.8345948664	-2.2325056895	-0.5187068455
C	4.8299644646	-3.917108262	-0.5183294391
H	-0.6528335466	5.1661173655	0.454316863
H	-4.153209424	-3.1626049211	0.4761599954
H	4.7938557296	-1.9844245796	0.4549518829
H	1.4861854399	1.3316534175	0.1141252688
H	-1.9293417787	0.6266056441	0.1252147835
H	0.3926880793	-1.9762032085	0.1324084727
O	2.206300011	5.892238835	-0.4733783672
O	-6.2436217228	-1.075551825	-0.4237244266
O	4.0380707208	-4.8537293229	-0.4161352492
N	0.51975475	7.3868661025	-0.7340837796
N	-6.6644951573	-3.2865842615	-0.7132749705
N	6.1587369406	-4.1025168002	-0.7128461207
C	-6.2842311415	-4.7017533577	-0.8425552262
C	-7.6315630057	-5.4388538502	-0.7708527101
C	-8.6218955849	-4.4292547989	-1.3758930167
C	-8.1180297443	-3.0784205107	-0.8506461483
H	-5.7833115816	-4.8855570115	-1.8045038459
H	-5.5989962259	-5.0071180098	-0.044152714
H	-7.8887929559	-5.6397656813	0.2756006484
H	-7.6072467659	-6.3956712941	-1.2995884327
H	-9.6590874044	-4.62539761	-1.0913362111
H	-8.5652278302	-4.4535081865	-2.4706315361
H	-8.5528848599	-2.8277740067	0.1253603553
H	-8.3131833656	-2.2384945326	-1.5220125129
C	-0.891186183	7.7903515001	-0.836160198
C	-0.8286836971	9.3229536256	-0.7336468749
C	0.5348759745	9.6649387791	-1.3578277252
C	1.4438593589	8.5281117771	-0.8717176834
H	-1.3191420253	7.4754800137	-1.7993576834
H	-1.4948545345	7.3434738819	-0.0386788333
H	-0.8482893618	9.6245376087	0.3200488072
H	-1.6714774439	9.8052604055	-1.2363640542
H	0.9058895372	10.6496023314	-1.0611719784
H	0.4641079177	9.650000156	-2.4519186577
H	1.9039755276	8.7537630876	0.098764502
H	2.2496939801	8.2755771654	-1.565455227
C	7.1881615457	-3.0611223768	-0.851288504
C	8.5043117905	-3.851014891	-0.7679991634
C	8.1350450968	-5.2195576911	-1.3651719937
C	6.7124982133	-5.4634236088	-0.8437361031
H	7.0965601079	-2.5468600588	-1.8194132177
H	7.1042414609	-2.3066007914	-0.0614365606
H	8.8029932064	-3.9640162684	0.2806563809
H	9.320225389	-3.3506406089	-1.2967548538
H	8.8268970403	-6.0140619801	-1.073129376
H	8.1312130346	-5.1651480333	-2.4602445561

H	6.7110875459	-5.9619657105	0.133931213
H	6.0880674096	-6.0577623501	-1.5154778396

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C	2.2767487508	5.8324773493	-0.1026199787
C	1.1503265222	4.8867119107	-0.3922530412
C	1.5453692876	3.3985434026	-0.3350250762
C	0.354701319	2.4611864022	-0.5615855871
N	0.8000122667	1.0813245671	-0.5668408658
C	-0.0673079978	0.1346665465	-0.4982227654
N	-1.4564210588	0.2803583508	-0.5456707081
C	-2.360950258	-0.6341600763	0.1585120804
C	-3.7897217704	-0.0886317085	0.1267023543
C	-4.7922071852	-1.0262413499	0.8287061236
C	-6.1885166057	-0.4823143437	0.8712422967
N	0.3568929062	-1.1853886192	-0.370507749
C	1.7837136652	-1.474524856	-0.4739835932
C	2.0417150481	-2.9680289121	-0.2721232503
C	3.5456037329	-3.308282046	-0.3116567167
C	3.828731103	-4.7685485348	-0.1218435425
H	-4.770882718	-2.0140782558	0.3474514846
H	-0.3989104535	2.6631004911	0.2255944767
H	-0.1290587256	2.7266177156	-1.5203180551
H	1.9944515665	3.1769534989	0.6399942525
H	2.3096614728	3.1697468516	-1.0884904687
H	0.3803435787	5.0924194828	0.358894397
H	0.7009346278	5.1092324709	-1.3718254577
H	-1.7387670828	1.2487924557	-0.4615321681
H	2.2965717089	-0.8877443115	0.2936529038
H	2.1942197053	-1.1372622616	-1.4395808403
H	1.6297719809	-3.2905518302	0.6909468449
H	1.5145363103	-3.5446590085	-1.0483416712
H	-2.0416766952	-0.8000788564	1.1985757915
H	-0.2300840553	-1.8506974338	-0.8609959432
H	-2.3470663236	-1.615263714	-0.3346977781
H	-3.8244680348	0.8896198467	0.6246600911
H	-4.0859918848	0.0760492882	-0.9178167596
H	-4.4840791569	-1.1738435949	1.8686926242
H	3.9818428316	-2.9501340984	-1.2538010753
H	4.0544049506	-2.7725511622	0.4963468273
N	3.8848411662	-5.6787383573	-1.1526172835
C	4.1293541095	-6.9144495571	-0.5799686369
C	4.1970385493	-6.6895792045	0.7700908778
N	4.0083857934	-5.3560305744	1.0477846025
H	4.3700029526	-7.4106048521	1.5580206016
H	4.2311948662	-7.8058833531	-1.1816245457
C	3.7992305861	-5.4053389191	-2.5774647693
H	3.6502580833	-6.346529624	-3.1109834203
H	2.9507795659	-4.7501751831	-2.7940097676
H	4.7147585699	-4.9324879253	-2.9516193836
N	-7.0902838602	-0.5706300236	-0.1657097791
C	-8.2359249213	0.0854969826	0.2476994656
C	-7.9705647245	0.5331082132	1.5152786494
N	-6.6987558301	0.1762711919	1.8965696595
H	-8.6252249207	1.0814664061	2.1794951919
H	-9.107169324	0.1548817322	-0.3872914495
C	-6.8921735648	-1.170094174	-1.4740489889

H	-7.8483272255	-1.5429834507	-1.8500493986
H	-6.4882046811	-0.447901964	-2.1934145369
H	-6.2021881995	-2.0136269841	-1.3985115824
N	3.2800895343	6.137894375	-0.9951646303
C	4.1373481369	7.0107231885	-0.3489121567
C	3.6056853887	7.1944418616	0.900211939
N	2.4505877377	6.4623987571	1.046258539
H	3.9821109723	7.8189063312	1.6997111942
H	5.0142710931	7.4076847764	-0.8395356504
C	3.4665160927	5.6181015563	-2.3384158566
H	3.9636169671	6.373022563	-2.9535504708
H	4.0741545995	4.7056145432	-2.3388129679
H	2.4971681584	5.3922860115	-2.7885869025

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N	-0.675823793	1.15914025	0.7274792686
N	-0.6659353234	-1.164851577	0.7274792686
N	1.3417564022	0.0057080024	0.7274792686
C	-2.1353323152	1.2979444392	0.6101142411
C	-0.0563890163	-2.4982251288	0.6101142411
C	2.1917186172	1.200277365	0.6101142411
C	-2.4873630174	2.7725729322	0.4157283331
C	-1.1574394013	-3.5404069064	0.4157283331
C	3.6447997044	0.7678306495	0.4157283331
C	-3.9978284773	3.0109499115	0.3066667664
C	-0.6086471911	-4.9676968558	0.3066667664
C	4.6064729541	1.9567436197	0.3066667664
C	-4.2835469494	4.4774422567	0.1508217169
C	-1.7358075805	-5.9483824836	0.1508217169
C	6.0193518155	1.4709369022	0.1508217169
H	-0.1516219411	2.0071185653	0.8944521
H	-1.6624070124	-1.1348686142	0.8944521
H	1.8140262391	-0.8722532758	0.8944521
H	-2.4745389533	0.7030766122	-0.2471192632
H	0.6283849528	-2.4945527811	-0.2471192632
H	1.8461512862	1.7914728442	-0.2471192632
H	-2.6219797421	0.9052919517	1.514702254
H	0.5269817262	-2.7233479195	1.514702254
H	2.0949953016	1.8180526432	1.514702254
H	-1.9962849231	3.1546707747	-0.4854505518
H	-1.7338848868	-3.3061697227	-0.4854505518
H	3.7301670956	0.1514956234	-0.4854505518
H	-2.098798218	3.3620969113	1.2543295102
H	-1.862264543	-3.4986619086	1.2543295102
H	3.9610600467	0.1365616727	1.2543295102
H	-4.4052268706	2.4474845688	-0.546407635
H	0.0830273065	-5.0387815426	-0.546407635
H	4.3221968498	2.5912936491	-0.546407635
H	-4.5041587436	2.6139223728	1.1999354025
H	-0.0116461235	-5.2076779598	1.1999354025
H	4.5158021528	2.5937522624	1.1999354025
N	-1.5524241596	-7.298538351	-0.005344426
C	-2.8136160211	-7.8565366816	-0.110855311
C	-3.6948990078	-6.8120627173	-0.0142657259
N	-3.015973507	-5.6257058725	0.1484606098
H	-4.7749709229	-6.8441299506	-0.0537562293

H	-2.9516438246	-8.9196447072	-0.2416583369
C	-0.2866905389	-8.0148194372	-0.0390583027
H	-0.4825204258	-9.0701147908	-0.2350550457
H	0.3586574216	-7.6294492909	-0.8353575769
H	0.2396982546	-7.9309170576	0.9179831719
N	-5.5445079401	4.9937054893	-0.005344426
C	-5.3971527389	6.3649288457	-0.110855311
C	-4.0519702588	6.6059053179	-0.0142657259
N	-3.3640178437	5.4247601646	0.1484606098
H	-3.53970534	7.557308651	-0.0537562293
H	-6.2488173942	7.0160184428	-0.2416583369
C	-6.7976923673	4.2556885625	-0.0390583027
H	-7.6136900086	4.9529298961	-0.2350550457
H	-6.786626011	3.5041157612	-0.8353575769
H	-6.9882251719	3.7578713052	0.9179831719
N	7.0969293854	2.304829537	-0.005344426
C	8.2107660457	1.4916045113	-0.110855311
C	7.7468665524	0.2061540747	-0.0142657259
N	6.3799886365	0.2009423832	0.1484606098
H	8.3146735486	-0.713182025	-0.0537562293
H	9.2004585046	1.9036229397	-0.2416583369
C	7.0843801919	3.7591275501	-0.0390583027
H	8.0962077201	4.1171815701	-0.2350550457
H	6.4279658751	4.125330205	-0.8353575769
H	6.748524203	4.1730424277	0.9179831719

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C	-1.1718262597	6.0457766251	-0.238197007
C	-0.2537704298	4.9107891282	0.1077448761
C	-0.9358948041	3.5333690098	0.0326562103
C	0.0234278091	2.3743096668	0.3192205815
N	-0.6889191257	1.1111040971	0.2862777173
C	-0.0218492047	0.0127837628	0.3412141544
N	1.3546544197	-0.1046405955	0.5466368673
C	2.1333109922	-1.2339096765	0.0311900976
C	3.6293989217	-0.9521900375	0.1752127211
C	4.5019243598	-2.1220180961	-0.312530663
C	5.9689611651	-1.8129076336	-0.2553451214
N	-0.6788940807	-1.2063118366	0.1931557029
C	-2.1385979424	-1.2153518972	0.1639137318
C	-2.6598189699	-2.6361886879	-0.0518301633
C	-4.1968045542	-2.6914594801	-0.1116459582
C	-4.7258052903	-4.0737421899	-0.3568934551
H	4.2948223815	-3.0183262766	0.2866489604
H	0.8465059175	2.4131260665	-0.422955319
H	0.4974133491	2.5406484876	1.3053454009
H	-1.375143955	3.3978360611	-0.9622103814
H	-1.7652167069	3.4879148211	0.749600639
H	0.6018445796	4.9264063988	-0.5819678171
H	0.1528963446	5.0689212713	1.1161032916
H	1.8332139973	0.7811821558	0.4447661777
H	-2.4559675426	-0.55869274	-0.6513685511
H	-2.5609525914	-0.7814547753	1.0848994335
H	-2.2500417152	-3.0457375422	-0.9820243805
H	-2.3125034959	-3.2912899373	0.7619165563
H	1.8860359238	-1.4492199934	-1.0197118829
H	-0.2816155682	-1.9540774712	0.7503440633

H	1.8883264199	-2.1396041036	0.6033245731
H	3.8968650563	-0.0575526234	-0.4021223095
H	3.8578323615	-0.7335735256	1.2264617122
H	4.2244078488	-2.3639693641	-1.3479332689
H	-4.620656481	-2.3015404143	0.8230753374
H	-4.5419454753	-2.0252638495	-0.9143551444
C	-5.5056257823	-4.8547736596	0.464217506
N	-5.7097149867	-6.0432031468	-0.213106758
C	-5.0463574773	-5.920756635	-1.4014212034
N	-4.44489126	-4.7582959736	-1.5245155265
H	-5.0441801106	-6.7179285104	-2.1346506111
C	-6.4824621746	-7.1835405273	0.2417355696
H	-5.9281867183	-4.6805631568	1.4434176909
C	6.9518741211	-2.4243177873	0.4873724959
N	8.1276409013	-1.7598320775	0.1907568841
C	7.7970920029	-0.7859610128	-0.7085585279
N	6.5150198113	-0.7851262943	-1.0002112714
H	8.5408390363	-0.111035512	-1.1137197151
C	9.4467017751	-2.0437714371	0.7249086872
H	6.9280946775	-3.2526630911	1.1808766262
C	-1.7082436483	7.0032352245	0.591346638
N	-2.5077111745	7.8023358984	-0.206122753
C	-2.4139143198	7.2902611466	-1.4696237752
N	-1.6251666242	6.2404482966	-1.5298553473
H	-2.944878168	7.7346818209	-2.3025562571
C	-3.2814656575	8.9545375205	0.213720355
H	-1.5993640375	7.1884685028	1.6504102551
H	10.1627123784	-1.343063355	0.2891775188
H	9.4607060713	-1.9262498372	1.8137523681
H	9.7581811492	-3.0633324522	0.4739545876
H	-6.4260778381	-7.9721128266	-0.5123825429
H	-6.0839972479	-7.573205188	1.1846166361
H	-7.5339331077	-6.9124890572	0.3866640637
H	-3.8049915131	9.3642373404	-0.6534743412
H	-4.0238169417	8.6733699918	0.9686706462
H	-2.6317157908	9.7326829906	0.6291567185

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C	0.0000001905	0.0000000606	0.5521922726
N	0.4849002569	1.2515498492	0.5357194723
N	-1.3263237538	-0.2058390579	0.5357194723
N	0.8414240683	-1.0457106095	0.5357194723
C	-0.320432424	2.4767527425	0.4202930627
C	-1.9847142437	-1.5158790647	0.4202930627
C	2.3051472391	-0.960873496	0.4202930627
C	0.5912653853	3.6767565928	0.1643618028
C	-3.4797969673	-1.3263275264	0.1643618028
C	2.8885321535	-2.3504288845	0.1643618028
C	-0.1816351876	5.0053183514	0.1186948942
C	-4.2439149143	-2.6599599365	0.1186948942
C	4.4255506734	-2.3453582331	0.1186948942
C	0.7519900416	6.1801049464	0.0604195911
C	-5.7281225642	-2.4388100679	0.0604195911
C	4.9761330941	-3.7412946967	0.0604195911
H	1.4652016395	1.3735963581	0.7508239665
H	-1.9221698222	0.5821035884	0.7508239665
H	0.4569687541	-1.9556997647	0.7508239665

H	-1.0285329286	2.3463314998	-0.4071453979
H	-1.517715882	-2.0639014688	-0.4071453979
H	2.5462493821	-0.2824298492	-0.4071453979
H	-0.8970158086	2.6358141844	1.3431040624
H	-1.8341738009	-2.0947456441	1.3431040624
H	2.7311901809	-0.5410683585	1.3431040624
H	1.1351711206	3.5287310642	-0.7767471433
H	-3.6235559668	-0.781278578	-0.7767471433
H	2.4883854176	-2.7474523043	-0.7767471433
H	1.3385051184	3.7530157578	0.9639892796
H	-3.9194592081	-0.7173285173	0.9639892796
H	2.5809546611	-3.0356870587	0.9639892796
H	-0.861994151	5.0252730803	-0.7416423889
H	-3.9210167348	-3.2591454469	-0.7416423889
H	4.7830114573	-1.7661274516	-0.7416423889
H	-0.8097178997	5.0795880018	1.0190809227
H	-3.9941929622	-3.241030346	1.0190809227
H	4.8039114334	-1.838557474	1.0190809227
C	-6.6618162442	-3.0141978852	-0.7687275211
N	-7.8805872118	-2.487051476	-0.3902707856
C	-7.6246606902	-1.6241652759	0.6351494663
N	-6.3436760743	-1.5669264635	0.9345533205
H	-8.4147164837	-1.0667771504	1.1218130574
C	-9.179513626	-2.7980217709	-0.9672953719
H	-6.5788410193	-3.7365162738	-1.5679530006
C	0.7205364147	7.2764013013	-0.7687275211
N	1.7864440804	8.068314716	-0.3902707856
C	2.4057621895	7.4152327468	0.6351494663
N	1.8148401471	6.2772481214	0.9345533205
H	3.2835023627	7.8207470716	1.1218130574
C	2.1665991123	9.3487031358	-0.9672953719
H	0.0535027281	7.5657018429	-1.5679530006
C	5.9412804009	-4.2622032342	-0.7687275211
N	6.0941437028	-5.5812630582	-0.3902707856
C	5.2188990722	-5.7910672891	0.6351494663
N	4.5288364986	-4.7103214761	0.9345533205
H	5.1312146925	-6.7539697394	1.1218130574
C	7.0129150851	-6.5506811831	-0.9672953719
H	6.5253388626	-3.8291853873	-1.5679530006
H	-9.9424692721	-2.2047683807	-0.4591109183
H	-9.196605806	-2.5535420853	-2.0338422042
H	-9.4156477371	-3.8588344247	-0.8387719103
H	3.0618494421	9.7128154122	-0.4591109183
H	2.3868708207	9.2412655551	-2.0338422042
H	1.365975461	10.0836076017	-0.8387719103
H	6.8806204014	-7.5080468497	-0.4591109183
H	6.8097355567	-6.687723288	-2.0338422042
H	8.0496728476	-6.2247729951	-0.8387719103

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C	1.2726203051	4.8540859115	-0.2663466927
C	1.6603652037	3.3637220135	-0.2690159595
C	0.4534924938	2.4343504864	-0.4295984688
N	0.88858661	1.0512788184	-0.4595421336
C	0.0038989226	0.1176573295	-0.4561424196
N	-1.3783584289	0.2961601999	-0.5370876188

C	-2.3318736218	-0.6606628398	0.0294570551
C	-3.7384735599	-0.0600414712	0.0299566076
C	-4.7973081008	-1.0345873122	0.5738865629
C	-6.1652914104	-0.395950317	0.681332631
N	0.3999069064	-1.2145402381	-0.3677554587
C	1.8227587648	-1.5285291444	-0.458007773
C	2.0480617847	-3.0292859183	-0.270889596
C	3.5404556672	-3.4038591195	-0.3198943303
H	-4.8513793398	-1.9256842551	-0.0637602213
H	-0.2528055248	2.6344682605	0.4011914659
H	-0.0838544468	2.7071807719	-1.3576088584
H	2.1769416289	3.1223380093	0.6669208725
H	2.3690472105	3.1604119939	-1.0817770584
H	0.5541375923	5.0383690334	0.5421184497
H	0.7757760621	5.1094571284	-1.2117302297
H	-1.6506921839	1.2594305733	-0.38934012
H	2.3355086795	-0.9603973153	0.3233178772
H	2.2508321815	-1.1869877235	-1.4141632894
H	1.6325236246	-3.3512333229	0.6904493286
H	1.5119579014	-3.5879435068	-1.053606562
H	-2.0472976684	-0.9598916351	1.0497537021
H	-0.1895014387	-1.8511349659	-0.8921087237
H	-2.3375220028	-1.5765764367	-0.5777729628
H	-3.7554415277	0.8449059454	0.6508758972
H	-4.0012360716	0.2446679953	-0.9916452196
H	-4.4918015408	-1.369724066	1.5738195405
H	3.9719905611	-3.0982041897	-1.2812367648
H	4.0695545301	-2.8475220141	0.4642286179
C	-7.2453325301	-0.824685004	-0.1001055491
C	-8.4794426	-0.1911569813	0.0391110617
C	-8.5979521706	0.8532366164	0.9537476552
C	-7.4658232811	1.2130546337	1.6868453955
N	-6.277992051	0.6130669708	1.5631516045
H	-7.1172512714	-1.6432577848	-0.8029173531
H	-9.3318830737	-0.5089532206	-0.5556943544
H	-9.5381163849	1.3766512445	1.0992804091
H	-7.5158159494	2.0234706473	2.4129741401
C	3.7735714435	-4.8820400354	-0.1002668228
C	4.2380008345	-5.716180031	-1.1256487679
C	4.4207285255	-7.0742365345	-0.8701324607
C	4.132844285	-7.5616032263	0.403142037
C	3.6732326619	-6.6562013462	1.3610949036
N	3.4946185409	-5.3522125786	1.128854908
H	4.455122144	-5.3017678804	-2.1063118984
H	4.7831698673	-7.7378874022	-1.6510891593
H	4.2608642374	-8.6107585008	0.6523885213
H	3.4389054395	-6.995633315	2.3694667732
C	3.0786687742	6.4285155074	-1.1231404743
C	4.1965438218	7.2231131787	-0.878226923
C	4.6725544566	7.3267114374	0.4277678799
C	3.997470213	6.62397229	1.4266061662
N	2.9236683324	5.8588205867	1.2050660204
H	2.6796959186	6.3258630062	-2.1286849934
H	4.6852389267	7.7531031891	-1.6919850315
H	5.5389097649	7.9350288122	0.6702120219
H	4.3347196975	6.6806354702	2.4611100096

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C	-0.0000000267	-0.0000000222	-0.0817170645
N	-0.0018378176	1.3421909927	-0.0639543772
N	1.1632903845	-0.6695039561	-0.0639543772
N	-1.1614526469	-0.6726871033	-0.0639543772
C	1.1966391375	2.1939421476	-0.0226393048
C	1.3016900447	-2.1332910224	-0.0226393048
C	-2.4983292622	-0.0606511918	-0.0226393048
C	0.7859380538	3.6584467966	0.128606506
C	2.7753388167	-2.5098657751	0.128606506
C	-3.5612769504	-1.1485810882	0.128606506
C	1.9914880753	4.6104272418	0.1165472903
C	2.9970030553	-4.0298929419	0.1165472903
C	-4.9884912107	-0.5805343666	0.1165472903
C	1.5658886919	6.0672615793	0.0698564523
C	4.4714582924	-4.3897302327	0.0698564523
C	-6.0373470643	-1.6775314133	0.0698564523
H	-0.8848654742	1.8095134753	-0.2163161835
H	2.0095173545	-0.1384408145	-0.2163161835
H	-1.1246519603	-1.6710727275	-0.2163161835
H	1.8192036306	1.8797271059	0.8247303952
H	0.7182895898	-2.5153401681	0.8247303952
H	-2.5374933004	0.6356129956	0.8247303952
H	1.7797809669	2.062875648	-0.9455136328
H	0.8966122118	-2.5727734109	-0.9455136328
H	-2.6763932587	0.5098976963	-0.9455136328
H	0.2230381965	3.7828554904	1.0625391266
H	3.1645298345	-2.0845845458	1.0625391266
H	-3.387568111	-1.6982710112	1.0625391266
H	0.1246836469	3.9488528693	-0.6963756293
H	3.3574650564	-2.0824056967	-0.6963756293
H	-3.4821487833	-1.8664472392	-0.6963756293
H	2.6298433273	4.4364141982	0.9907856359
H	2.5271257129	-4.4957182849	0.9907856359
H	-5.1569691202	0.0593040201	0.9907856359
H	2.6048733612	4.3984052725	-0.7713480135
H	2.5066940008	-4.4550891971	-0.7713480135
H	-5.1115674419	0.056683858	-0.7713480135
C	5.0155953018	-5.3594806553	0.917394904
C	6.370223823	-5.6719335176	0.8034515335
C	7.1354728781	-5.0033726233	-0.1495451435
C	6.5049797686	-4.045559329	-0.9453893462
N	5.2068106697	-3.7391790354	-0.8466326908
H	4.3897920715	-5.8624672379	1.6492474512
H	6.8173402993	-6.4232847641	1.4482447955
H	8.1929800704	-5.212833365	-0.2755401969
H	7.067971871	-3.4991929019	-1.7000839275
C	2.1336486884	7.0233732638	0.917394904
C	1.7269265441	8.3527424071	0.8034515335
C	0.7653112981	8.6811870819	-0.1495451435
C	0.2510672078	7.656257385	-0.9453893462
N	0.6348186399	6.3788198201	-0.8466326908
H	2.8821494619	6.73290506	1.6492474512
H	2.1540575725	9.1156322572	1.4482447955
H	0.4179560253	9.701745546	-0.2755401969
H	-0.5035960489	7.8706396342	-1.7000839275
C	-7.1492440702	-1.6638926752	0.917394904

C	-8.0971504471	-2.6808089562	0.8034515335
C	-7.9007842562	-3.6778145252	-0.1495451435
C	-6.7560470565	-3.6106981227	-0.9453893462
N	-5.8416293895	-2.6396408514	-0.8466326908
H	-7.2719416134	-0.8704378887	1.6492474512
H	-8.9713979518	-2.6923475598	1.4482447955
H	-8.6109361758	-4.4889122476	-0.2755401969
H	-6.5643759021	-4.371446799	-1.7000839275

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C	2.6148070031	5.7018944919	-0.0269397887
C	1.3902900384	4.8561363448	-0.2798957641
C	1.7228314823	3.3526586203	-0.3239805712
C	0.4837831089	2.4729048785	-0.5192175686
N	0.8779165924	1.079283227	-0.578218639
C	-0.0250805054	0.1644409092	-0.5558762532
N	-1.4056425634	0.3686673245	-0.6034134684
C	-2.3576561745	-0.5481316528	0.0280952552
C	-3.7696208968	0.036475725	-0.0373710305
C	-4.8170162852	-0.8998704777	0.5907264295
C	-6.1999025588	-0.2886644142	0.610727694
N	0.3473013573	-1.1762894451	-0.4822081234
C	1.7626643742	-1.5122950881	-0.6041132723
C	1.9773324679	-3.0063625917	-0.3574190064
C	3.4629136936	-3.3998722786	-0.4637812278
H	-4.8430436107	-1.8538022147	0.0508699992
H	-0.2239239072	2.6780735304	0.3088833628
H	-0.0320356116	2.7846042299	-1.4463548967
H	2.2217339152	3.0640012086	0.6082016394
H	2.4291014503	3.1458083117	-1.1376024591
H	0.6716969439	5.0450057605	0.5271138146
H	0.9170347293	5.1623941526	-1.221370005
H	-1.6531995261	1.3417782596	-0.476483528
H	2.3052437665	-0.9172807865	0.1353072409
H	2.1646592794	-1.2189988032	-1.5872140913
H	1.6056598515	-3.2747222055	0.6378377488
H	1.3972885677	-3.5943162876	-1.0849357248
H	-2.0837833181	-0.763025026	1.0727866449
H	-0.2603554815	-1.7941834451	-1.0087149738
H	-2.3485102242	-1.5084224484	-0.5031492904
H	-3.8028300574	0.9956425117	0.4950262799
H	-4.0279678304	0.2392534797	-1.0846380209
H	-4.5235677466	-1.1210343558	1.6253113008
H	3.8448708948	-3.1549501875	-1.4619822522
H	4.0394867872	-2.812399343	0.2610585198
C	-7.2637132963	-0.8602440246	-0.0986317127
C	-8.4997669031	-0.2309934002	-0.0268950613
C	-8.6776708075	0.9256717993	0.7194508599
C	-7.5512934851	1.4126145021	1.3851196976
N	-6.3486950993	0.8322719743	1.3389728503
H	-7.1441492438	-1.762292261	-0.6857127493
N	-9.648535415	-0.8067158022	-0.7608238735
H	-9.6422043349	1.4136749037	0.7748146876
H	-7.6250050557	2.3153381398	1.9879163786
C	3.6880436227	-4.8653554936	-0.1746983803
C	4.0182047496	-5.7702461594	-1.1925638313
C	4.1831977396	-7.1041532758	-0.8434513274

C	4.0280318098	-7.5303608553	0.4686965485
C	3.6989173258	-6.5476897491	1.4037001165
N	3.5315071537	-5.2565491869	1.102881713
H	4.146312308	-5.454830337	-2.2206290183
N	4.5320167911	-8.089425098	-1.8904570583
H	4.1595684839	-8.5700698491	0.739150817
H	3.5662128758	-6.816755466	2.4496157844
C	3.2521036632	6.3950122772	-1.0658482047
C	4.3916189485	7.123913917	-0.75410803
C	4.8876277941	7.1673864938	0.5423538586
C	4.1779175118	6.4421274993	1.5001260443
N	3.0776708087	5.7306473901	1.2358430139
H	2.8781249178	6.3735173948	-2.0819511848
N	5.0884129796	7.8716359487	-1.8232599748
H	5.7746209582	7.7385541823	0.7839439862
H	4.5130640518	6.4380605117	2.5353840406
O	4.6689903656	-9.2595728095	-1.5417959404
O	4.6603044876	-7.673801217	-3.039611542
O	-10.7251270339	-0.2221458968	-0.6718411256
O	-9.4493451094	-1.830424099	-1.4102717129
O	6.0945584554	8.5030988176	-1.5083220633
O	4.6168859761	7.8133203143	-2.9565835803

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C	-0.0000000997	0.0000000206	0.5803118935
N	0.6381094549	1.1811614827	0.563755851
N	-1.341970709	-0.0379616257	0.563755851
N	0.7038609551	-1.1431997951	0.563755851
C	-0.0046299065	2.4961112977	0.4166212113
C	-2.1593809729	-1.2520651483	0.4166212113
C	2.1640105804	-1.2440460876	0.4166212113
C	1.0527064752	3.5654501928	0.1372883571
C	-3.6141238122	-0.8710544289	0.1372883571
C	2.561417038	-2.6943957021	0.1372883571
C	0.4379076608	4.9685307758	0.0099563642
C	-4.5218278334	-2.1050261119	0.0099563642
C	4.0839198736	-2.8635046021	0.0099563642
C	1.4994593695	6.0462669541	-0.0960563027
C	-5.9859505967	-1.7245634539	-0.0960563027
C	4.4864909282	-4.3217034383	-0.0960563027
H	1.62182938	1.1806461448	0.7978317268
H	-1.8333843758	0.8142224885	0.7978317268
H	0.2115546969	-1.9948685714	0.7978317268
H	-0.7198162618	2.4367949325	-0.4124404068
H	-1.7504183161	-1.8417765178	-0.4124404068
H	2.4702342789	-0.5950183528	-0.4124404068
H	-0.5593323175	2.7493006976	1.3316787209
H	-2.1012982196	-1.8590462277	1.3316787209
H	2.6606302382	-0.890254408	1.3316787209
H	1.5927561308	3.309177281	-0.7828237597
H	-3.6622097881	-0.2752212519	-0.7828237597
H	2.0694533582	-3.0339559672	-0.7828237597
H	1.7837149736	3.5899512723	0.9545007482
H	-4.0008466186	-0.2502330386	0.9545007482
H	2.217131346	-3.3397181718	0.9545007482
H	-0.2304436112	5.0185809106	-0.8570967655
H	-4.2309968855	-2.7088603595	-0.8570967655

H	4.4614401978	-2.3097204892	-0.8570967655
H	-0.1737609337	5.1750072867	0.8993336596
H	-4.3948074398	-2.7379849089	0.8993336596
H	4.5685680746	-2.4370223159	0.8993336596
C	-6.7929620331	-2.2144826516	-1.1268966604
C	-8.1288910207	-1.8327004274	-1.1302697431
C	-8.642345663	-0.9973998893	-0.1490621605
C	-7.7463137451	-0.5609136132	0.8293048747
N	-6.4555929806	-0.907801244	0.8616121463
H	-6.4124584643	-2.8691949699	-1.9012534586
N	-9.0176683436	-2.3273040739	-2.2082735547
H	-9.6845206048	-0.7042848752	-0.1539180593
H	-8.0871307846	0.0980513007	1.6244104255
C	1.4786826166	6.990118958	-1.1268966604
C	2.4772802154	7.9561762868	-1.1302697431
C	3.4573990223	7.9831907817	-0.1490621605
C	3.3873912669	6.9889612401	0.8293048747
N	2.4416173841	6.0446080843	0.8616121463
H	0.7214333324	6.9879493604	-1.9012534586
N	2.4933295541	8.97318185	-2.2082735547
H	4.2323315417	8.7391832495	-0.1539180593
H	4.1284801423	6.9546349975	1.6244104255
C	5.3142791175	-4.7756362446	-1.1268966604
C	5.6516105063	-6.1234757976	-1.1302697431
C	5.1849463417	-6.9857908306	-0.1490621605
C	4.3589221792	-6.4280475651	0.8293048747
N	4.0139752975	-5.1368067784	0.8616121463
H	5.6910248329	-4.1187543286	-1.9012534586
N	6.5243384905	-6.6458777142	-2.2082735547
H	5.4521887642	-8.0348983124	-0.1539180593
H	3.9586503434	-7.0526862364	1.6244104255
O	6.8081159019	-7.838190706	-2.1701369844
O	6.8976487235	-5.8465903553	-3.0624277677
O	-10.1921303894	-1.9769060254	-2.1701369844
O	-8.5121203023	-3.0502438987	-3.0624277677
O	3.3840141885	9.8150967932	-2.1701369844
O	1.6144712798	8.8968343158	-3.0624277677

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C	2.5268413164	5.7014662845	-0.0439220299
C	1.3261998619	4.8371507526	-0.3463203864
C	1.6760961829	3.3370298361	-0.3513769629
C	0.455107465	2.4426998415	-0.5907520572
N	0.863092466	1.0527079812	-0.6284465415
C	-0.0307737121	0.1288468957	-0.6025229986
N	-1.4127920341	0.31637109	-0.6622481317
C	-2.3581724858	-0.6076329363	-0.0305562118
C	-3.7644114547	-0.0060213726	-0.0425128493
C	-4.8089160963	-0.9477053505	0.5823910007
C	-6.1787375634	-0.3125103096	0.6658943621
N	0.3545803342	-1.2069629348	-0.5098042377
C	1.7738530811	-1.5304653723	-0.6185606381
C	2.0015377326	-3.0209958113	-0.3633746469
C	3.4916368007	-3.3992345332	-0.4586131205
H	-4.8663839811	-1.8809655122	0.0093583883
H	-0.2866343405	2.6470477604	0.2074392321
H	-0.0262542232	2.7441312726	-1.5394489184

H	2.1340235991	3.0674467599	0.6072456759
H	2.4213988578	3.1256201533	-1.1282016344
H	0.5661476174	5.0303532311	0.4203934538
H	0.8971456162	5.12258481	-1.315453539
H	-1.6740886991	1.2874585718	-0.5490260737
H	2.3050169843	-0.9265488954	0.1219923592
H	2.1807609489	-1.2381358139	-1.59999471
H	1.6269667173	-3.2890409666	0.6308342205
H	1.4319549901	-3.6181867652	-1.0917047041
H	-2.0585833081	-0.8512285697	1.0002687372
H	-0.2446656876	-1.8383809883	-1.0297990878
H	-2.3734010444	-1.5545429428	-0.5866104654
H	-3.7705931684	0.9362774361	0.520329689
H	-4.0466458587	0.2328763951	-1.0760984371
H	-4.4897706151	-1.2103786404	1.5992653591
H	3.877086805	-3.1558784342	-1.4561104249
H	4.0571268597	-2.7994943063	0.2650325173
C	-7.2637232123	-0.8086585946	-0.0634673868
C	-8.5073412709	-0.1724454362	0.0529188503
C	-8.6224468962	0.9408514635	0.8947235407
C	-7.4796138978	1.3575843037	1.5753033043
N	-6.2898945696	0.7581829031	1.4723599653
H	-7.1507397796	-1.6737091096	-0.7084522187
C	-9.6425636639	-0.6575577942	-0.6797503659
H	-9.5679207889	1.4585896131	1.0122474694
H	-7.5257676145	2.2179846994	2.2402001159
C	3.7348185368	-4.8598215316	-0.1575345695
C	4.093991187	-5.7649120242	-1.1622864606
C	4.2882356009	-7.1114839628	-0.8264733946
C	4.1170757977	-7.5087461775	0.5057812543
C	3.7573510646	-6.5297924199	1.4302920947
N	3.5683531636	-5.2435562735	1.1211592099
H	4.2246705486	-5.4330965741	-2.1869864468
C	4.6574412367	-8.0658972557	-1.8333758437
H	4.2613255388	-8.5408779517	0.8054051338
H	3.6163138223	-6.7955173012	2.4763681644
C	3.2387015266	6.3466740209	-1.0622930463
C	4.3649986831	7.1089174849	-0.7271988213
C	4.7444906264	7.2018696391	0.6184576376
C	3.9691495192	6.52219556	1.5554073024
N	2.8924889624	5.792179667	1.2475114209
H	2.9244025697	6.2612554538	-2.0972941718
C	5.114479285	7.7864901127	-1.7472265722
H	5.6086665179	7.7845821672	0.9177088341
H	4.2270573494	6.5703987441	2.6118597126
N	4.9540845805	-8.8388568461	-2.6497179079
N	-10.560958577	-1.0512425179	-1.2741261549
N	5.72122819	8.3353493225	-2.5734378375

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C	-0.0000000996	0.0000000307	0.5356781121
N	0.6402683951	1.1799920795	0.5190343731
N	-1.3420374376	-0.0355072121	0.5190343731
N	0.7017687436	-1.1444847755	0.5190343731
C	-0.0001229593	2.4968199801	0.3783988384
C	-2.1622481746	-1.2485163437	0.3783988384
C	2.1623708351	-1.2483035444	0.3783988384

C	1.0585899151	3.5631505897	0.093501518
C	-3.6150740086	-0.8648094039	0.093501518
C	2.5564837947	-2.6983410938	0.093501518
C	0.451095874	4.9706763262	-0.013233223
C	-4.5302800323	-2.0946775444	-0.013233223
C	4.0791838595	-2.8759986898	-0.013233223
C	1.5179227234	6.0437384481	-0.1241051994
C	-5.9929925145	-1.7073094523	-0.1241051994
C	4.4750694922	-4.3364289038	-0.1241051994
H	1.6243158601	1.1774545076	0.7517046783
H	-1.8318635683	0.817971677	0.7517046783
H	0.2075474094	-1.9954260927	0.7517046783
H	-0.7212551686	2.4407154786	-0.4457300614
H	-1.7530941464	-1.8449829057	-0.4457300614
H	2.4743490162	-0.5957324809	-0.4457300614
H	-0.5479250107	2.7495885701	1.297744769
H	-2.1072511692	-1.8493111315	1.297744769
H	2.6551758811	-0.9002773467	1.297744769
H	1.5852402805	3.311621244	-0.8356253083
H	-3.6605683881	-0.2829521357	-0.8356253083
H	2.0753278088	-3.0286690163	-0.8356253083
H	1.8012024984	3.5776256845	0.9003131732
H	-3.9989161001	-0.228925589	0.9003131732
H	2.1977133029	-3.3487000036	0.9003131732
H	-0.2299083479	5.0324280864	-0.8698618363
H	-4.2432565144	-2.7153203808	-0.8698618363
H	4.4731645635	-2.3171076136	-0.8698618363
H	-0.1477360591	5.1726840744	0.8861306776
H	-4.4058079075	-2.7142850852	0.8861306776
H	4.5535436677	-2.4583988973	0.8861306776
C	-6.8152273188	-2.2458497055	-1.1153115897
C	-8.1658714575	-1.8693194819	-1.1484803619
C	-8.640182515	-0.9670484576	-0.1884583693
C	-7.7335391202	-0.4838120565	0.7537653406
N	-6.4442298	-0.8363160746	0.7935896265
H	-6.4256457064	-2.9447506298	-1.8480136642
C	-9.039344932	-2.4004065458	-2.1556462119
H	-9.6779257735	-0.653101079	-0.1809075581
H	-8.0618831533	0.2207221185	1.514760214
C	1.4626505854	7.0250848031	-1.1153115897
C	2.4640573937	8.0065118269	-1.1484803619
C	3.4826025505	7.9661417399	-0.1884583693
C	3.4477758525	6.9393473272	0.7537653406
N	2.4978437579	5.9990247116	0.7935896265
H	0.662593824	7.0371476921	-1.8480136642
C	2.440859242	9.0285055773	-2.1556462119
H	4.2733605851	8.707880075	-0.1809075581
H	4.2220923625	6.8714345136	1.514760214
C	5.3525764346	-4.7792350056	-1.1153115897
C	5.701813765	-6.1371922531	-1.1484803619
C	5.1575796656	-6.9990931903	-0.1884583693
C	4.2857629688	-6.4555351788	0.7537653406
N	3.9463857433	-5.1627085451	0.7935896265
H	5.7630515836	-4.0923969703	-1.8480136642
C	6.5984853912	-6.6280989396	-2.1556462119
H	5.4045648895	-8.0547789041	-0.1809075581
H	3.839790492	-7.0921565401	1.514760214
N	7.3222693433	-7.0194243783	-2.9765719902

N -9.7401346791	-2.8315591158	-2.9765719902
N 2.417865037	9.850983586	-2.9765719902

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C 2.6078980049	5.6997729319	-0.052649804
C 1.4028743435	4.8421732454	-0.3641931516
C 1.7344101662	3.338750098	-0.3494009278
C 0.5065644165	2.4549076848	-0.5912429767
N 0.894100466	1.0577776566	-0.6107506182
C -0.0156492935	0.1493484983	-0.5815446149
N -1.3943296945	0.360325829	-0.6555042182
C -2.3608863495	-0.5388216035	-0.0188496272
C -3.7579318118	0.0825165696	-0.0541988609
C -4.8233721204	-0.8300135423	0.5766277156
C -6.1867553681	-0.1752369438	0.6278401651
N 0.3453885049	-1.1914853816	-0.4712898765
C 1.757758048	-1.5461152077	-0.575397104
C 1.9510316179	-3.0436113996	-0.3335343138
C 3.4298099183	-3.4598441509	-0.4313503386
H -4.8850784277	-1.7754637363	0.0237709758
H -0.2406177765	2.6769748183	0.1973115528
H 0.0367519261	2.7519348442	-1.547481862
H 2.1800335642	3.0757172305	0.6166433959
H 2.4856791565	3.1116219449	-1.1161299787
H 0.6325267337	5.0489269024	0.3895119858
H 0.9893696141	5.1222462034	-1.3418759052
H -1.6376819324	1.3367675889	-0.5474376949
H 2.2995456781	-0.960720495	0.172616964
H 2.1753590445	-1.2534356527	-1.5524102375
H 1.5696132543	-3.3132980974	0.6573986336
H 1.3677904943	-3.620061573	-1.0681555424
H -2.0749086114	-0.7713351526	1.0185381667
H -0.2671065237	-1.8197825116	-0.9790771887
H -2.3844755521	-1.4942202633	-0.5601839025
H -3.756648636	1.035036031	0.4909035037
H -4.0271299749	0.3068995629	-1.0946625681
H -4.5188045816	-1.0743546891	1.6030069286
H 3.8216488127	-3.2183076091	-1.4270396527
H 4.0091567161	-2.8775359077	0.2964074905
C -7.2677017351	-0.6931399185	-0.0801063379
C -8.5110395833	-0.0492140738	-0.0040198799
C -8.618107427	1.10037248	0.784634814
C -7.4691151413	1.5350207	1.4501516818
N -6.2806663376	0.9343324475	1.3904712782
H -7.1724232503	-1.5868676992	-0.6883591085
O -9.5219430508	-0.6081630415	-0.7153261379
H -9.5463204389	1.6487189215	0.8907677557
H -7.5217660295	2.42744129	2.0729717863
C 3.6373184544	-4.9292322416	-0.1396066821
C 4.0156854938	-5.8211321064	-1.1403451804
C 4.1816140034	-7.1772812714	-0.8269415634
C 3.9576832577	-7.5882214046	0.4905498008
C 3.5799249794	-6.6108111497	1.4148246121
N 3.4179922809	-5.3178897923	1.13453669
H 4.1895936324	-5.4893458109	-2.1589856057
O 4.5534034465	-7.99062654	-1.8483886194
H 4.0687394941	-8.6187700686	0.8059245529

H	3.400625335	-6.9004538426	2.4499109687
C	3.3034927791	6.3656752378	-1.0600645802
C	4.4354439373	7.1224828678	-0.7307683998
C	4.8291647344	7.1837517985	0.6096022432
C	4.0596085547	6.4795359747	1.5389045481
N	2.9804444729	5.754728301	1.2438672907
H	2.9872886959	6.31114554	-2.0969537766
O	5.0647997361	7.7462036959	-1.760705987
H	5.6921038019	7.7508242256	0.9377356473
H	4.3394887007	6.5108813772	2.5916842553
C	4.7373501014	-9.3735714671	-1.5736722966
H	5.0314005251	-9.8285474103	-2.5208908537
H	5.5298027388	-9.5330843155	-0.8315867943
H	3.8090726618	-9.8390005189	-1.2188791464
C	-10.8023062519	0.0096354402	-0.6660694337
H	-11.4504190917	-0.5989863811	-1.2985169889
H	-11.2005294802	0.0247432954	0.3562220869
H	-10.7681830611	1.0338435321	-1.0581842804
C	6.2201837821	8.521270407	-1.4706212885
H	6.5590280828	8.9208366237	-2.4279519796
H	5.9869578711	9.3516608557	-0.7919620659
H	7.0159224982	7.9066873196	-1.0307295386

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C	-0.0000000586	0.0000000183	0.4999320871
N	0.6490728031	1.1747901879	0.4837579745
N	-1.3419346205	-0.0252814793	0.4837579745
N	0.6928616415	-1.1495086537	0.4837579745
C	0.01660863	2.4971152097	0.3619475992
C	-2.1708695948	-1.2341740311	0.3619475992
C	2.154260789	-1.2629411236	0.3619475992
C	1.0842349446	3.5626231747	0.1141030029
C	-3.6274397177	-0.8423365035	0.1141030029
C	2.5432045973	-2.7202866163	0.1141030029
C	0.4923847138	4.9779175637	0.0392241665
C	-4.5571954971	-2.062541033	0.0392241665
C	4.0648106075	-2.9153764758	0.0392241665
C	1.5749831977	6.0408927105	-0.0065528317
C	-6.0190582197	-1.6564708173	-0.0065528317
C	4.4440748463	-4.3844218383	-0.0065528317
H	1.6364105899	1.1638367447	0.7009848855
H	-1.8261175538	0.8352548477	0.7009848855
H	0.1897067881	-1.9990915375	0.7009848855
H	-0.6958324853	2.4621370832	-0.4712261876
H	-1.7843570911	-1.8336770724	-0.4712261876
H	2.4801894006	-0.6284599558	-0.4712261876
H	-0.5406790267	2.7333621854	1.280123748
H	-2.096821649	-1.8349227869	1.280123748
H	2.6375004999	-0.8984393435	1.280123748
H	1.6190134916	3.3311026759	-0.8158239796
H	-3.6943263578	-0.2634444469	-0.8158239796
H	2.0753126904	-3.0676581741	-0.8158239796
H	1.8190127071	3.5530741877	0.9280800742
H	-3.9865589336	-0.2012258015	0.9280800742
H	2.1675460508	-3.3518483312	0.9280800742
H	-0.1666798387	5.0756056299	-0.8313009174
H	-4.3122635678	-2.6821517114	-0.8313009174

H	4.4789432307	-2.3934538636	-0.8313009174
H	-0.1270566683	5.1530264573	0.9307242508
H	-4.3991235563	-2.6865474529	0.9307242508
H	4.5261800488	-2.4664789494	0.9307242508
C	-6.8860923828	-2.1936259745	-0.9501452781
C	-8.2376586348	-1.8119805464	-0.9317838456
C	-8.6544954576	-0.8958300986	0.0408508238
C	-7.6954897833	-0.4149972764	0.9335666326
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H	-6.5493265258	-2.904617165	-1.6977035979
O	-9.0288539605	-2.3706319173	-1.8719102206
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C	2.5496080292	8.0400118953	-0.9317838456
C	3.5514360022	7.9429279492	0.0408508238
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O	2.4613994131	9.0045328323	-1.8719102206
H	4.3581668718	8.6618183569	0.1149001877
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C	5.3427819397	-4.8667178708	-0.9501452781
C	5.6880504297	-6.228031294	-0.9317838456
C	5.1030592796	-7.0470977957	0.0408508238
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H	7.6677684915	-8.0966923618	-2.7175036072
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H	6.1017088709	-8.6623197417	-2.0716202742
C	-10.4135056824	-2.0257666192	-1.8921585713
H	-10.8458256214	-2.5921361464	-2.7175036072
H	-10.9065064155	-2.3099490986	-0.955052523
H	-10.5526434913	-0.9530750411	-2.0716202742
C	3.452387383	10.0312437497	-1.8921585713
H	3.1780569541	10.6888285631	-2.7175036072
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H	4.4509344445	9.6153948378	-2.0716202742

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C	1.7014136638	3.3254541781	-0.3274887238
C	0.4702845308	2.4395087261	-0.5416889325
N	0.8570486925	1.0419627537	-0.5748744688
C	-0.0590316559	0.138767679	-0.5771122799
N	-1.434060338	0.3633143494	-0.667923949
C	-2.4221746008	-0.5584012933	-0.1010967944
C	-3.8041617428	0.0964896396	-0.0871356768
C	-4.898214386	-0.840327302	0.45215323
C	-6.2403278983	-0.1478959649	0.5689383086
N	0.2906503835	-1.20590499	-0.4856045629

C	1.7010933704	-1.5718195732	-0.5743539696
C	1.8764481645	-3.0766755145	-0.3676229194
C	3.3532438282	-3.5040869289	-0.4326297328
H	-4.9858839565	-1.7251925839	-0.1908481812
H	-0.2574358178	2.6559302186	0.2664103311
H	-0.02507539	2.7405975281	-1.4843247767
H	2.1734475338	3.0594237703	0.6250144728
H	2.4333007923	3.1038966414	-1.1146747887
H	0.6219307122	5.030379707	0.4533575042
H	0.918666982	5.1089743288	-1.2887231769
H	-1.6741479375	1.3356349786	-0.5233880038
H	2.2353799452	-1.0108481358	0.1975746819
H	2.1382198248	-1.2577061677	-1.5362281621
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H	-2.4678098234	-1.4697816316	-0.7139618525
H	-3.7836878825	0.9954419742	0.5419914176
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H	-4.6036125377	-1.1921631977	1.4496420249
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C	-8.5639240248	0.1231493336	-0.1018406
C	-8.6160980437	1.1819606423	0.8320239346
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H	-7.5147270075	2.3048632493	2.2863648564
C	3.5405981906	-4.9844651121	-0.176144467
C	3.9944289185	-5.833365513	-1.1850042947
C	4.1495992141	-7.2162470285	-0.9363561509
C	3.8349520717	-7.6500210517	0.3703991485
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N	3.2343415138	-5.4097482525	1.0640429266
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H	3.9343681041	-8.686990594	0.6669665184
H	3.1469963784	-7.0497150719	2.3082258773
C	3.2393001462	6.3454289896	-1.0926679205
C	4.3908979534	7.1203052634	-0.8313165613
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N	2.9881568711	5.7458295985	1.2295299627
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H	5.6959548498	7.7181877027	0.8180308172
H	4.408051564	6.5088707806	2.5129549815
C	4.8707560999	-9.4708785269	-1.5656495155
H	5.1665872529	-10.0119094059	-2.4663317489
H	5.6839877962	-9.5578781863	-0.8289340856
H	3.9849527942	-9.969520146	-1.15357259
C	-10.8825074604	0.5377504712	-0.7728128776
H	-11.6399193023	0.0837625152	-1.4140669622
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H 5.2921085673	-8.4115976197	-3.8454886924
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H-10.5005057522	-1.4339201871	-2.3419069514
H -8.8178311409	-0.9722335054	-2.6681041754
H -9.1882251399	-2.2166036456	-1.4531889022
C 4.6837454639	7.5834967251	-3.2201518031
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C -2.4319330278	-0.5722984045	0.5478367873
C 1.711591546	-1.8199664148	0.5478367873
C 2.0479970605	3.116232408	0.3273752942
C -3.7227348845	0.2155014426	0.3273752942
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C 3.0750404809	-3.9607628637	0.3106104395
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H -1.5151358134	1.3197864774	0.8498805435
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H 2.214395811	-1.316996612	-0.2872995834
H 0.2448173074	2.7571789775	1.4699484689
H -2.5101956157	-1.166571316	1.4699484689
H 2.265378278	-1.5906073484	1.4699484689
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C	-7.4312270457	1.8398500426	1.2600563408
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H	-7.4595483656	2.6500681531	1.9873864341
C	3.486495675	6.4176999206	-0.5328951677
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H	6.6426795063	7.0407001214	0.5818721174
H	6.0248004196	5.1351244567	1.9873864341
C	3.814643222	-6.2282436372	-0.5328951677
C	3.7720116815	-7.6434775523	-0.4823853815
C	2.8804620987	-8.2017658597	0.4644702741
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H	1.4347479157	-7.7851922966	1.9873864341
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C	-8.5525671795	1.9991189016	0.2677576501
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C	3.0431431902	-7.9669843961	0.3165317202
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