

Supporting Information for:

**On the Properties and Atmospheric Implication of Amine-Hydrated
Clusters**

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Table S1 Topological parameters at intermolecular bond critical points for the global minimum of $(\text{CH}_3)_2\text{NH}(\text{H}_2\text{O})_{n=1-6}$.

Isomer	BCPs	$\rho/\text{a.u.}$	$\nabla^2\rho/\text{a.u.}$	$G/\text{a.u.}$	$V/\text{a.u.}$	$H/\text{a.u.}$	$G/ V $
1a	O-H2 $\cdots$ N1	0.0409	0.0735	0.0256	-0.0328	-0.0072	0.7805
2a	O3-H4 $\cdots$ N1	0.0532	0.0662	0.0316	-0.0466	-0.0150	0.6781
	O2-H5 $\cdots$ O3	0.0378	0.098	0.0285	-0.0324	-0.0040	0.8796
	C-H6 $\cdots$ O2	0.0065	0.0194	0.0042	-0.0035	0.0007	1.200
	C-H7 $\cdots$ O2	0.0058	0.0198	0.0042	-0.0033	0.0008	1.2727
3a	O2-H5 $\cdots$ N1	0.0634	0.0517	0.0354	-0.0579	-0.0225	0.6114
	O3-H6 $\cdots$ O2	0.0504	0.1029	0.0369	-0.0481	-0.0112	0.7672
	O4-H7 $\cdots$ O3	0.0445	0.1014	0.0330	-0.0407	-0.0077	0.8108
	N1-H8 $\cdots$ O4	0.0267	0.0831	0.0202	-0.0197	0.0006	1.0254
4a	O5-H10 $\cdots$ N1	0.0683	0.0447	0.0373	-0.0635	-0.0262	0.5874
	N1-H6 $\cdots$ O2	0.0298	0.0886	0.0226	-0.0230	-0.0004	0.9826
	O2-H7 $\cdots$ O3	0.0474	0.1033	0.0352	-0.0445	-0.0093	0.7910
	O3-H8 $\cdots$ O4	0.0516	0.1043	0.0380	-0.0498	-0.0119	0.7631
	O4-H9 $\cdots$ O5	0.0549	0.1033	0.0399	-0.0540	-0.0141	0.7389
5a	O5-H7 $\cdots$ N1	0.0884	0.0051	0.0439	-0.0866	-0.0426	0.5069
	N1-H14 $\cdots$ O2	0.0326	0.0890	0.0238	-0.0254	-0.0016	0.9370
	O2-H10 $\cdots$ O3	0.0337	0.0955	0.0258	-0.0278	-0.0019	0.9281
	C-H13 $\cdots$ O3	0.0053	0.0171	0.0036	-0.0029	0.0007	1.2414
	O3-H9 $\cdots$ O4	0.0454	0.0992	0.0331	-0.0414	-0.0083	0.7995
	O6-H12 $\cdots$ O5	0.0407	0.1048	0.0314	-0.0365	-0.0052	0.8603
	O4-H8 $\cdots$ O5	0.0329	0.0972	0.0255	-0.0268	-0.0012	0.9515
	O2-H11 $\cdots$ O6	0.0244	0.0787	0.0187	-0.0177	0.0010	1.0565
6a	O4-H15 $\cdots$ O6	0.0143	0.0506	0.0110	-0.0094	0.0016	1.1702
	O2-H16 $\cdots$ N1	0.0695	0.0424	0.0378	-0.0649	-0.0271	0.5824
	O5-H11 $\cdots$ O4	0.0408	0.1014	0.0307	-0.0361	-0.0054	0.8504
	O3-H15 $\cdots$ O2	0.0306	0.0915	0.0236	-0.0243	-0.0007	0.9712
	O5-H14 $\cdots$ O2	0.0370	-0.0273	0.0844	-0.0852	-0.767	0.9906
	O4-H12 $\cdots$ O3	0.0492	0.1001	0.0355	-0.0460	-0.0105	0.7717
	N1-H8 $\cdots$ O7	0.0208	0.0698	0.0158	-0.0142	0.0016	1.1127
	O3-H13 $\cdots$ O7	0.0318	0.0922	0.0243	-0.0255	-0.0012	0.9529
	C-H17 $\cdots$ O6	0.0520	0.0168	0.0035	-0.0282	0.0007	0.1241
	O7-H9 $\cdots$ O6	0.0535	0.1031	0.0389	-0.0520	-0.0131	0.7481
	O6-H10 $\cdots$ O5	0.0618	0.0963	0.0428	-0.0616	-0.0188	0.6948

Table S2 Binding mean isotropic, anisotropic polarizabilities, Rayleigh scattering activities of the $R_{p\parallel}$, $R_{p\perp}$ components of the linearly polarized light, depolarization ratio of natural light σ_n ,

and circularly polarized light σ_c for $(\text{CH}_3)_2\text{NH}(\text{H}_2\text{O})_{n=1-6}$ calculated at the level of CAM-B3LYP /aug-cc-pVDZ

isomer	$\bar{\alpha}_{\text{Binding}}$	$\Delta\alpha_{\text{Binding}}$	$R_{p \perp}$	$R_{p \parallel}$	σ_n	σ_c
1a	-0.02	0.18	103177.95	377.52	0.00366	0.00367
2a	0.15	-4.21	147813.66	129.90	0.00088	0.00088
3a	1.60	-0.87	208987.67	498.12	0.00238	0.00239
4a	2.32	-0.24	275315.17	707.73	0.00257	0.00258
5a	1.81	-1.80	340727.73	650.80	0.00191	0.00191
5b	1.20	-3.04	335764.39	505.60	0.00151	0.00151
5c	1.81	-2.40	340626.94	577.83	0.00170	0.00170
5d	2.68	0.79	347992.93	1015.40	0.00292	0.00293
5e	2.13	-3.49	342959.2	456.51	0.00133	0.00133
5f	2.60	-0.96	347047.47	760.11	0.00219	0.00220
5g	2.63	0.47	347544.75	965.29	0.00278	0.00279
5h	2.20	-2.77	343651.28	535.83	0.00156	0.00156
5i	2.44	-1.99	345649.94	628.04	0.00182	0.00182
5j	2.53	0.05	346680.88	903.54	0.00261	0.00261
6a	2.43	-6.50	422545.98	280.65	0.00066	0.00066

Cartesian Coordinates of optimized Structures

1a

N	0.465271	-0.018088	0.444128
H	0.671176	-0.008475	1.442624
C	0.857446	1.263980	-0.144583
H	1.949963	1.431298	-0.136876
H	0.514243	1.299596	-1.185935
H	0.369286	2.081781	0.3963020
C	1.136433	-1.157045	-0.182296
H	0.857870	-2.081959	0.335235
H	0.803954	-1.240665	-1.224549
H	2.238497	-1.070218	-0.181591
O	-2.313566	-0.007085	-0.124897
H	-1.362702	-0.088971	0.153297
H	-2.753928	-0.780699	0.253042

1b

N	0.418811	-0.002694	-0.359421
H	0.436695	-0.001339	-1.379150
C	1.079636	-1.209906	0.135200
H	2.163646	-1.236428	-0.080229
H	0.952946	-1.270729	1.223830
H	0.610259	-2.094857	-0.308172
C	1.031862	1.228646	0.137640
H	0.526224	2.095088	-0.302204
H	0.904338	1.281372	1.226547
H	2.113490	1.298767	-0.079609
O	-2.407373	-0.008698	-0.033103
H	-2.635326	-0.077405	0.904297
H	-1.413949	-0.018462	-0.061583

2a

N	-1.198997	0.443689	-0.028902
H	-1.967955	1.113196	-0.059742
C	-1.236250	-0.279342	1.249353
H	-2.138137	-0.906642	1.359390
H	-0.352205	-0.925357	1.310201
H	-1.199753	0.436965	2.077606
C	-1.293671	-0.461802	-1.180932
H	-1.308316	0.121240	-2.108988
H	-0.409996	-1.110723	-1.192633
H	-2.194275	-1.099983	-1.151365

O	1.338672	1.482361	0.018363
H	0.364534	1.218976	-0.055898
H	1.545365	1.960493	-0.797128
O	1.976652	-1.210455	-0.022295
H	1.909850	-0.223775	0.003061
H	2.800792	-1.418598	0.438738

2b

N	-0.769463	-0.069773	0.027855
H	-0.116351	-0.814041	0.293626
C	-1.527620	-0.481702	-1.152319
H	-2.226754	-1.312861	-0.948395
H	-2.115246	0.366394	-1.527995
H	-0.836188	-0.797242	-1.941579
C	-1.624427	0.273100	1.163154
H	-1.002628	0.515019	2.032163
H	-2.224066	1.159214	0.917511
H	-2.319379	-0.539732	1.441919
O	1.485866	1.451444	-0.240879
H	0.556310	1.052570	-0.238369
H	1.619923	1.817607	-1.126474
O	2.037482	-1.212073	0.224357
H	2.693298	-1.383670	0.914053
H	2.082817	-0.238207	0.055719

3a

N	-1.164335	0.033302	-0.006372
H	-0.507729	0.827582	-0.041064
C	-1.923057	0.084694	1.244177
H	-2.602529	0.953869	1.295962
H	-2.527289	-0.825897	1.350327
H	-1.229802	0.135088	2.090607
C	-2.024238	0.058535	-1.188792
H	-1.406423	0.087598	-2.093806
H	-2.639658	-0.850589	-1.222611
H	-2.706352	0.927377	-1.205159
O	1.091717	1.952288	0.045188
H	1.348357	2.597467	-0.627962
H	1.781289	1.234427	-0.003659
O	0.705373	-1.906730	0.067486
H	-0.068289	-1.232534	0.000738

H	0.598702	-2.521145	-0.672316
O	2.755213	-0.193460	-0.088384
H	3.320216	-0.332352	0.684818
H	2.055199	-0.910159	-0.037892

3b

N	-1.169612	0.032628	0.014811
H	-0.517759	0.828299	0.077291
C	-2.002804	-0.017300	1.215965
H	-2.684857	0.847652	1.300895
H	-2.613712	-0.929575	1.207361
H	-1.363648	-0.046083	2.105438
C	-1.955261	0.149136	-1.213743
H	-1.281676	0.263100	-2.070309
H	-2.553577	-0.760056	-1.361976
H	-2.646913	1.010155	-1.199729
O	1.077823	1.946860	-0.039612
H	1.381529	2.655295	0.543700
H	1.790040	1.252136	-0.012564
O	2.770058	-0.192181	-0.072247
H	2.062371	-0.902265	-0.035706
H	3.351117	-0.373305	0.679750
O	0.709895	-1.899394	0.036150
H	0.615484	-2.481754	-0.730877
H	-0.064929	-1.225299	-0.014604

3c

N	1.163689	0.035220	-0.005055
H	0.504251	0.827422	0.024290
C	1.990276	0.136904	-1.207267
H	2.675307	1.003149	-1.184784
H	2.599774	-0.770049	-1.319532
H	1.346565	0.230990	-2.089039
C	1.955695	0.011425	1.224839
H	1.286092	-0.010493	2.091742
H	2.574567	-0.895094	1.251280
H	2.626496	0.884096	1.319632
O	-1.094008	1.953663	-0.069728
H	-1.779736	1.233187	-0.010699
H	-1.333966	2.588077	0.619771
O	-0.698308	-1.913026	0.050300

H	0.069845	-1.234160	-0.023379
H	-0.576087	-2.545332	-0.671426
O	-2.757660	-0.191023	0.088971
H	-3.343007	-0.325996	-0.669266
H	-2.071946	-0.919218	0.035020

3d

N	-1.809670	-0.005301	0.372567
H	-2.581906	-0.044501	1.037212
C	-1.898145	-1.145167	-0.545363
H	-2.775594	-1.093854	-1.214469
H	-0.994008	-1.179656	-1.165387
H	-1.946834	-2.076891	0.028975
C	-1.832060	1.284631	-0.324326
H	-1.842521	2.098403	0.409270
H	-0.920175	1.386132	-0.925692
H	-2.703428	1.398943	-0.993318
O	0.719219	-0.188119	1.517599
H	1.149447	0.625648	1.185387
H	-0.229159	-0.114546	1.192906
O	2.105107	1.410621	-0.460677
H	2.977518	1.828251	-0.455177
H	2.268167	0.459269	-0.676572
O	1.981014	-1.350905	-0.537683
H	2.702787	-1.941226	-0.279809
H	1.501900	-1.118417	0.312927

3e

N	1.726585	0.369653	-0.360161
H	2.118259	0.985378	-1.072634
C	2.712456	-0.655299	-0.010804
H	3.607740	-0.244711	0.489656
H	2.248914	-1.381453	0.668521
H	3.027147	-1.189304	-0.914233
C	1.304836	1.169392	0.795137
H	0.599980	1.942407	0.470239
H	0.781202	0.520278	1.507587
H	2.150271	1.649240	1.319225
O	-1.833510	-1.091912	1.134589
H	-1.326930	-1.197126	0.274694
H	-2.383249	-1.884124	1.213460

O	-0.630717	-0.820986	-1.242833
H	-1.249166	-0.068925	-1.346840
H	0.244499	-0.389619	-1.003051
O	-2.538501	1.150735	-0.336540
H	-3.471086	1.254668	-0.571540
H	-2.515605	0.428467	0.338326

3f

N	1.597474	-0.116160	-0.310767
H	1.344228	-0.480940	-1.229348
C	2.871201	-0.700337	0.111132
H	3.725772	-0.377467	-0.510506
H	3.076424	-0.405426	1.147815
H	2.805422	-1.793437	0.078041
C	1.629702	1.348117	-0.367444
H	0.657848	1.725212	-0.704582
H	1.812210	1.740645	0.640870
H	2.419923	1.738767	-1.032833
O	-0.667826	-0.780769	1.169531
H	0.192606	-0.571096	0.695185
H	-1.113595	0.087555	1.242889
O	-2.302490	1.405177	0.206849
H	-2.558239	0.596067	-0.301650
H	-3.132968	1.780045	0.531528
O	-2.360509	-1.136963	-0.878712
H	-3.054180	-1.790176	-0.710975
H	-1.716582	-1.222865	-0.114537

3g

N	1.826276	0.291925	-0.253426
H	2.114617	0.990028	-0.938951
C	2.848131	-0.752997	-0.167469
H	3.805794	-0.392434	0.249138
H	2.482515	-1.561433	0.478083
H	3.031277	-1.172873	-1.162465
C	1.575009	0.951381	1.030552
H	0.828007	1.741876	0.899361
H	1.166444	0.216848	1.736143
H	2.484613	1.386492	1.481385
O	-2.372131	1.287972	-0.315557
H	-3.055279	1.522526	-0.959675

H	-1.704980	0.735034	-0.819585
O	-0.654019	-0.556579	-1.229544
H	-1.061813	-1.127065	-0.546455
H	0.251946	-0.315708	-0.876340
O	-2.543776	-1.206294	0.871075
H	-2.677257	-0.259844	0.615576
H	-2.429246	-1.198015	1.831484

3h

N	1.973240	-0.142525	0.359407
H	2.525999	-0.393722	1.178738
C	2.376500	1.184380	-0.111425
H	3.404719	1.209459	-0.514538
H	1.692331	1.507488	-0.906270
H	2.302495	1.904786	0.710496
C	2.122369	-1.177270	-0.664916
H	1.860787	-2.154291	-0.243633
H	1.430703	-0.967082	-1.490605
H	3.143460	-1.233816	-1.083237
O	-0.703299	-0.003743	1.209950
H	0.248756	-0.051389	0.909796
H	-1.092285	0.759135	0.731159
O	-2.382599	1.405154	-0.626831
H	-3.139952	1.924779	-0.322031
H	-2.689283	0.463851	-0.602465
O	-2.690799	-1.280147	-0.077494
H	-1.877619	-1.045006	0.453947
H	-2.402428	-1.939284	-0.724161

4a

N	-1.583938	0.029229	0.011716
H	-0.932534	0.830613	0.015243
C	-2.297393	-0.012462	1.289402
H	-2.957625	0.860515	1.438348
H	-2.915407	-0.918295	1.342392
H	-1.574275	-0.046672	2.111795
C	-2.489959	0.160066	-1.130470
H	-1.906314	0.262075	-2.052220
H	-3.117841	-0.737380	-1.215072
H	-3.159352	1.034339	-1.047112
O	2.798390	1.187514	0.019983

H	2.720713	0.187749	0.041649
H	3.339057	1.381795	-0.758575
O	-0.019020	-2.138096	-0.128863
H	-0.219264	-2.615905	-0.946016
H	-0.636489	-1.307421	-0.117200
O	2.540711	-1.469979	0.043854
H	2.870225	-1.898725	0.846077
H	1.571868	-1.736996	-0.023986
O	0.324684	2.263970	-0.083774
H	1.250412	1.891175	-0.051686
H	0.320375	2.975637	0.571151

4b

N	1.601757	0.012526	0.025686
H	0.947820	0.810971	0.063678
C	2.493010	0.186683	-1.123219
H	3.152590	1.066426	-1.021535
H	3.127932	-0.701538	-1.241806
H	1.895693	0.303787	-2.033562
C	2.329620	-0.066478	1.292317
H	1.617353	-0.135578	2.122425
H	2.961272	-0.965191	1.306704
H	2.984040	0.806370	1.465962
O	-2.799638	1.188805	-0.077585
H	-3.268399	1.336360	-0.911066
H	-2.735078	0.192609	0.015203
O	-2.569658	-1.463615	0.185615
H	-1.619391	-1.733121	0.000276
H	-2.751659	-1.752961	1.090565
O	-0.313913	2.240023	-0.001748
H	-0.351006	2.948233	0.655685
H	-1.242626	1.875861	-0.041138
O	-0.047811	-2.052536	-0.401617
H	0.621216	-1.289050	-0.208093
H	0.360325	-2.873512	-0.095008

4c

N	-1.585993	0.022709	0.021458
H	-0.938286	0.819571	-0.087470
C	-2.230777	0.111370	1.333414
H	-2.881166	0.998450	1.428693

H	-2.843381	-0.782780	1.508471
H	-1.464698	0.158273	2.114839
C	-2.551919	0.043378	-1.077451
H	-2.019953	0.041859	-2.035916
H	-3.186827	-0.852074	-1.035361
H	-3.214253	0.926830	-1.048715
O	0.313377	2.261044	-0.158776
H	1.238818	1.892568	-0.095174
H	0.343355	2.884927	-0.897134
O	-0.012695	-2.144896	-0.020815
H	-0.635565	-1.318577	-0.037811
H	-0.262884	-2.687005	-0.782317
O	2.549951	-1.458085	-0.123046
H	1.580690	-1.727941	-0.083651
H	2.994690	-2.004394	0.539714
O	2.792993	1.208778	0.042606
H	3.197502	1.419059	0.895838
H	2.741070	0.209052	0.010259

4d

N	-1.413212	-0.110945	0.029358
H	-0.763925	-0.109655	0.838108
C	-2.265824	-1.299196	0.077756
H	-2.958764	-1.288332	0.936216
H	-2.865190	-1.368156	-0.839833
H	-1.641344	-2.196937	0.148638
C	-2.175836	1.140770	0.022485
H	-1.482505	1.988583	0.047163
H	-2.774581	1.207968	-0.895596
H	-2.861113	1.220694	0.883103
O	2.223334	-1.666960	-0.022759
H	2.096596	-2.619376	-0.133702
H	1.692734	-1.240465	-0.739691
O	0.615035	-0.101298	-1.622468
H	-0.287283	-0.131941	-1.072454
H	0.399090	-0.110106	-2.565221
O	0.868661	0.041750	1.850116
H	1.171184	0.848766	1.377536
H	1.397148	-0.665586	1.420226
O	1.502084	2.048236	-0.106016
H	2.443062	2.250549	-0.207666

H 1.304422 1.367337 -0.794770

4e

N -1.539712 0.015214 0.054557
H -0.956322 0.820035 -0.224571
C -1.769590 0.082148 1.500237
H -2.376418 0.956324 1.793297
H -2.288621 -0.824917 1.836512
H -0.807133 0.139508 2.020330
C -2.787059 0.035301 -0.710088
H -2.563028 0.049622 -1.783285
H -3.371735 -0.868983 -0.494562
H -3.417552 0.911039 -0.475614
O -0.015826 -2.137163 -0.388587
H -0.210577 -2.495334 -1.265993
H -0.629901 -1.311854 -0.266337
O 0.262558 2.271208 -0.557034
H 0.405791 2.557204 -1.469746
H 1.147067 1.926414 -0.252860
O 2.580865 1.206306 0.364331
H 3.416560 1.535313 0.005484
H 2.590665 0.216755 0.203355
O 2.520413 -1.433904 -0.071397
H 1.563732 -1.718941 -0.209759
H 2.831279 -1.954946 0.682448

4f

N -1.471695 -0.153445 0.012752
H -1.116950 0.802745 0.173736
C -1.617155 -0.828496 1.306414
H -2.387181 -0.360355 1.942897
H -1.897650 -1.878045 1.147168
H -0.660573 -0.805879 1.839135
C -2.728084 -0.086329 -0.734797
H -2.575395 0.476359 -1.662853
H -3.061036 -1.099425 -0.997491
H -3.539039 0.397344 -0.163089
O 0.637850 -1.130125 -1.254401
H 0.406072 -1.740290 -1.967704
H -0.251851 -0.803902 -0.812348
O -0.016673 2.342193 0.519395

H	-0.090370	3.252904	0.203345
H	0.849906	2.003473	0.157554
O	2.190534	1.162688	-0.531373
H	1.727179	0.556861	-1.145926
H	2.513624	0.523944	0.142211
O	2.380040	-1.298871	0.863637
H	3.136555	-1.891816	0.753847
H	1.785988	-1.477936	0.092487

4g

N	1.524091	-0.147993	0.091789
H	0.888304	-0.175208	0.893363
C	2.261356	1.116527	0.103123
H	2.961484	1.201625	0.954269
H	2.843854	1.207453	-0.822791
H	1.553212	1.951480	0.143791
C	2.399969	-1.317538	0.112120
H	1.796645	-2.231213	0.163411
H	2.986795	-1.351560	-0.814897
H	3.108265	-1.316636	0.961103
O	-1.402095	1.961298	-0.175100
H	-1.136020	1.294657	-0.895629
H	-2.258105	2.319381	-0.449460
O	-1.232996	0.064060	1.675433
H	-1.643971	0.272344	2.526010
H	-1.383462	0.866387	1.085868
O	-0.563251	0.022833	-1.744069
H	-1.159640	-0.694644	-1.431668
H	0.267702	-0.110209	-1.192219
O	-2.238414	-1.695756	-0.208524
H	-2.023930	-2.621307	-0.026379
H	-1.943678	-1.190014	0.589333

4h

N	2.329891	-0.404744	-0.169088
H	2.901783	-1.026517	-0.740137
C	2.028357	-1.055115	1.108301
H	2.922336	-1.208377	1.738928
H	1.320509	-0.431046	1.667949
H	1.550179	-2.023732	0.926142
C	3.017605	0.877712	-0.004301

H	3.266444	1.291629	-0.987703
H	2.343995	1.582737	0.498835
H	3.943461	0.801786	0.593805
O	-0.123524	0.126093	-1.398031
H	0.768076	-0.105807	-1.005452
H	-0.713233	-0.638819	-1.182133
O	-1.912571	-1.791299	-0.479078
H	-2.444919	-1.135915	0.053368
H	-2.537089	-2.168893	-1.114494
O	-3.161974	0.203519	0.861624
H	-3.163909	0.153090	1.827827
H	-2.514474	0.935297	0.631538
O	-1.282419	1.948439	0.095869
H	-0.792366	1.307510	-0.522969
H	-1.591900	2.670662	-0.468964

4i

N	2.133394	-0.395600	0.176489
H	2.852657	-0.916110	0.678075
C	2.652251	0.925968	-0.187154
H	3.459136	0.881485	-0.940378
H	1.834342	1.532487	-0.595787
H	3.032274	1.431202	0.707696
C	1.693937	-1.170526	-0.988304
H	1.348984	-2.158856	-0.665798
H	0.846177	-0.659909	-1.461476
H	2.486352	-1.296268	-1.747632
O	-1.179743	2.102943	0.097502
H	-1.823777	2.726098	0.461542
H	-1.702461	1.485188	-0.482769
O	-1.826984	-1.709978	0.530520
H	-2.495133	-1.992026	1.170610
H	-1.194536	-1.102302	1.045726
O	-2.345031	0.123098	-1.345679
H	-3.248712	0.101669	-1.688349
H	-2.276881	-0.628096	-0.684504
O	-0.186205	0.002606	1.662774
H	0.694444	-0.154507	1.205617
H	-0.520049	0.837141	1.253815

4j

N	1.564457	-0.158068	0.034534
H	1.145314	0.759376	0.256474
C	2.636851	0.023999	-0.944971
H	3.488691	0.599857	-0.543114
H	3.016624	-0.953723	-1.270549
H	2.246433	0.549898	-1.823449
C	2.031507	-0.785838	1.272177
H	1.207549	-0.831699	1.992516
H	2.368051	-1.810810	1.067282
H	2.869764	-0.238990	1.737869
O	-0.636885	-1.285468	-0.957130
H	-0.441219	-2.001616	-1.576890
H	0.267238	-0.923491	-0.597166
O	-0.054847	2.204068	0.638762
H	0.036452	3.145884	0.440028
H	-0.877244	1.906705	0.153815
O	-2.143575	1.151986	-0.720156
H	-1.639628	0.463686	-1.200755
H	-2.643316	0.593916	-0.082872
O	-2.837130	-1.180715	0.711382
H	-2.613131	-1.293727	1.645819
H	-2.013428	-1.406725	0.213158

5a

N	-1.725153	0.013226	-0.068024
H	-1.144998	0.239274	0.763072
C	-2.930673	-0.703228	0.353235
H	-3.600024	-0.076737	0.966118
H	-3.494641	-1.040048	-0.527035
H	-2.648867	-1.584948	0.939899
C	-2.020908	1.253751	-0.793442
H	-1.087037	1.793670	-0.982620
H	-2.497939	1.020274	-1.754479
H	-2.697631	1.915144	-0.227067
O	0.274876	0.543305	1.980903
H	0.729971	1.236452	1.445977
H	0.819257	-0.257667	1.834571
O	0.092804	-1.450067	-1.211220
H	-0.247314	-2.057527	-1.882247
H	-0.723523	-0.879530	-0.818388
O	2.419202	0.090904	-1.253833

H	2.764727	-0.449520	-0.520283
H	1.588025	-0.391945	-1.479108
O	1.403448	2.241669	0.059218
H	2.081233	2.913469	0.217018
H	1.850734	1.524496	-0.471953
O	1.709245	-1.771865	0.936791
H	1.074180	-1.887495	0.181278
H	1.822803	-2.644644	1.337781

5b

N	1.734048	-0.046705	-0.083769
H	1.115728	-0.720669	-0.561284
C	2.846350	-0.771458	0.535441
H	3.505584	-1.252688	-0.206959
H	3.457474	-0.078820	1.129050
H	2.454318	-1.545352	1.204736
C	2.180162	0.964539	-1.048040
H	1.307610	1.446134	-1.502329
H	2.766572	1.735166	-0.530900
H	2.808994	0.537020	-1.847317
O	-1.405439	2.245759	-0.446667
H	-2.047087	2.907537	-0.152325
H	-0.951362	1.925582	0.375832
O	-0.061237	0.958284	1.559313
H	0.325995	1.355051	2.352288
H	0.727487	0.586146	0.970170
O	-2.491118	-0.274028	-1.030473
H	-2.570160	-0.563406	-0.090460
H	-2.189803	0.663482	-0.952578
O	-1.809176	-1.288313	1.512858
H	-1.209758	-0.528045	1.691758
H	-1.267035	-1.877724	0.957660
O	-0.355072	-1.849366	-1.110067
H	-0.399406	-2.509983	-1.815039
H	-1.156229	-1.249672	-1.240040

5c

N	-1.925222	-0.251623	0.139731
H	-1.624699	0.713863	0.364062
C	-3.179059	-0.200953	-0.616185
H	-3.452233	-1.208669	-0.957074

H	-4.017559	0.194513	-0.018428
H	-3.050167	0.440610	-1.494714
C	-2.044237	-1.020593	1.380566
H	-1.101242	-0.966036	1.936172
H	-2.854591	-0.651512	2.032293
H	-2.248753	-2.074570	1.149984
O	2.309913	-1.969780	0.098102
H	2.025198	-2.562234	0.807732
H	1.480477	-1.712892	-0.391721
O	0.173659	-1.010148	-1.249238
H	-0.076744	-1.404113	-2.096588
H	-0.712031	-0.761130	-0.731380
O	-0.824828	2.408202	0.429560
H	0.045155	2.193240	-0.023165
H	-0.586853	2.907393	1.222661
O	1.358299	1.578626	-0.888710
H	2.104564	1.306195	-0.297835
H	0.998459	0.721624	-1.205466
O	3.313877	0.477696	0.754940
H	3.026947	-0.458581	0.580242
H	4.213040	0.536167	0.401599

5d

N	-2.032330	-0.173108	-0.075809
H	-1.709112	0.752066	-0.383403
C	-3.254020	-0.032505	0.713459
H	-4.114984	0.325466	0.119391
H	-3.526468	-1.002435	1.149903
H	-3.081931	0.671616	1.535371
C	-2.203071	-1.044204	-1.237997
H	-1.272951	-1.071518	-1.816230
H	-2.424585	-2.066460	-0.903903
H	-3.022816	-0.719661	-1.904578
O	1.880362	-2.130196	-0.191115
H	1.187977	-1.716509	0.429715
H	2.299084	-2.839810	0.316120
O	0.197314	-0.850761	1.358774
H	-0.663395	-0.644222	0.857388
H	0.659369	0.012263	1.395158
O	3.298927	0.054941	-0.634833
H	3.294680	0.217771	-1.588972

H	2.835303	-0.833656	-0.510561
O	1.673294	1.585180	0.774085
H	2.188503	2.131729	1.383528
H	2.342103	1.075079	0.214231
O	-0.506109	2.329361	-0.764102
H	0.296783	2.189900	-0.205656
H	-0.669011	3.282188	-0.752080

5e

N	-1.738467	-0.235460	0.104145
H	-1.201248	0.204226	0.857637
C	-1.883497	-1.663558	0.383813
H	-2.538708	-1.870444	1.250076
H	-2.314680	-2.168504	-0.490758
H	-0.898522	-2.100813	0.581851
C	-3.022173	0.443804	-0.057049
H	-2.856900	1.517096	-0.205633
H	-3.534006	0.055570	-0.947210
H	-3.698208	0.308925	0.807698
O	0.126894	0.312914	-1.897616
H	-0.602249	0.098659	-1.237751
H	0.487638	1.168962	-1.567005
O	2.074257	-1.151986	1.317046
H	3.011762	-1.054683	1.537209
H	2.059228	-1.309480	0.317166
O	2.003142	-1.408352	-1.298648
H	1.278857	-0.758000	-1.602292
H	1.789476	-2.258904	-1.706231
O	0.574258	0.990737	1.769844
H	1.182173	0.193979	1.646720
H	0.702616	1.282443	2.683224
O	1.119009	2.531607	-0.461986
H	0.615607	3.357700	-0.454515
H	0.939990	2.100646	0.411089

5f

N	1.896964	-0.244501	-0.101252
H	1.180592	-0.558611	0.579402
C	3.202085	-0.173866	0.556285
H	3.575566	-1.165093	0.866427
H	3.942675	0.266931	-0.124963

H	3.132254	0.460510	1.447405
C	1.891719	-1.151023	-1.252073
H	0.871667	-1.241422	-1.640919
H	2.532979	-0.749940	-2.048039
H	2.254435	-2.161227	-0.995209
O	-0.354275	-0.820705	1.660450
H	-0.751369	0.070202	1.591055
H	-0.953356	-1.378439	1.106496
O	0.776621	2.075372	-0.700955
H	1.387962	2.806403	-0.534487
H	1.297304	1.191132	-0.484738
O	-1.388521	1.760091	0.729043
H	-1.673742	2.562231	1.187828
H	-0.551228	1.995757	0.205077
O	-3.125442	0.327017	-0.798865
H	-3.015223	0.594301	-1.722539
H	-2.531276	0.931735	-0.278624
O	-2.064993	-2.097252	-0.145582
H	-2.766532	-2.656130	0.217603
H	-2.521398	-1.263679	-0.441022

5g

N	-1.971948	-0.297461	-0.113938
H	-1.182660	-0.656172	0.454748
C	-2.091851	-1.101978	-1.330090
H	-2.386852	-2.145632	-1.123395
H	-2.847285	-0.665210	-1.997316
H	-1.131534	-1.113620	-1.858879
C	-3.195518	-0.303212	0.689722
H	-3.026570	0.255548	1.616518
H	-4.008600	0.186250	0.137370
H	-3.525296	-1.323269	0.952602
O	2.530461	-2.043507	-0.000495
H	2.333688	-2.599886	-0.767157
H	2.809817	-1.167784	-0.377552
O	0.398896	-0.919880	1.456041
H	0.745288	-0.005485	1.406453
H	1.095631	-1.449274	1.000307
O	1.287885	1.752031	0.705973
H	1.464280	2.487910	1.308365
H	0.423409	1.977675	0.218354

O	3.112971	0.486451	-0.871215
H	4.010550	0.791987	-0.678370
H	2.514211	1.039103	-0.302014
O	-1.001165	2.143548	-0.480488
H	-0.954473	2.354841	-1.423745
H	-1.438144	1.197247	-0.405049

5h

N	-1.775838	-0.059649	0.091040
H	-1.027391	-0.757997	0.269519
C	-2.437849	-0.406374	-1.169901
H	-2.974902	-1.368214	-1.112748
H	-3.165007	0.371875	-1.439089
H	-1.689257	-0.475408	-1.967304
C	-2.701257	-0.043296	1.225888
H	-2.146899	0.162308	2.148329
H	-3.446596	0.751833	1.091191
H	-3.237859	-0.999769	1.346126
O	2.316473	-0.392018	1.872455
H	2.043043	0.043083	2.692388
H	2.279424	0.311928	1.179533
O	0.416384	-1.934748	0.407775
H	1.049082	-1.538763	1.048507
H	0.842615	-1.754772	-0.460586
O	2.051672	1.312310	-0.302905
H	1.110255	1.713100	-0.254634
H	2.661597	2.048771	-0.449492
O	1.638943	-0.896553	-1.944248
H	1.908631	-0.076769	-1.462990
H	2.466299	-1.319863	-2.214286
O	-0.386435	2.165195	-0.095679
H	-0.983724	1.293293	-0.040883
H	-0.720103	2.677438	-0.845957

5i

N	-2.296659	-0.434505	-0.282812
H	-2.477502	-1.437984	-0.256145
C	-1.617361	-0.098324	-1.537552
H	-2.253535	-0.251185	-2.427835
H	-1.319656	0.957511	-1.509105
H	-0.708557	-0.701708	-1.639930

C	-3.553410	0.292658	-0.100568
H	-4.038328	-0.034065	0.825949
H	-3.337918	1.364727	-0.009881
H	-4.261145	0.158044	-0.938676
O	1.222602	-2.126114	1.223520
H	1.975194	-2.251637	1.818297
H	1.617065	-1.855583	0.348662
O	2.664206	1.329117	-0.853994
H	2.517532	1.877801	-1.637422
H	2.011108	1.675611	-0.165903
O	-0.420543	0.052258	1.724647
H	0.177683	-0.732912	1.648644
H	-1.138550	-0.125315	1.046425
O	2.103457	-1.258560	-1.187847
H	2.340790	-0.285958	-1.101616
H	2.885102	-1.684353	-1.566792
O	0.873093	2.157466	0.898657
H	0.368655	1.343593	1.254865
H	1.200788	2.625610	1.679003

5j

N	2.160391	-0.005241	0.291611
H	1.785387	0.875192	-0.071046
C	3.590690	-0.091205	0.005770
H	4.192554	0.652225	0.560723
H	3.958566	-1.089530	0.276229
H	3.761050	0.052311	-1.067017
C	1.854117	-0.117249	1.716148
H	0.776017	0.004552	1.871752
H	2.137934	-1.115616	2.074181
H	2.386456	0.626866	2.337261
O	-3.105197	-0.331612	0.960641
H	-2.613732	-1.072447	0.485275
H	-4.027781	-0.422495	0.682768
O	0.013781	1.708230	-1.324509
H	-0.773171	1.868757	-0.726384
H	-0.089388	2.330630	-2.057794
O	-1.803987	-2.211901	-0.365755
H	-1.512860	-2.996636	0.118526
H	-0.970012	-1.821646	-0.791870
O	-2.094412	2.037358	0.293778

H	-2.490423	1.148263	0.547206
H	-1.925964	2.491707	1.131021
O	0.306917	-1.096043	-1.471071
H	0.040619	-0.172932	-1.681676
H	1.036351	-0.920056	-0.806624

5k

N	-2.775485	-0.489752	0.098344
H	-3.503656	-1.121994	-0.232657
C	-3.220473	0.897377	-0.069111
H	-4.058002	1.166587	0.599157
H	-2.380125	1.571593	0.138451
H	-3.530927	1.059143	-1.107147
C	-2.444606	-0.810927	1.487641
H	-2.181885	-1.871566	1.571074
H	-1.571842	-0.220956	1.794239
H	-3.267539	-0.594298	2.192660
O	-0.409838	-0.532524	-1.422895
H	-1.266163	-0.600708	-0.913340
H	-0.097327	0.391172	-1.245864
O	2.625069	1.771552	0.687198
H	2.899635	0.805090	0.705800
H	2.565341	2.040520	1.614484
O	0.372304	2.029139	-0.748337
H	0.606139	2.598380	-1.495086
H	1.207958	1.961775	-0.201856
O	3.310073	-0.802522	0.704214
H	2.629052	-1.336419	0.186968
H	4.149947	-0.957060	0.248965
O	1.520831	-2.154206	-0.698889
H	0.744789	-1.558311	-0.974526
H	1.125956	-2.914894	-0.251245

5l

N	-2.778696	-0.418925	0.052703
H	-3.442526	-1.064645	-0.373886
C	-3.367571	0.920661	0.112465
H	-4.220696	0.990582	0.811131
H	-2.600503	1.635694	0.435534
H	-3.704897	1.218518	-0.886375
C	-2.381277	-0.925267	1.367885

H	-1.977733	-1.938689	1.266654
H	-1.585873	-0.285765	1.770529
H	-3.210596	-0.939803	2.097866
O	0.584459	2.164681	-0.619337
H	0.846856	2.755733	-1.339185
H	1.428310	1.980843	-0.114934
O	-0.425452	-0.256724	-1.456219
H	-0.054347	0.627544	-1.203695
H	-1.290205	-0.328667	-0.958118
O	2.849982	1.610956	0.718535
H	3.026942	0.624033	0.705875
H	2.827705	1.860891	1.652611
O	1.215706	-2.137784	-0.699629
H	0.571269	-1.408339	-1.003552
H	1.488477	-2.588839	-1.511127
O	3.269479	-1.027851	0.551858
H	2.495587	-1.464953	0.075223
H	3.392804	-1.540259	1.362759

5m

N	-2.657764	-0.083392	-0.543948
H	-2.340167	-0.243715	-1.499711
C	-3.087233	1.309536	-0.401702
H	-3.978070	1.555158	-1.007262
H	-3.329017	1.502632	0.650938
H	-2.266909	1.978465	-0.684370
C	-3.711998	-1.043431	-0.214404
H	-3.350846	-2.062613	-0.391025
H	-3.959960	-0.952479	0.850510
H	-4.639692	-0.889863	-0.795012
O	-0.395845	-0.375138	1.082886
H	-1.204511	-0.296981	0.499114
H	0.058632	0.503366	1.011059
O	0.852549	2.054942	0.744049
H	1.721909	1.882873	0.280129
H	1.091692	2.507953	1.564959
O	3.174747	1.531827	-0.507155
H	3.185607	1.840757	-1.423683
H	3.315881	0.540061	-0.554916
O	1.229262	-2.258849	0.294272
H	0.584122	-1.531883	0.600132

H	1.366271	-2.817403	1.072506
O	3.485848	-1.125365	-0.506465
H	2.634314	-1.573823	-0.204925
H	3.737990	-1.574726	-1.324865

5n

N	-2.012702	-0.015420	-0.231630
H	-1.678628	-0.767169	0.391110
C	-1.655192	-0.336713	-1.615297
H	-2.246954	-1.176485	-2.019407
H	-1.826753	0.537572	-2.257445
H	-0.595308	-0.609133	-1.663580
C	-3.446333	0.202522	-0.045122
H	-3.660143	0.367655	1.017134
H	-3.764086	1.093557	-0.603106
H	-4.055919	-0.649258	-0.393968
O	-0.303071	1.626286	0.961145
H	-0.742572	2.369313	1.397696
H	-1.033232	1.093123	0.447418
O	2.038869	2.113621	-0.222070
H	1.135840	1.970987	0.187540
H	1.877363	2.539778	-1.075343
O	3.373761	-0.202237	-0.423281
H	4.024497	-0.195420	0.292897
H	2.895095	0.673866	-0.347295
O	-0.315687	-1.405388	1.718566
H	-0.069496	-0.479961	1.890639
H	0.364125	-1.715457	1.069805
O	1.455815	-2.097507	-0.296686
H	1.866002	-2.973112	-0.316025
H	2.210732	-1.444975	-0.335543

5o

N	2.701837	0.493307	0.125900
H	3.182424	1.391125	0.071459
C	3.250870	-0.413539	-0.887132
H	4.298508	-0.700201	-0.688746
H	2.645491	-1.328134	-0.915750
H	3.194965	0.059515	-1.873665
C	2.823068	-0.040132	1.486271
H	2.447156	0.695027	2.206046

H	2.206606	-0.943203	1.572922
H	3.860405	-0.305674	1.755768
O	-2.159411	2.309477	-0.936301
H	-1.968412	3.257676	-0.932133
H	-1.277838	1.864207	-0.883389
O	-0.013719	0.664559	-0.388840
H	-0.223621	-0.220583	-0.790784
H	0.976865	0.674448	-0.221505
O	-0.786204	-1.804316	-1.271757
H	-1.208401	-1.784924	-2.142415
H	-1.535843	-1.923264	-0.619391
O	-2.125263	0.644712	1.401194
H	-2.552539	1.305374	0.817574
H	-1.221706	0.622951	0.997909
O	-2.664557	-1.872400	0.660052
H	-2.584117	-0.924664	0.985283
H	-3.603196	-2.007060	0.469895

5p

N	2.629066	-0.238726	0.131050
H	2.520507	-0.385475	1.135124
C	4.045676	-0.023466	-0.173303
H	4.669618	-0.913554	0.021522
H	4.151175	0.235144	-1.234514
H	4.428638	0.814699	0.419067
C	2.058128	-1.389904	-0.578367
H	1.034648	-1.563440	-0.228427
H	2.031157	-1.173060	-1.654127
H	2.647559	-2.312705	-0.434598
O	-1.106425	-1.510356	1.040839
H	-1.382270	-1.939764	1.863219
H	-1.894996	-1.591975	0.429022
O	-3.259293	-1.457721	-0.571159
H	-3.165706	-1.800612	-1.470988
H	-3.344185	-0.459879	-0.669974
O	1.149021	2.068179	-0.147948
H	1.013014	2.271866	-1.084353
H	1.704608	1.223981	-0.123393
O	-3.239548	1.200578	-0.681480
H	-3.995983	1.657533	-0.287429
H	-2.470198	1.338440	-0.034511

O	-1.229889	1.298953	1.010700
H	-0.383684	1.624875	0.607351
H	-1.101106	0.328166	1.132058

5q

N	-2.611569	0.030608	-0.281013
H	-1.670082	-0.047144	-0.678370
C	-3.185648	1.329479	-0.626856
H	-3.395280	1.437857	-1.706570
H	-4.130989	1.470093	-0.086496
H	-2.498423	2.128280	-0.325450
C	-3.433391	-1.094070	-0.726237
H	-2.928028	-2.035949	-0.486227
H	-4.393815	-1.079060	-0.195062
H	-3.645125	-1.073193	-1.810669
O	0.467321	-0.106743	0.028596
H	0.006279	-0.248256	0.894551
H	1.111252	-0.855999	-0.085252
O	2.505530	-1.893002	-0.301592
H	3.236333	-1.212552	-0.327333
H	2.568900	-2.370884	-1.140432
O	-1.322471	-0.385131	2.094323
H	-1.405489	0.325189	2.746171
H	-1.969771	-0.167665	1.350374
O	2.232607	1.886529	0.055953
H	2.046936	2.470179	-0.693160
H	1.495289	1.199856	0.055949
O	4.257765	0.164558	-0.334911
H	4.859488	0.214285	0.421441
H	3.581717	0.888558	-0.186771

5r

N	-2.880087	-0.150623	-0.273599
H	-3.164571	-0.244723	-1.248598
C	-3.608981	0.963431	0.337797
H	-4.694604	0.778794	0.420868
H	-3.216176	1.138077	1.347034
H	-3.451406	1.875034	-0.249189
C	-3.104192	-1.423478	0.418939
H	-2.573071	-2.226126	-0.104124
H	-2.694985	-1.354917	1.434320

H	-4.172294	-1.692107	0.496989
O	2.351131	1.137407	1.218119
H	2.925191	0.362435	0.976552
H	1.465564	0.737277	1.297925
O	1.360863	-1.907792	-0.883299
H	0.757686	-1.137603	-0.655118
H	1.483649	-1.857503	-1.842182
O	3.635253	-1.135207	0.372015
H	3.865045	-1.788975	1.047264
H	2.839003	-1.508660	-0.101101
O	-0.129083	0.177464	-0.124064
H	-1.125829	0.124658	-0.227159
H	0.187065	0.999318	-0.574667
O	1.391146	2.278578	-1.024481
H	1.219122	3.220522	-0.886642
H	1.915777	1.985545	-0.223716

6a

N	-2.177614	-0.159149	-0.054698
H	-1.670039	0.054562	0.812617
C	-2.644733	1.096125	-0.653644
H	-3.057965	0.897022	-1.650897
H	-3.429656	1.584936	-0.050968
H	-1.800573	1.786289	-0.755001
C	-3.267079	-1.093908	0.235012
H	-2.865801	-1.985652	0.729491
H	-4.046910	-0.654434	0.880757
H	-3.745191	-1.406586	-0.702586
O	3.562737	-0.504187	0.067276
H	2.816416	-1.034658	0.476893
H	4.200171	-1.155083	-0.257852
O	-0.135944	-1.248083	-1.378941
H	-0.420935	-1.859351	-2.072313
H	-0.988549	-0.852942	-0.939149
O	1.349047	-1.721477	0.987997
H	0.837800	-1.749392	0.147012
H	0.902726	-1.003713	1.494724
O	-0.068332	0.496300	2.023991
H	-0.010364	0.795216	2.941929
H	0.281937	1.251098	1.454998
O	0.692837	2.322178	0.262231

H	1.153448	1.781645	-0.468605
H	1.311172	3.031576	0.486546
O	1.796922	0.802573	-1.570061
H	2.542168	0.351753	-1.091596
H	1.126186	0.090032	-1.681276

6b

N	2.228156	0.012962	-0.114018
H	1.626047	-0.676532	-0.584183
C	2.500528	1.124490	-1.030985
H	3.047337	1.914803	-0.500823
H	3.103130	0.817621	-1.902627
H	1.555040	1.545496	-1.389460
C	3.447169	-0.648733	0.356067
H	3.181208	-1.503960	0.987313
H	4.083860	-1.007337	-0.470991
H	4.041045	0.051524	0.957927
O	-0.003282	-1.747290	-1.056115
H	-0.454355	-1.782655	-0.147266
H	-0.053889	-2.641691	-1.421446
O	-1.164448	-1.546271	1.302932
H	-0.632821	-0.796799	1.659606
H	-2.037053	-1.141926	1.072181
O	-1.838665	0.278176	-1.846203
H	-1.492188	1.031827	-1.307227
H	-1.164078	-0.431719	-1.745271
O	0.464882	0.695321	1.748180
H	1.234639	0.467619	1.084654
H	0.863910	1.037048	2.560509
O	-1.363610	2.134997	0.196012
H	-0.703663	1.727205	0.806779
H	-2.218067	1.807464	0.528574
O	-3.353661	-0.165580	0.294829
H	-4.259535	-0.476047	0.158943
H	-2.933577	-0.082034	-0.616640

6c

N	-2.163958	-0.466697	-0.408709
H	-1.306776	-0.268000	-0.938278
C	-2.396697	-1.914593	-0.400439
H	-3.244718	-2.147369	0.256710

H	-2.624363	-2.312889	-1.403856
H	-1.505934	-2.419672	-0.011751
C	-3.275093	0.291244	-0.990858
H	-3.017138	1.355636	-1.017609
H	-3.523896	-0.037359	-2.014267
H	-4.171344	0.167721	-0.369020
O	-1.251497	0.483036	1.901406
H	-1.714721	0.088540	1.055085
H	-1.921587	0.541630	2.596829
O	0.934900	-1.177471	0.979124
H	0.361481	-0.758385	1.649830
H	0.788910	-0.600652	0.177898
O	-0.247256	2.590490	0.488348
H	-0.603566	1.944970	1.153970
H	0.427555	3.103747	0.954644
O	0.595086	0.509114	-1.156280
H	1.549538	0.529702	-1.431581
H	0.424938	1.361821	-0.686240
O	3.595118	-1.030609	0.757548
H	2.626543	-1.115866	1.000523
H	4.012545	-0.570126	1.498824
O	3.302823	0.418327	-1.510294
H	3.677139	-0.082098	-2.248922
H	3.510451	-0.117473	-0.692859

6d

N	-1.796851	-0.565204	-0.209296
H	-1.169844	-0.681638	0.613647
C	-3.189545	-0.711258	0.220040
H	-3.866051	-0.485207	-0.615177
H	-3.414430	-1.731135	0.573661
H	-3.397990	-0.009575	1.035312
C	-1.417438	-1.528329	-1.248858
H	-0.351461	-1.422750	-1.478815
H	-1.609036	-2.569771	-0.939968
H	-1.992234	-1.335305	-2.164400
O	2.306055	-1.857623	1.118505
H	2.351873	-1.569136	0.166293
H	2.215590	-2.820503	1.091924
O	0.477403	2.239989	1.442294
H	-0.221884	2.275834	0.737574

H	0.290576	2.965387	2.054227
O	-1.045496	1.846915	-0.760476
H	-1.441146	0.856828	-0.594973
H	-1.705020	2.376049	-1.229293
O	0.020071	-0.555135	2.025003
H	0.259848	0.394706	1.999442
H	0.850178	-1.032782	1.777052
O	2.289914	-0.919780	-1.433288
H	3.116065	-0.972642	-1.934165
H	2.083395	0.061334	-1.367200
O	1.666135	1.669430	-1.207683
H	0.681462	1.746700	-1.271590
H	1.827316	1.957191	-0.290417

6e

N	-2.280366	-0.082722	-0.122090
H	-1.797880	0.013095	0.776665
C	-2.739102	1.231001	-0.570993
H	-3.113586	1.158392	-1.600656
H	-3.551522	1.642970	0.055738
H	-1.901041	1.937071	-0.558812
C	-3.365952	-1.054299	-0.000752
H	-2.973381	-1.998019	0.394235
H	-4.184551	-0.709688	0.657774
H	-3.792987	-1.254133	-0.992137
O	0.895841	2.241388	0.709967
H	0.552238	1.497425	1.292270
H	1.589505	2.672091	1.229905
O	-0.062932	0.139797	2.038895
H	-0.009832	0.046576	3.000112
H	0.447371	-0.661025	1.634767
O	-0.117304	-1.170015	-1.486971
H	-0.937830	-0.747524	-1.081806
H	0.470176	-0.417420	-1.698057
O	3.566327	-0.697187	-0.063520
H	4.061818	-1.293301	-0.643213
H	3.090374	-0.077118	-0.668935
O	1.138010	-1.797135	0.833816
H	0.670823	-1.710593	-0.049580
H	2.063301	-1.522527	0.626967
O	1.868762	1.003606	-1.443239

H	1.513262	1.535420	-0.666470
H	2.087000	1.643522	-2.135246

6f

N	1.606180	-0.367284	-0.021210
H	0.913469	-0.575832	0.772266
C	2.103653	-1.651840	-0.553251
H	2.734794	-1.471713	-1.430730
H	2.688813	-2.175947	0.210962
H	1.245764	-2.269422	-0.836771
C	2.666510	0.534711	0.473610
H	2.203614	1.470918	0.800284
H	3.197996	0.068234	1.310651
H	3.376718	0.747755	-0.333366
O	0.040922	2.822737	0.145790
H	0.047308	2.217356	-0.668961
H	-0.276620	3.684152	-0.158236
O	-0.232829	-0.969716	1.874191
H	-0.839153	-0.174118	1.838144
H	-0.716254	-1.648733	1.346416
O	0.070762	0.928019	-1.658389
H	0.341385	1.070996	-2.575280
H	1.005365	0.161388	-0.801286
O	-1.409484	-2.532643	-0.134426
H	-1.789625	-1.730177	-0.591182
H	-2.160411	-3.118787	0.033714
O	-2.162362	-0.155453	-1.167721
H	-1.269620	0.298489	-1.485633
H	-2.820642	-0.009927	-1.860684
O	-1.847753	1.166636	1.373581
H	-1.224790	1.865769	1.053665
H	-2.196396	0.786715	0.538140

6g

N	1.763063	-0.340600	-0.054115
H	1.590360	0.679601	-0.158486
C	1.648848	-0.962346	-1.383619
H	2.432859	-0.603751	-2.068025
H	1.737233	-2.052274	-1.291024
H	0.669889	-0.724597	-1.812618
C	3.087377	-0.534823	0.547632

H	3.132452	-0.015789	1.511730
H	3.267083	-1.604385	0.718098
H	3.893984	-0.150843	-0.096120
O	-1.407347	1.020284	2.245038
H	-2.248807	0.781063	2.657839
H	-0.949535	0.159119	2.044753
O	-1.917052	-2.303162	-0.218257
H	-1.251079	-1.975946	0.455794
H	-2.732716	-2.455916	0.279225
O	-1.470863	2.108704	-0.327290
H	-1.696951	1.340017	-0.903573
H	-1.549159	1.765442	0.595558
O	1.158167	2.403740	-0.602259
H	1.426272	3.188510	-0.104873
H	0.153430	2.368906	-0.520149
O	-0.101131	-1.235801	1.445821
H	0.742354	-0.852578	0.807416
H	0.282925	-1.804800	2.128226
O	-1.885643	-0.168303	-1.899795
H	-2.590781	-0.203275	-2.560599
H	-1.998270	-0.978387	-1.331688

6h

N	-2.186469	-0.085104	-0.166444
H	-1.455708	-0.406179	-0.833418
C	-3.112886	-1.190322	0.094855
H	-3.820553	-0.907196	0.885486
H	-3.693715	-1.471120	-0.799283
H	-2.547775	-2.066440	0.431210
C	-2.851503	1.106337	-0.698746
H	-2.103600	1.878330	-0.911949
H	-3.414421	0.895994	-1.623414
H	-3.554905	1.506018	0.043798
O	0.088219	-1.078703	-1.618909
H	0.411544	-1.525931	-0.792346
H	0.748105	-0.369924	-1.747116
O	-0.509336	0.413588	1.746803
H	-1.282351	0.224381	1.022960
H	-0.932086	0.511986	2.611708
O	0.884171	2.382941	0.623083
H	1.435660	2.828865	1.281090

H	0.362813	1.687776	1.130751
O	0.966386	-1.919444	0.878531
H	1.912187	-1.666377	0.765741
H	0.556548	-1.162429	1.348477
O	2.176095	1.005795	-1.266060
H	2.531523	1.593486	-1.947235
H	1.723985	1.590043	-0.586652
O	3.508962	-0.961978	0.151438
H	3.165365	-0.208885	-0.388510
H	4.133022	-0.570342	0.778060

6i

N	3.138154	-0.261360	-0.481984
H	3.401431	-0.869919	-1.257066
C	3.489793	1.123391	-0.812923
H	3.087180	1.790650	-0.040670
H	4.579224	1.288860	-0.876977
H	3.033377	1.399476	-1.769598
C	3.785841	-0.731737	0.745609
H	3.533097	-1.783948	0.916479
H	4.885009	-0.630276	0.722115
H	3.409411	-0.148933	1.595343
O	-3.503637	0.440106	-1.266058
H	-4.370973	0.124344	-1.555089
H	-2.864778	-0.300739	-1.466199
O	-0.538614	2.110423	0.571364
H	-1.399899	1.714848	0.923384
H	-0.816448	2.695775	-0.148214
O	-2.732698	0.818726	1.358703
H	-2.341695	-0.061696	1.558865
H	-3.164632	0.690549	0.476460
O	-1.629876	-1.510379	-1.558004
H	-0.820787	-1.046926	-1.216626
H	-1.839966	-2.119774	-0.830625
O	0.393827	-0.296527	-0.161309
H	0.136758	0.650336	0.041857
H	1.391312	-0.317383	-0.294637
O	-1.248787	-1.620390	1.508465
H	-0.488714	-1.192290	1.024695
H	-0.891511	-1.939029	2.348985

6j

N	2.472693	-0.317444	-0.233129
H	1.696716	-0.700244	0.319971
C	2.537562	-1.011877	-1.518376
H	3.287579	-0.532435	-2.161342
H	2.810546	-2.078301	-1.420033
H	1.565923	-0.947077	-2.021626
C	3.715211	-0.428402	0.531966
H	3.593774	0.063793	1.503253
H	4.024832	-1.475404	0.702751
H	4.525880	0.080612	-0.005254
O	1.652863	2.290337	-0.279892
H	1.999191	1.337668	-0.355395
H	1.485058	2.585718	-1.186237
O	-0.654858	1.653257	1.061113
H	0.157358	1.975743	0.585876
H	-0.469195	0.702051	1.237149
O	-2.761718	1.805904	-0.485656
H	-1.944865	1.769963	0.118138
H	-3.305506	2.528717	-0.143260
O	-3.816573	-0.612643	-0.680416
H	-4.619520	-0.643310	-0.141639
H	-3.466523	0.329748	-0.595773
O	-2.002528	-2.362094	0.127072
H	-1.778608	-2.891905	-0.650687
H	-2.700717	-1.705687	-0.185316
O	-0.029397	-1.089287	1.357654
H	-0.032545	-1.421651	2.266560
H	-0.757181	-1.598002	0.884221

6k

N	-2.985368	-0.213536	-0.380093
H	-3.304366	-0.641188	-1.249448
C	-3.661208	-0.855110	0.751443
H	-3.231415	-0.477205	1.687226
H	-4.748399	-0.663941	0.771980
H	-3.493358	-1.937006	0.716069
C	-3.222685	1.231702	-0.438195
H	-2.735045	1.650019	-1.325571
H	-4.294666	1.494776	-0.463424
H	-2.777865	1.703129	0.446938

O	-0.263225	-0.606452	-0.076222
H	-1.248652	-0.480677	-0.232503
H	0.232530	-0.061127	-0.757049
O	1.486261	0.626030	1.772572
H	2.241930	0.124537	1.398772
H	0.719166	0.199390	1.323456
O	1.240935	-2.800754	-0.090555
H	0.544407	-2.077547	-0.103234
H	1.134487	-3.273283	-0.928472
O	3.148963	-0.911427	-0.039147
H	2.572154	-1.728744	-0.066706
H	4.065191	-1.218897	-0.002001
O	1.421208	0.778416	-1.661481
H	1.500249	1.629051	-1.160080
H	2.197329	0.266687	-1.351688
O	1.728923	2.804866	0.190630
H	1.622516	2.098472	0.891951
H	1.100233	3.503307	0.418571

6l

N	3.078233	0.109687	0.387458
H	3.443334	0.218611	1.333610
C	3.612715	-1.123486	-0.198778
H	3.118871	-1.307491	-1.160880
H	4.702008	-1.082336	-0.373363
H	3.392776	-1.970501	0.460122
C	3.410949	1.301755	-0.398922
H	3.026494	2.195608	0.104251
H	4.495802	1.422133	-0.563599
H	2.923429	1.231459	-1.379016
O	0.329328	-0.118332	0.381437
H	1.329931	-0.018995	0.444958
H	-0.067487	0.796213	0.468514
O	-0.931350	2.258097	0.596375
H	-1.158087	2.417310	1.524050
H	-1.807499	2.042762	0.152608
O	-0.716075	-1.338124	-1.823315
H	-0.258248	-0.848370	-1.086452
H	-0.779429	-0.699632	-2.548558
O	-1.454873	-1.442417	1.963449
H	-0.687117	-1.037291	1.478099

H	-1.204963	-2.364111	2.120031
O	-3.072461	-1.141202	-0.311342
H	-2.347174	-1.343442	-0.952313
H	-2.643283	-1.306828	0.563471
O	-3.147335	1.472496	-0.651257
H	-4.027392	1.821757	-0.455674
H	-3.199447	0.471585	-0.498647

6m

N	-2.781542	-0.546772	0.206607
H	-3.334540	-1.076242	0.880299
C	-3.399754	0.765940	-0.000983
H	-2.743965	1.374327	-0.636028
H	-4.388262	0.707573	-0.489457
H	-3.513683	1.277472	0.961439
C	-2.662585	-1.316902	-1.037805
H	-2.268525	-2.314555	-0.815623
H	-3.623300	-1.424478	-1.570549
H	-1.949386	-0.816687	-1.704401
O	0.754950	2.381863	1.464994
H	0.341260	1.477117	1.357178
H	0.024149	2.983646	1.664005
O	-0.131823	-0.099023	0.875824
H	0.254288	-0.068364	-0.063660
H	-1.111928	-0.284999	0.741652
O	1.819831	2.612899	-1.027869
H	2.758874	2.834808	-0.957893
H	1.475599	2.625428	-0.092777
O	1.613821	-1.997334	1.674733
H	0.887117	-1.335035	1.491209
H	1.165121	-2.820116	1.914604
O	0.985857	0.013252	-1.514553
H	1.397044	0.912602	-1.479127
H	1.722004	-0.637641	-1.396511
O	2.782025	-1.968455	-0.783164
H	2.430512	-2.049916	0.145732
H	3.725146	-1.777373	-0.683331

6n

N	2.479488	-0.300883	-0.032843
H	2.252886	0.693444	0.118062

C	2.820897	-0.924604	1.247515
H	2.946232	-2.006445	1.111683
H	3.753473	-0.523887	1.681219
H	2.007090	-0.763165	1.963326
C	3.560112	-0.404794	-1.016565
H	3.280743	0.136876	-1.927066
H	4.513656	0.009014	-0.646111
H	3.726222	-1.458449	-1.276254
O	0.097884	-1.105696	-0.907840
H	1.064341	-0.866339	-0.603046
H	0.119095	-1.127811	-1.876069
O	1.362794	2.446848	0.090978
H	1.403068	3.172981	0.728168
H	0.408235	2.181040	0.049795
O	-2.676545	-1.708078	-0.095500
H	-2.642498	-1.296502	0.801641
H	-1.732432	-1.782112	-0.340809
O	-1.063619	1.205578	0.005326
H	-0.645603	0.377031	-0.360194
H	-1.888231	1.278246	-0.544390
O	-3.267288	0.577291	-1.456445
H	-4.174960	0.869556	-1.292741
H	-3.187757	-0.315868	-1.012480
O	-2.358576	-0.018673	2.104128
H	-1.789357	-0.203375	2.864127
H	-1.813861	0.530176	1.480158

6o

N	-2.781542	-0.546772	0.206607
H	-3.334540	-1.076242	0.880299
C	-3.399754	0.765940	-0.000983
H	-2.743965	1.374327	-0.636028
H	-4.388262	0.707573	-0.489457
H	-3.513683	1.277472	0.961439
C	-2.662585	-1.316902	-1.037805
H	-2.268525	-2.314555	-0.815623
H	-3.623300	-1.424478	-1.570549
H	-1.949386	-0.816687	-1.704401
O	0.754950	2.381863	1.464994
H	0.341260	1.477117	1.357178
H	0.024149	2.983646	1.664005

O	-0.131823	-0.099023	0.875824
H	0.254288	-0.068364	-0.063660
H	-1.111928	-0.284999	0.741652
O	1.819831	2.612899	-1.027869
H	2.758874	2.834808	-0.957893
H	1.475599	2.625428	-0.092777
O	1.613821	-1.997334	1.674733
H	0.887117	-1.335035	1.491209
H	1.165121	-2.820116	1.914604
O	0.985857	0.013252	-1.514553
H	1.397044	0.912602	-1.479127
H	1.722004	-0.637641	-1.396511
O	2.782025	-1.968455	-0.783164
H	2.430512	-2.049916	0.145732
H	3.725146	-1.777373	-0.683331