

ELECTRONIC SUPPLEMENTARY INFORMATION

The aromaticity of verdazyl radicals and their closed-shell charged species

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Table S1. The calculated bond lengths (in Å) of the verdazyl heterocycle in the radical as well as in the anionic and cationic forms of the studied compounds.

Molecule	Neutral radical			Anions			Cations		
Bond	N ₁ -N ₂	N ₁ -C ₁	N ₂ -C ₂	N ₁ -N ₂	N ₁ -C ₁	N ₂ -C ₂	N ₁ -N ₂	N ₁ -C ₁	N ₂ -C ₂
1	1.355	1.385	1.333	1.431	1.372	1.323	1.290	1.408	1.347
2	1.355	1.385	1.330	1.431	1.372	1.324	1.290	1.409	1.345
3	1.355	1.385	1.330	1.431	1.372	1.324	1.290	1.410	1.344
4	1.353	1.388	1.329	1.427	1.374	1.324	1.289	1.412	1.343
5	1.354	1.386	1.329	1.433	1.373	1.322	1.288	1.411	1.344
6	1.354	1.389	1.329	1.433	1.373	1.323	1.288	1.411	1.342
7	1.353	1.387	1.329	1.432	1.373	1.323	1.288	1.412	1.340
8	1.353	1.389	1.328	1.428	1.375	1.323	1.288	1.411	1.340
9	1.345	1.458	1.335	1.397	1.451	1.329	1.296	1.473	1.340
10	1.344	1.453	1.335	1.397	1.450	1.330	1.295	1.473	1.340
11	1.342	1.460	1.335	1.393	1.452	1.330	1.294	1.475	1.340
12	1.340	1.451	1.335	1.393	1.447	1.329	1.294	1.462	1.340
13	1.343	1.450	1.335	1.398	1.446	1.328	1.295	1.460	1.345
14	1.344	1.450	1.336	1.398	1.446	1.328	1.296	1.459	1.348
15	1.360	1.388	1.322	1.445	1.370	1.318	1.290	1.419	1.329

2. The Cartesian coordinates of atoms in Å for the radicals and their charged forms of 1-15 compounds.

2.1. The 1-15 radicals

		1	
O	4.249417000	-0.007267000	0.006049000
C	3.032480000	-0.004375000	0.000349000
N	2.269355000	1.151834000	-0.004214000
C	2.918175000	2.453580000	0.001595000
H	3.991442000	2.303600000	-0.041313000
H	2.649720000	2.991487000	0.911686000
H	2.580145000	3.027531000	-0.861261000
N	0.914416000	1.182344000	-0.002264000
C	0.301401000	0.001683000	-0.001898000
N	0.909127000	-1.182231000	-0.002738000
N	2.264197000	-1.157481000	-0.003848000
C	2.907610000	-2.461767000	0.000734000
H	2.578336000	-3.029226000	-0.869947000
H	2.625808000	-3.004195000	0.904007000
H	3.981888000	-2.315819000	-0.028489000
C	-1.178434000	0.005135000	-0.000757000
C	-1.893688000	1.208005000	-0.000782000
H	-1.351531000	2.142753000	-0.001539000
C	-3.277575000	1.217638000	0.000109000
H	-3.829254000	2.148323000	0.000043000
C	-3.979726000	0.014311000	0.001046000
C	-3.282676000	-1.191977000	0.001140000
H	-3.824821000	-2.131629000	0.001895000

C	-1.896255000	-1.192888000	0.000251000
H	-1.359877000	-2.130943000	0.000296000
O	-5.342002000	0.076715000	0.001820000
H	-5.708707000	-0.814781000	0.002392000

2

O	4.270626000	0.000221000	0.003954000
C	3.053969000	0.000088000	0.002866000
N	2.288316000	-1.154868000	0.001773000
C	2.934306000	-2.458090000	0.002685000
H	4.008657000	-2.309846000	0.004162000
H	2.630672000	-3.013665000	-0.885047000
H	2.628238000	-3.013603000	0.889628000
N	0.933496000	-1.182169000	-0.000787000
C	0.323591000	-0.000105000	-0.002288000
N	0.933320000	1.182052000	-0.001020000
N	2.288110000	1.154963000	0.002769000
C	2.933968000	2.458251000	0.002047000
H	2.611506000	3.021508000	0.878039000
H	2.646828000	3.005896000	-0.896227000
H	4.008135000	2.310245000	0.023738000
C	-1.158412000	-0.000230000	-0.004056000
C	-1.873510000	-1.200292000	-0.007259000
H	-1.334600000	-2.137006000	-0.010493000
C	-3.260509000	-1.194817000	-0.010497000
H	-3.793247000	-2.138894000	-0.016915000
C	-3.981994000	-0.000282000	-0.008667000
C	-3.260392000	1.194551000	-0.009926000
H	-3.793350000	2.138534000	-0.015881000
C	-1.873693000	1.200069000	-0.006682000

H	-1.334600000	2.136676000	-0.009461000
C	-5.486933000	0.000263000	0.021381000
H	-5.895481000	-0.892468000	-0.454040000
H	-5.895542000	0.874894000	-0.486774000
H	-5.857244000	0.019671000	1.050869000

3

H	5.467935000	-0.000004000	-0.000128000
O	-3.842297000	-0.000007000	-0.000275000
C	-2.626036000	0.000010000	-0.000007000
N	-1.860227000	1.155274000	0.000198000
C	-2.506215000	2.458686000	-0.000073000
H	-3.580552000	2.310447000	0.001956000
H	-2.202999000	3.013226000	-0.888575000
H	-2.199708000	3.014921000	0.886199000
N	-0.505725000	1.181961000	0.000082000
C	0.103434000	0.000002000	0.000090000
N	-0.505732000	-1.181971000	0.000158000
N	-1.860223000	-1.155272000	0.000200000
C	-2.506252000	-2.458664000	-0.000036000
H	-3.580588000	-2.310408000	0.001617000
H	-2.200066000	-3.014758000	0.886439000
H	-2.202744000	-3.013356000	-0.888339000
C	1.587182000	-0.000004000	0.000025000
C	2.297106000	1.204219000	0.000031000
H	1.752906000	2.137686000	0.000082000
C	3.685165000	1.201620000	-0.000025000
H	4.221872000	2.142077000	-0.000017000
C	4.385161000	-0.000004000	-0.000087000
C	3.685166000	-1.201628000	-0.000095000

H	4.221871000	-2.142086000	-0.000144000
C	2.297105000	-1.204227000	-0.000041000
H	1.752907000	-2.137694000	-0.000048000

4

O	-4.493359000	-0.000334000	-0.000696000
C	-3.279102000	0.000064000	0.000159000
N	-2.513567000	1.157429000	-0.000820000
C	-3.161402000	2.460992000	-0.000464000
H	-4.235381000	2.311436000	-0.016156000
H	-2.844566000	3.021493000	-0.880047000
H	-2.870169000	3.010397000	0.895109000
N	-1.160634000	1.182765000	0.000208000
C	-0.554896000	0.000261000	0.000341000
N	-1.160519000	-1.182684000	0.000480000
N	-2.513103000	-1.157611000	0.001566000
C	-3.161095000	-2.460999000	-0.000183000
H	-2.839620000	-3.023617000	0.876305000
H	-2.873696000	-3.008206000	-0.898382000
H	-4.235018000	-2.311639000	0.021162000
C	0.927889000	0.000122000	0.000206000
C	1.637370000	1.205087000	0.000636000
H	1.093827000	2.138492000	0.001080000
C	3.021147000	1.208780000	0.000522000
H	3.564308000	2.144007000	0.000898000
C	3.725493000	-0.000006000	-0.000085000
C	3.021044000	-1.208709000	-0.000567000
H	3.564110000	-2.143992000	-0.001066000
C	1.637247000	-1.204898000	-0.000399000

H	1.093618000	-2.138245000	-0.000750000
C	5.154795000	-0.000062000	-0.000221000
N	6.307612000	-0.000076000	-0.000326000

5

N	1.713996000	1.154681000	-0.000214000
C	-2.449966000	1.209995000	-0.000533000
H	-1.907651000	2.144467000	-0.000959000
O	-5.900137000	0.082473000	-0.000047000
H	-6.267265000	-0.808785000	0.000957000
N	0.360254000	1.181457000	-0.000099000
C	-3.834027000	1.221221000	-0.000511000
H	-4.384640000	2.152572000	-0.000949000
O	3.691135000	-0.009607000	0.000425000
N	0.353035000	-1.180596000	-0.000082000
C	-4.537521000	0.018876000	0.000065000
H	-4.384015000	-2.127007000	0.001149000
N	1.706976000	-1.161692000	-0.000049000
C	-3.841262000	-1.187662000	0.000663000
C	-2.454625000	-1.189434000	0.000659000
H	-1.919752000	-2.128160000	0.001142000
C	-1.734650000	0.007223000	0.000040000
C	-0.253897000	0.002534000	-0.000065000
C	2.368751000	-2.482904000	-0.000206000
H	3.431055000	-2.251140000	-0.000077000
C	2.472883000	-0.005678000	0.000108000
H	3.444263000	2.234510000	-0.000550000
C	2.383297000	2.472329000	-0.000065000
C	2.036274000	3.244716000	-1.271194000
H	2.323058000	2.682323000	-2.161058000

H	2.574321000	4.193850000	-1.281613000
H	0.967209000	3.452704000	-1.321386000
C	2.037279000	3.243959000	1.271785000
H	2.324859000	2.681094000	2.161097000
H	0.968236000	3.451811000	1.322971000
H	2.575249000	4.193133000	1.282297000
C	2.018053000	-3.253383000	1.271080000
H	2.307745000	-2.692283000	2.160803000
H	2.551309000	-4.205226000	1.281631000
H	0.947920000	-3.455859000	1.321493000
C	2.018212000	-3.252868000	-1.271878000
H	2.550940000	-4.205009000	-1.282484000
H	0.947973000	-3.454739000	-1.322757000
H	2.308570000	-2.691661000	-2.161311000

6

C	-6.049225000	-0.000023000	0.021725000
H	-1.897017000	-2.136365000	-0.010348000
N	1.727438000	-1.158435000	0.000494000
C	-2.435357000	-1.199493000	-0.007304000
C	-3.822336000	-1.194393000	-0.010323000
O	3.707818000	0.000021000	0.004812000
N	0.373823000	-1.180881000	-0.002094000
H	-4.354962000	-2.138600000	-0.016265000
C	-4.544234000	-0.000059000	-0.008793000
N	0.373790000	1.180871000	-0.002059000
C	-3.822345000	1.194326000	-0.010680000
N	1.727423000	1.158460000	0.000488000
H	-4.355005000	2.138516000	-0.016913000
C	-2.435405000	1.199452000	-0.007672000

H	-1.897056000	2.136319000	-0.010997000
C	-1.718991000	-0.000028000	-0.004631000
C	-0.236231000	0.000005000	-0.003124000
C	2.392647000	2.478200000	0.002163000
H	3.454380000	2.243845000	0.003831000
C	2.489862000	0.000028000	0.002154000
C	2.392715000	-2.478152000	0.002112000
H	3.454437000	-2.243752000	0.003916000
C	2.041368000	-3.248577000	1.273232000
H	2.328789000	-2.686632000	2.163170000
H	2.576213000	-4.199499000	1.284977000
H	0.971514000	-3.452846000	1.321969000
C	2.045847000	-3.249450000	-1.269695000
H	2.580762000	-4.200362000	-1.278912000
H	0.976184000	-3.453805000	-1.322043000
H	2.336353000	-2.688108000	-2.159010000
C	2.045611000	3.249612000	-1.269526000
H	2.335984000	2.688343000	-2.158930000
H	2.580545000	4.200513000	-1.278729000
H	0.975945000	3.453994000	-1.321716000
C	2.041396000	3.248478000	1.273400000
H	0.971527000	3.452635000	1.322294000
H	2.576146000	4.199453000	1.285159000
H	2.328993000	2.686480000	2.163247000
H	-6.419619000	0.002558000	1.051344000
H	-6.457900000	-0.884986000	-0.468101000
H	-6.457992000	0.882478000	-0.472477000
7			
H	-5.964070000	0.000008000	0.000195000

N	1.365549000	1.158810000	-0.000195000
C	-2.792745000	1.203535000	-0.000828000
H	-2.249187000	2.137192000	-0.001526000
O	3.345585000	-0.000021000	0.000412000
C	-4.180884000	1.201323000	-0.000760000
N	0.012248000	1.180768000	-0.000071000
H	-4.717346000	2.141964000	-0.001456000
C	-4.881303000	0.000017000	0.000167000
N	0.012230000	-1.180762000	-0.000251000
N	1.365537000	-1.158816000	-0.000291000
C	-4.180876000	-1.201299000	0.001049000
H	-4.717348000	-2.141933000	0.001824000
C	-2.792745000	-1.203508000	0.000977000
H	-2.249168000	-2.137152000	0.001669000
C	-2.081573000	0.000020000	0.000023000
C	-0.597157000	0.000008000	-0.000124000
C	2.030898000	-2.478747000	-0.000370000
H	3.092589000	-2.244235000	-0.000562000
C	2.128012000	-0.000007000	0.000031000
C	2.030946000	2.478744000	0.000042000
H	3.092624000	2.244179000	-0.000308000
C	1.681506000	3.249781000	-1.271198000
H	0.611810000	3.454524000	-1.321391000
H	2.216594000	4.200555000	-1.281611000
H	1.970084000	2.688314000	-2.161049000
C	1.682200000	3.249058000	1.271897000
H	1.971270000	2.687099000	2.161282000
H	0.612535000	3.453766000	1.322784000
H	2.217303000	4.199819000	1.282547000

C	1.682058000	-3.249443000	1.271229000
H	0.612484000	-3.454718000	1.321712000
H	2.217651000	-4.199927000	1.281921000
H	1.970511000	-2.687484000	2.160813000
H	2.216648000	-4.200204000	-1.282483000
H	0.611860000	-3.454159000	-1.322173000
H	1.970193000	-2.687725000	-2.161528000
C	1.681553000	-3.249435000	-1.271850000

8

C	-5.442294000	-0.111999000	-0.028091000
C	-1.856998000	1.182713000	-0.055475000
H	-1.320855000	2.119374000	-0.095840000
O	-6.119026000	1.003533000	0.350000000
N	2.294931000	1.166937000	-0.013271000
N	0.942948000	1.179762000	-0.018898000
C	-3.243000000	1.172726000	-0.054475000
O	4.280038000	0.018219000	0.010957000
H	-3.761985000	2.122073000	-0.124642000
N	0.957276000	-1.183099000	0.012696000
C	-3.948346000	-0.032062000	-0.016126000
N	2.308736000	-1.154576000	0.019119000
H	-3.778546000	-2.160871000	0.018789000
C	-3.230217000	-1.228888000	0.006955000
C	-1.846458000	-1.222027000	0.016698000
H	-1.299452000	-2.152937000	0.044765000
C	-1.139533000	-0.015161000	-0.012859000
C	0.343856000	-0.005673000	-0.006085000
C	2.983189000	-2.471230000	0.037153000
H	4.043070000	-2.229035000	0.044472000

C	3.064136000	0.010590000	0.005885000
C	2.954491000	2.490791000	-0.025840000
H	4.017055000	2.260591000	-0.023295000
C	2.602795000	3.247396000	-1.304869000
H	2.892342000	2.677891000	-2.189189000
H	3.136205000	4.198793000	-1.324732000
H	1.532903000	3.450606000	-1.357180000
C	2.601819000	3.271032000	1.238763000
H	3.133768000	4.223472000	1.241090000
H	1.531532000	3.473528000	1.286891000
H	2.892078000	2.718539000	2.133613000
C	2.627865000	-3.232078000	1.312627000
H	2.901612000	-2.659183000	2.199839000
H	3.172761000	-4.176797000	1.337734000
H	1.560159000	-3.448677000	1.354092000
H	2.943376000	-2.698782000	-2.122882000
C	2.650447000	-3.254517000	-1.230908000
H	1.582937000	-3.468339000	-1.289169000
H	3.192324000	-4.201331000	-1.228388000
O	-6.050646000	-1.095938000	-0.347848000
H	-5.511961000	1.671730000	0.691532000

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N	0.621250000	-1.184760000	0.421935000
C	-1.296524000	0.000021000	-0.386924000
H	5.352258000	-2.138052000	0.377583000
C	-1.473029000	2.223962000	0.787082000
N	-0.715895000	1.160483000	0.278425000
H	5.351943000	2.138821000	0.367423000
N	-0.715569000	-1.160882000	0.277474000

C	-1.065204000	0.000679000	-1.899581000
H	2.893163000	2.135989000	0.348545000
C	1.233789000	0.000026000	0.365019000
N	0.620877000	1.184589000	0.422944000
H	2.893782000	-2.135722000	0.358794000
H	0.114825000	-2.931276000	2.041490000
C	3.432132000	1.199179000	0.364512000
C	7.046915000	-0.000269000	0.428443000
C	3.432724000	-1.198839000	0.370406000
H	-1.184394000	-4.825015000	2.942546000
C	2.715220000	0.000300000	0.369407000
H	-3.529748000	-5.194460000	2.217038000
C	-1.472480000	-2.224811000	0.785435000
H	-4.541006000	-3.655561000	0.553719000
H	-3.248981000	-1.816036000	-0.385183000
C	-0.901754000	3.099567000	1.721446000
C	-0.901196000	-3.100707000	1.719540000
H	0.114408000	2.930288000	2.043034000
C	4.819609000	-1.193618000	0.380111000
H	-1.185216000	4.823179000	2.945384000
C	-1.640515000	-4.160318000	2.219468000
H	-3.530782000	5.192332000	2.220534000
C	5.541861000	0.000750000	0.386954000
H	-4.542045000	3.653810000	0.556856000
C	-2.792118000	-2.444797000	0.366348000
H	-3.249733000	1.815054000	-0.383186000
C	-2.956531000	-4.368898000	1.816460000
H	-1.027186000	2.143123000	-2.070052000
C	4.819539000	1.194349000	0.374385000

H	-0.798151000	2.143637000	-4.517538000
C	-0.794637000	0.001741000	-4.682903000
H	-0.686467000	0.002158000	-5.760117000
C	-2.792857000	2.443668000	0.368469000
H	-0.797346000	-2.140270000	-4.519120000
C	-0.993641000	1.202195000	-2.602725000
H	-1.026298000	-2.141609000	-2.071580000
H	-2.361123000	-0.000272000	-0.173712000
C	-1.641286000	4.158708000	2.222072000
C	-3.523806000	3.501341000	0.891887000
C	-3.522882000	-3.502929000	0.889100000
C	-0.993172000	-1.200307000	-2.603608000
C	-2.957468000	4.367055000	1.819500000
C	-0.858944000	-1.199406000	-3.986971000
C	-0.859411000	1.202342000	-3.986106000
H	7.458339000	0.909327000	-0.011353000
H	7.460270000	-0.855073000	-0.109396000
H	7.411342000	-0.058159000	1.458677000

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N	0.869560000	1.184962000	-0.480036000
C	-1.015689000	0.000020000	0.400826000
H	5.599746000	2.142358000	-0.601575000
N	-0.460509000	-1.160448000	-0.286153000
C	-1.236149000	-2.226039000	-0.762026000
H	5.599685000	-2.141535000	-0.607583000
N	-0.460543000	1.160867000	-0.285662000
C	-0.726292000	-0.000231000	1.903344000
H	3.133168000	-2.136427000	-0.502026000
C	1.483521000	0.000257000	-0.445800000

N	0.869583000	-1.184479000	-0.480415000
H	3.133141000	2.136960000	-0.495649000
C	3.676818000	-1.202763000	-0.529440000
H	6.846445000	0.000553000	-0.658640000
H	0.298558000	2.930274000	-2.083013000
C	3.676835000	1.203428000	-0.526040000
H	-1.034342000	4.825973000	-2.929010000
C	2.965118000	0.000294000	-0.503263000
H	-3.346707000	5.198705000	-2.106467000
C	-1.236379000	2.226109000	-0.761945000
H	-4.290715000	3.660748000	-0.403221000
C	-0.702800000	-3.100633000	-1.719360000
H	-2.963451000	1.819155000	0.481035000
C	-0.702955000	3.101032000	-1.718970000
H	0.298475000	-2.929426000	-2.083863000
C	5.063830000	1.201382000	-0.584212000
H	-1.034097000	-4.825542000	-2.929495000
H	-3.345832000	-5.199387000	-2.105799000
C	-1.460876000	4.161810000	-2.187630000
C	5.764412000	0.000432000	-0.616451000
H	-4.289609000	-3.662106000	-0.401813000
C	-2.537210000	2.447452000	-0.288660000
H	-2.962748000	-1.819911000	0.481877000
C	-2.758676000	4.372138000	-1.730163000
H	-0.680127000	-2.142787000	2.073050000
C	5.063840000	-1.200567000	-0.587604000
H	-0.357434000	-2.142454000	4.509562000
C	-0.349676000	-0.000507000	4.674474000
H	-0.200078000	-0.000631000	5.746703000

C	-2.536654000	-2.447961000	-0.288110000
H	-0.361517000	2.141499000	4.510615000
C	-0.626855000	-1.201536000	2.603543000
H	-0.684089000	2.142331000	2.074023000
H	-2.087617000	0.000070000	0.228815000
C	-1.460513000	-4.161674000	-2.187787000
C	-3.286759000	-3.507571000	-0.779555000
C	-3.287524000	3.506787000	-0.780381000
C	-0.629085000	1.200967000	2.604126000
C	-2.757998000	-4.372584000	-1.729704000
C	-0.442063000	1.200438000	3.981367000
C	-0.439805000	-1.201271000	3.980807000

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N	0.156014000	1.186541000	-0.398278000
C	-1.780332000	-0.000090000	0.358177000
H	4.895927000	2.135705000	-0.247314000
C	-1.925985000	-2.231036000	-0.812594000
N	-1.181389000	-1.162019000	-0.291905000
H	4.895836000	-2.135482000	-0.244537000
N	-1.181451000	1.162116000	-0.291581000
C	-1.585471000	-0.000303000	1.875698000
H	2.408989000	-2.138474000	-0.280677000
C	0.762924000	0.000117000	-0.326320000
N	0.156081000	-1.186322000	-0.398666000
H	2.409061000	2.138766000	-0.283559000
N	6.485949000	0.000095000	-0.222570000
H	-0.317420000	2.926740000	-2.047796000
C	2.953470000	-1.205680000	-0.278286000
H	-1.594828000	4.824945000	-2.969112000

C	2.953505000	1.205956000	-0.279924000
C	2.242441000	0.000139000	-0.295692000
H	-3.948023000	5.205024000	-2.277281000
C	-1.926120000	2.231209000	-0.811968000
H	-4.990875000	3.673925000	-0.627246000
H	-3.719953000	1.829559000	0.333771000
C	-1.336584000	-3.100704000	-1.740089000
C	-1.336703000	3.101342000	-1.739032000
H	-0.317380000	-2.925811000	-2.048955000
C	4.337518000	1.211783000	-0.258413000
H	-1.594670000	-4.823874000	-2.970798000
C	-2.063745000	4.163560000	-2.251445000
H	-3.947654000	-5.204613000	-2.278653000
C	5.015807000	0.000107000	-0.248086000
H	-4.990438000	-3.674353000	-0.627817000
C	-3.250259000	2.455551000	-0.412124000
H	-3.719640000	-1.830100000	0.333664000
C	-3.384344000	4.377644000	-1.867206000
H	-1.550787000	-2.143490000	2.048441000
C	4.337480000	-1.211541000	-0.256825000
H	-1.374966000	-2.142543000	4.499189000
C	-1.375634000	-0.000685000	4.663933000
H	-1.290898000	-0.000828000	5.743144000
C	-3.250006000	-2.455742000	-0.412572000
H	-1.376120000	2.141229000	4.499878000
C	-1.528834000	-1.201854000	2.580390000
H	-1.551892000	2.142862000	2.049124000
H	-2.838555000	-0.000073000	0.115020000
C	-2.063550000	-4.162848000	-2.252778000

C	-3.968398000	-3.516113000	-0.947823000
C	-3.968724000	3.516007000	-0.947107000
C	-1.529472000	1.201074000	2.580778000
C	-3.384038000	-4.377292000	-1.868368000
C	-1.425430000	1.200331000	3.966696000
C	-1.424785000	-1.201492000	3.966323000
O	7.056192000	-1.081557000	-0.212515000
O	7.056245000	1.081728000	-0.213680000

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C	3.677481000	-4.658880000	0.522830000
H	4.234394000	-5.557791000	0.751483000
N	0.172425000	-1.188039000	-0.174354000
C	4.213942000	-3.695212000	-0.320909000
H	5.190767000	-3.843024000	-0.763597000
N	1.502258000	-1.166477000	-0.337952000
C	3.503367000	-2.540561000	-0.622488000
H	3.934408000	-1.829738000	-1.313224000
N	1.502261000	1.166470000	-0.337917000
N	0.172426000	1.188017000	-0.174328000
C	2.237149000	2.329925000	-0.062753000
H	3.934630000	1.829519000	-1.312834000
C	3.503478000	2.540437000	-0.622270000
H	5.190996000	3.842756000	-0.763172000
C	4.214040000	3.695095000	-0.320720000
H	4.234364000	5.557862000	0.751354000
H	1.980513000	5.196923000	1.726476000
C	3.677459000	4.658931000	0.522765000
C	2.411967000	4.455008000	1.066412000
H	0.717859000	3.140906000	1.214817000

H	-2.083693000	2.139046000	-0.145219000
C	1.694202000	3.304552000	0.784884000
C	-1.915029000	-0.000010000	-0.142414000
H	-4.567366000	2.135530000	-0.038304000
N	-6.156443000	-0.000022000	0.028880000
C	-2.626530000	1.205780000	-0.117157000
C	-4.009435000	1.211475000	-0.059310000
H	-4.567373000	-2.135559000	-0.038792000
C	-4.687503000	-0.000022000	-0.030305000
H	-2.083701000	-2.139058000	-0.145676000
C	-4.009445000	-1.211500000	-0.059568000
H	3.151479000	-0.000015000	-0.840368000
H	1.839212000	0.000032000	-2.054337000
C	-2.626537000	-1.205795000	-0.117412000
C	2.078304000	0.000004000	-0.981261000
H	0.718097000	-3.140588000	1.215272000
C	-0.436565000	-0.000016000	-0.202180000
H	1.980771000	-5.196634000	1.726974000
C	2.237172000	-2.329913000	-0.062742000
C	1.694339000	-3.304378000	0.785160000
C	2.412104000	-4.454822000	1.066716000
O	-6.726221000	-1.081726000	0.052205000
O	-6.726231000	1.081678000	0.052192000

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C	2.817729000	-4.640778000	0.523890000
N	-0.707569000	-1.186781000	-0.166271000
H	3.379587000	-5.535690000	0.756387000
C	3.349636000	-3.675535000	-0.321035000
N	0.622398000	-1.163531000	-0.350531000

H	4.328697000	-3.817939000	-0.760899000
C	2.632807000	-2.526144000	-0.627749000
N	0.621075000	1.164244000	-0.350897000
H	3.062309000	-1.814927000	-1.319002000
N	-0.708811000	1.185992000	-0.166331000
C	1.360922000	2.320943000	-0.072000000
H	3.060971000	1.817633000	-1.318107000
C	2.630439000	2.528562000	-0.627215000
H	4.325104000	3.821956000	-0.759945000
C	3.345969000	3.678725000	-0.320498000
H	3.373727000	5.539105000	0.756583000
C	2.812794000	4.643628000	0.524033000
H	1.114135000	5.186420000	1.723191000
C	1.544421000	4.443913000	1.062758000
H	-0.157671000	3.138405000	1.201379000
C	0.821403000	3.298079000	0.776317000
H	-2.972699000	2.135550000	-0.117902000
C	-2.802120000	-0.001455000	-0.116067000
H	-5.437089000	2.139216000	0.008684000
H	-6.682845000	-0.003221000	0.072703000
C	-3.514754000	1.201207000	-0.084898000
H	-5.435122000	-2.144548000	0.008807000
C	-4.901225000	1.198341000	-0.015171000
H	-2.970709000	-2.138617000	-0.117759000
C	-5.601261000	-0.002742000	0.021048000
C	-4.900122000	-1.203184000	-0.015098000
H	2.257639000	0.001171000	-0.900852000
C	-3.513643000	-1.204773000	-0.084829000
H	0.910811000	0.000281000	-2.076402000

C	1.181048000	0.000532000	-1.010253000
H	-0.153805000	-3.138132000	1.202375000
C	-1.320905000	-0.000749000	-0.188887000
H	1.120236000	-5.184910000	1.724046000
C	1.363415000	-2.319616000	-0.071962000
C	0.825205000	-3.297041000	0.776875000
C	1.549420000	-4.442112000	1.063229000

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C	3.819338000	-4.410584000	0.545693000
H	4.446585000	-5.258539000	0.786765000
N	0.042961000	-1.239712000	-0.180553000
C	4.285265000	-3.405774000	-0.292062000
N	1.368928000	-1.116250000	-0.361281000
H	5.278820000	-3.469787000	-0.717634000
C	3.484640000	-2.316262000	-0.609779000
H	3.867327000	-1.573203000	-1.294965000
N	1.193659000	1.203458000	-0.359361000
H	3.571736000	2.041598000	-1.332458000
C	1.847681000	2.408029000	-0.072704000
N	-0.135183000	1.126526000	-0.174757000
C	3.095429000	2.713283000	-0.632434000
H	4.690525000	4.127879000	-0.762454000
C	3.727157000	3.909718000	-0.318986000
H	3.625278000	5.757875000	0.775118000
C	3.129965000	4.825916000	0.537007000
H	1.402981000	5.232701000	1.749310000
C	1.882445000	4.529329000	1.079909000
H	0.280668000	3.101500000	1.215250000
C	1.243008000	3.336320000	0.786806000

H	-2.475407000	1.897323000	-0.144799000
C	-2.132791000	-0.214837000	-0.139316000
H	-4.914388000	1.731810000	-0.033299000
O	-6.277261000	-0.635015000	0.042376000
C	-2.939317000	0.921509000	-0.113770000
C	-4.325223000	0.826486000	-0.051203000
H	-4.618600000	-2.543303000	-0.024794000
H	-2.152536000	-2.361478000	-0.137715000
C	-4.932699000	-0.427842000	-0.016455000
H	2.910806000	0.167612000	-0.916719000
C	-4.135476000	-1.575193000	-0.047648000
C	-2.759745000	-1.467804000	-0.109685000
H	1.562860000	0.065500000	-2.086972000
C	1.836979000	0.085878000	-1.021899000
H	0.729331000	-3.146726000	1.180805000
C	-0.658170000	-0.102950000	-0.203313000
H	2.152588000	-5.086805000	1.721424000
C	2.194805000	-2.209659000	-0.072242000
C	1.723719000	-3.227495000	0.769420000
C	2.531692000	-4.312201000	1.066483000
C	-7.136331000	0.491800000	0.076030000
H	-7.029781000	1.103922000	-0.824597000
H	-6.949154000	1.112044000	0.957727000
H	-8.148347000	0.096029000	0.123549000

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N	-1.152453000	0.490313000	-0.058281000
N	-1.116505000	-0.869479000	-0.081302000
C	0.097980000	-1.390965000	-0.075725000
N	1.256944000	-0.756801000	-0.048243000

N	1.165524000	0.600657000	-0.020009000
C	-0.030586000	1.303386000	0.017710000
C	-2.476619000	1.090806000	-0.012114000
C	2.430641000	1.313681000	0.056513000
O	-0.094046000	2.514012000	0.099017000
H	0.149458000	-2.471338000	-0.097284000
H	-2.843057000	1.138293000	1.016056000
H	-2.423732000	2.096863000	-0.416637000
H	-3.144514000	0.468816000	-0.602584000
H	3.116059000	0.877606000	-0.667749000
H	2.253794000	2.361380000	-0.162997000
H	2.859849000	1.216913000	1.055978000

2.2. The 1-15 anions

1			
O	4.271865000	0.010990000	0.000296000
C	3.034991000	0.006519000	-0.000157000
N	2.289948000	-1.134336000	-0.161151000
C	2.923899000	-2.418533000	-0.061735000
H	3.975038000	-2.315914000	-0.318501000
H	2.434023000	-3.116014000	-0.746687000
H	2.837713000	-2.833109000	0.954388000
N	0.892896000	-1.184825000	0.146025000
C	0.314616000	-0.003754000	-0.000146000
N	0.884213000	1.181993000	-0.147440000
N	2.281697000	1.141761000	0.160434000
C	2.906198000	2.430445000	0.061731000
H	2.410418000	3.124212000	0.746311000
H	2.817928000	2.844656000	-0.954484000

H	3.957858000	2.335759000	0.319367000
C	-1.175874000	-0.008866000	0.000602000
C	-1.894963000	-1.206407000	0.056690000
H	-1.334810000	-2.130635000	0.091781000
C	-3.284943000	-1.218135000	0.065017000
H	-3.836896000	-2.148916000	0.115968000
C	-3.984194000	-0.018707000	0.000997000
C	-3.288215000	1.183865000	-0.063270000
H	-3.834310000	2.122496000	-0.114764000
C	-1.897049000	1.184906000	-0.055394000
H	-1.342094000	2.112210000	-0.090429000
O	-5.366435000	-0.067346000	0.003841000
H	-5.696391000	0.835962000	-0.047140000

2

O	4.292140000	0.000109000	0.005833000
C	3.055515000	0.000016000	0.003240000
N	2.306001000	-1.137702000	0.166296000
C	2.935897000	-2.424201000	0.070010000
H	3.985863000	-2.325865000	0.333151000
H	2.854454000	-2.838265000	-0.946790000
H	2.438965000	-3.119755000	0.751697000
N	0.910039000	-1.183864000	-0.146394000
C	0.335354000	-0.000233000	-0.002695000
N	0.909226000	1.183512000	0.143121000
N	2.306541000	1.137586000	-0.162796000
C	2.935696000	2.424273000	-0.064423000
H	2.848881000	2.839160000	0.951591000
H	2.442241000	3.119233000	-0.749257000
H	3.987030000	2.325854000	-0.322004000

C	-1.155289000	-0.000272000	-0.004486000
C	-1.876222000	-1.195149000	-0.073060000
H	-1.319485000	-2.121066000	-0.118865000
C	-3.266345000	-1.191136000	-0.083893000
H	-3.801347000	-2.134064000	-0.149235000
C	-3.989329000	0.000228000	-0.009454000
C	-3.265990000	1.192093000	0.061595000
H	-3.800663000	2.136087000	0.114284000
C	-1.876279000	1.195427000	0.057376000
H	-1.319388000	2.121552000	0.095820000
C	-5.497021000	-0.000697000	0.025321000
H	-5.906926000	-0.876160000	-0.483604000
H	-5.908327000	0.890319000	-0.455231000
H	-5.876989000	-0.016707000	1.053002000

3

H	5.480839000	-0.000021000	0.000005000
O	-3.863361000	-0.000035000	-0.000010000
C	-2.626916000	-0.000006000	-0.000010000
N	-1.877596000	-1.137322000	-0.167346000
C	-2.507304000	-2.424144000	-0.072506000
H	-3.557266000	-2.325722000	-0.335585000
H	-2.425918000	-2.839423000	0.943779000
H	-2.010135000	-3.118551000	-0.755087000
N	-0.481387000	-1.183809000	0.142827000
C	0.092956000	0.000012000	-0.000010000
N	-0.481391000	1.183829000	-0.142841000
N	-1.877606000	1.137337000	0.167348000
C	-2.507288000	2.424169000	0.072530000
H	-3.557478000	2.325537000	0.334603000

H	-2.424929000	2.839862000	-0.943493000
H	-2.010846000	3.118378000	0.755883000
C	1.584254000	0.000004000	-0.000004000
C	2.301028000	-1.198791000	0.072228000
H	1.739292000	-2.121503000	0.119049000
C	3.691452000	-1.197984000	0.080264000
H	4.228672000	-2.138258000	0.145037000
C	4.396391000	-0.000014000	0.000006000
C	3.691467000	1.197963000	-0.080259000
H	4.228700000	2.138230000	-0.145037000
C	2.301043000	1.198790000	-0.072229000
H	1.739316000	2.121508000	-0.119043000

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O	-4.509718000	0.000061000	0.000080000
C	-3.275927000	0.000014000	0.000012000
N	-2.528064000	-1.138471000	-0.180821000
C	-3.160587000	-2.426278000	-0.097610000
H	-4.210623000	-2.322450000	-0.357111000
H	-3.077386000	-2.851202000	0.913797000
H	-2.667107000	-3.113209000	-0.789632000
N	-1.133648000	-1.188123000	0.118039000
C	-0.563092000	-0.000022000	-0.000008000
N	-1.133645000	1.188058000	-0.118016000
N	-2.527981000	1.138507000	0.180714000
C	-3.160481000	2.426317000	0.097599000
H	-2.666577000	3.113338000	0.789253000
H	-4.210377000	2.322601000	0.357701000
H	-3.077854000	2.851084000	-0.913895000
C	0.921161000	-0.000022000	-0.000026000

C	1.636820000	-1.198689000	0.112932000
H	1.073874000	-2.117938000	0.190099000
C	3.020959000	-1.203465000	0.121973000
H	3.565697000	-2.134174000	0.218585000
C	3.730750000	-0.000035000	0.000009000
C	3.020965000	1.203403000	-0.121982000
H	3.565710000	2.134109000	-0.218577000
C	1.636826000	1.198636000	-0.112971000
H	1.073893000	2.117892000	-0.190157000
C	5.156759000	-0.000037000	0.000028000
N	6.312419000	0.000104000	0.000022000

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N	1.726808000	1.133811000	0.167896000
C	-2.459403000	1.209418000	-0.077111000
H	-1.899860000	2.132901000	-0.129360000
O	-5.932002000	0.077551000	-0.005900000
H	-6.264579000	-0.823880000	0.059644000
N	0.331411000	1.182767000	-0.152801000
C	-3.849186000	1.223286000	-0.086729000
H	-4.399463000	2.153923000	-0.154570000
O	3.706879000	-0.015373000	0.000084000
N	0.319237000	-1.178715000	0.156445000
C	-4.550532000	0.026391000	-0.001562000
H	-4.403116000	-2.112609000	0.152408000
N	1.715067000	-1.144015000	-0.164920000
C	-3.856113000	-1.175670000	0.084430000
C	-2.465048000	-1.178517000	0.076419000
H	-1.913481000	-2.106698000	0.129119000
C	-1.741154000	0.012484000	0.000003000

C	-0.250042000	0.005218000	0.001174000
C	2.362892000	-2.444653000	-0.112925000
H	3.404322000	-2.251987000	-0.367762000
C	2.469378000	-0.009048000	0.001003000
H	3.427455000	2.224953000	0.368419000
C	2.388151000	2.427771000	0.112795000
C	2.344128000	3.032823000	-1.297637000
H	2.850020000	2.374731000	-2.006796000
H	2.843058000	4.006492000	-1.317155000
H	1.309874000	3.157330000	-1.620679000
C	1.792917000	3.378962000	1.153345000
H	1.875702000	2.948309000	2.153340000
H	0.736922000	3.557542000	0.948596000
H	2.322221000	4.336339000	1.142319000
C	2.312259000	-3.053031000	1.295907000
H	2.824728000	-2.402140000	2.006961000
H	2.801052000	-4.031894000	1.312922000
H	1.276677000	-3.167495000	1.618467000
C	1.758170000	-3.387141000	-1.156044000
H	2.276716000	-4.350425000	-1.146629000
H	0.700030000	-3.554231000	-0.952439000
H	1.846534000	-2.955282000	-2.155027000

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C	-6.067704000	0.001501000	0.020892000
H	-1.891575000	2.120219000	-0.160151000
N	1.737785000	1.138147000	0.169405000
C	-2.446263000	1.194507000	-0.095376000
C	-3.836818000	1.190643000	-0.106801000
O	3.722887000	-0.002385000	0.004275000

N	0.343179000	1.181562000	-0.155270000
H	-4.371353000	2.132204000	-0.190763000
C	-4.560003000	0.001818000	-0.008938000
N	0.340782000	-1.180261000	0.151963000
C	-3.836494000	-1.188685000	0.086926000
N	1.736290000	-1.139281000	-0.168184000
H	-4.370764000	-2.131584000	0.159068000
C	-2.447361000	-1.191931000	0.082350000
H	-1.892400000	-2.117851000	0.140985000
C	-1.724963000	0.002021000	-0.003417000
C	-0.233693000	0.001206000	-0.002101000
C	2.389706000	-2.437343000	-0.113897000
H	3.430451000	-2.240760000	-0.368507000
C	2.485612000	-0.001141000	0.001944000
C	2.393562000	2.435097000	0.117774000
H	3.433086000	2.236707000	0.375979000
C	2.350597000	3.041908000	-1.291942000
H	2.860902000	2.386894000	-2.000792000
H	2.845664000	4.017598000	-1.308801000
H	1.316647000	3.162633000	-1.617368000
C	1.790926000	3.382057000	1.157931000
H	2.315015000	4.342332000	1.148996000
H	0.734404000	3.554830000	0.950904000
H	1.873842000	2.950865000	2.157681000
C	2.340795000	-3.043803000	1.295787000
H	2.849618000	-2.389477000	2.006332000
H	2.834266000	-4.020264000	1.314569000
H	1.305516000	-3.162881000	1.617585000
C	1.789099000	-3.383551000	-1.155912000

H	0.731552000	-3.554439000	-0.952555000
H	2.311438000	-4.344756000	-1.144827000
H	1.876296000	-2.952828000	-2.155497000
H	-6.479692000	-0.841772000	-0.539346000
H	-6.473394000	0.919903000	-0.408841000
H	-6.450864000	-0.075488000	1.044433000

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H	-5.985398000	-0.000060000	0.000111000
N	1.374176000	1.138594000	0.169950000
C	-2.805699000	1.196216000	-0.100279000
H	-2.245858000	2.118350000	-0.169888000
O	3.359976000	0.000024000	-0.000171000
C	-4.196055000	1.195460000	-0.108832000
N	-0.020406000	1.180822000	-0.153488000
H	-4.732945000	2.134018000	-0.196031000
C	-4.901041000	-0.000051000	0.000049000
N	-0.020362000	-1.180810000	0.153457000
N	1.374176000	-1.138563000	-0.169857000
C	-4.196032000	-1.195549000	0.108902000
H	-4.732908000	-2.134115000	0.196089000
C	-2.805676000	-1.196282000	0.100275000
H	-2.245822000	-2.118415000	0.169829000
C	-2.088058000	-0.000029000	-0.000013000
C	-0.596161000	-0.000008000	-0.000016000
C	2.028754000	-2.436268000	-0.119048000
H	3.068628000	-2.238469000	-0.376272000
C	2.122886000	0.000026000	-0.000063000
C	2.028693000	2.436307000	0.118971000
H	3.068657000	2.238566000	0.375876000

C	1.983705000	3.044644000	-1.289972000
H	0.949352000	3.165539000	-1.614033000
H	2.478412000	4.020515000	-1.306275000
H	2.493354000	2.390704000	-2.000267000
C	1.426232000	3.381427000	1.160866000
H	1.510956000	2.949358000	2.160067000
H	0.369239000	3.553240000	0.955416000
H	1.949136000	4.342340000	1.152216000
C	1.984190000	-3.044490000	1.289962000
H	0.949902000	-3.164326000	1.614673000
H	2.477917000	-4.020864000	1.306008000
H	2.494959000	-2.391002000	1.999854000
H	1.950035000	-4.341838000	-1.153136000
H	0.369510000	-3.554602000	-0.954143000
H	1.509137000	-2.948832000	-2.159786000
C	1.426067000	-3.381502000	-1.160697000

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C	-5.444770000	-0.121726000	-0.006594000
C	-1.866602000	1.158953000	-0.168684000
H	-1.313930000	2.080590000	-0.280417000
O	-6.109193000	1.057244000	0.201264000
N	2.294600000	1.152494000	0.171662000
N	0.903607000	1.178263000	-0.151841000
C	-3.251625000	1.147088000	-0.175915000
O	4.290400000	0.033146000	0.018562000
H	-3.768384000	2.087968000	-0.342370000
N	0.928377000	-1.189134000	0.136173000
C	-3.963345000	-0.051092000	-0.023341000
N	2.323390000	-1.131932000	-0.164732000

H	-3.782725000	-2.166669000	0.222109000
C	-3.236451000	-1.239000000	0.112968000
C	-1.852032000	-1.228013000	0.112435000
H	-1.286481000	-2.143120000	0.213554000
C	-1.140698000	-0.028679000	-0.020995000
C	0.344087000	-0.012552000	-0.011727000
C	2.995192000	-2.422094000	-0.096595000
H	4.034610000	-2.211363000	-0.344301000
C	3.055898000	0.018526000	0.008947000
C	2.938639000	2.456829000	0.113373000
H	3.978530000	2.269045000	0.377046000
C	2.895833000	3.052919000	-1.300267000
H	3.411802000	2.396754000	-2.003760000
H	3.385488000	4.030859000	-1.321823000
H	1.862654000	3.167491000	-1.630458000
C	2.324197000	3.404013000	1.145773000
H	2.843305000	4.366580000	1.135293000
H	1.268170000	3.572075000	0.932275000
H	2.403740000	2.978272000	2.147988000
C	2.943383000	-3.018723000	1.316434000
H	3.433455000	-2.351218000	2.027795000
H	3.454325000	-3.985452000	1.346006000
H	1.907942000	-3.156620000	1.630070000
H	2.502491000	-2.954811000	-2.139000000
C	2.417380000	-3.382259000	-1.137970000
H	1.362387000	-3.574111000	-0.940472000
H	2.957704000	-4.332923000	-1.119539000
O	-6.092478000	-1.127448000	-0.152721000
H	-5.469268000	1.750153000	0.407267000

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N	0.660995000	1.203806000	-0.359176000
C	-1.350040000	0.000485000	0.240415000
H	5.356094000	2.136105000	-0.228790000
C	-1.428725000	-2.253558000	-0.820273000
N	-0.737047000	-1.167662000	-0.363057000
H	5.354816000	-2.141341000	-0.210325000
N	-0.735727000	1.166828000	-0.365137000
C	-1.240646000	0.001512000	1.772405000
H	2.882737000	-2.128718000	-0.267977000
C	1.220781000	-0.001684000	-0.346004000
N	0.659687000	-1.206599000	-0.355487000
H	2.884566000	2.124508000	-0.285998000
H	0.320739000	3.180021000	-1.653927000
C	3.433374000	-1.198646000	-0.269235000
C	7.054013000	-0.002532000	-0.220686000
C	3.434666000	1.194133000	-0.279377000
H	-0.866772000	5.155327000	-2.520658000
C	2.711801000	-0.002307000	-0.295655000
H	-3.326143000	5.399509000	-2.202332000
C	-1.426309000	2.253887000	-0.821357000
H	-4.549130000	3.616845000	-0.965220000
H	-3.390774000	1.691900000	-0.070913000
C	-0.745610000	-3.288256000	-1.506754000
C	-0.742882000	3.286780000	-1.510170000
H	0.318564000	-3.183591000	-1.647958000
C	4.823065000	1.190297000	-0.244427000
H	-0.870537000	-5.157286000	-2.516169000
C	-1.425062000	4.389615000	-1.992115000

H	-3.331224000	-5.396477000	-2.203967000
C	5.546367000	-0.003088000	-0.224111000
H	-4.553822000	-3.610696000	-0.971001000
C	-2.819691000	2.420385000	-0.629691000
H	-3.394115000	-1.687286000	-0.075341000
C	-2.801815000	4.532976000	-1.819944000
H	-1.217270000	-2.134471000	1.943649000
C	4.822372000	-1.195464000	-0.234219000
H	-1.187272000	-2.139483000	4.409347000
C	-1.187105000	0.003401000	4.574600000
H	-1.163676000	0.004131000	5.658082000
C	-2.822911000	-2.417335000	-0.631948000
H	-1.155860000	2.145736000	4.405785000
C	-1.227139000	-1.197457000	2.483703000
H	-1.186344000	2.137081000	1.940005000
H	-2.400795000	0.000945000	-0.033810000
C	-1.428695000	-4.390121000	-1.989594000
C	-3.484622000	-3.527146000	-1.133771000
C	-3.480533000	3.531094000	-1.130653000
C	-1.209795000	1.201272000	2.481668000
C	-2.806132000	-4.530824000	-1.820640000
C	-1.185676000	1.203076000	3.871966000
C	-1.203174000	-1.197382000	3.873947000
H	7.451328000	-0.915307000	0.228435000
H	7.452167000	0.848032000	0.337539000
H	7.458093000	0.061231000	-1.236938000
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N	0.938253000	1.205161000	-0.384614000
C	-1.060335000	-0.000111000	0.251442000

H	5.634561000	2.143333000	-0.341954000
N	-0.457770000	-1.167466000	-0.364023000
C	-1.157462000	-2.254242000	-0.807263000
H	5.635116000	-2.142056000	-0.341812000
N	-0.458044000	1.167254000	-0.364276000
C	-0.923474000	0.000020000	1.781185000
H	3.154476000	-2.127188000	-0.351592000
C	1.498883000	0.000108000	-0.383493000
N	0.938568000	-1.205134000	-0.384002000
H	3.153921000	2.127830000	-0.351849000
C	3.709662000	-1.199940000	-0.354677000
H	6.888431000	0.000785000	-0.333549000
H	0.571756000	3.180783000	-1.674809000
C	3.709357000	1.200724000	-0.354795000
H	-0.634014000	5.154583000	-2.519076000
C	2.991257000	0.000291000	-0.360491000
H	-3.086814000	5.397073000	-2.152813000
C	-1.158012000	2.253886000	-0.807462000
H	-4.283990000	3.614500000	-0.890553000
C	-0.487977000	-3.287105000	-1.509521000
H	-3.106692000	1.690816000	-0.018135000
C	-0.488909000	3.286755000	-1.510064000
H	0.572722000	-3.180959000	-1.673948000
C	5.099030000	1.200317000	-0.346384000
H	-0.632418000	-5.155165000	-2.518193000
H	-3.085340000	-5.397954000	-2.152733000
C	-1.181245000	4.388803000	-1.979209000
C	5.804380000	0.000660000	-0.341782000
H	-4.283180000	-3.615449000	-0.891070000

C	-2.547383000	2.419450000	-0.588491000
H	-3.106480000	-1.691422000	-0.018565000
C	-2.554451000	4.531213000	-1.780127000
H	-0.881596000	-2.135862000	1.950243000
C	5.099348000	-1.199179000	-0.346279000
H	-0.807797000	-2.142430000	4.414919000
C	-0.820330000	0.000248000	4.582045000
H	-0.777967000	0.000336000	5.664944000
C	-2.546864000	-2.420039000	-0.588643000
H	-0.807130000	2.142897000	4.414535000
C	-0.888667000	-1.199315000	2.491112000
H	-0.881041000	2.135940000	1.949908000
H	-2.115844000	-0.000231000	-0.004202000
C	-1.179962000	-4.389366000	-1.978671000
C	-3.217945000	-3.530143000	-1.077202000
C	-3.218819000	3.529342000	-1.077038000
C	-0.888336000	1.199463000	2.490899000
C	-2.553191000	-4.532022000	-1.779909000
C	-0.839746000	1.200433000	3.880534000
C	-0.840096000	-1.200061000	3.880735000

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N	0.207991000	1.207204000	-0.359860000
C	-1.806935000	0.000033000	0.212467000
H	4.903385000	2.137410000	-0.170317000
C	-1.871201000	-2.266345000	-0.829730000
N	-1.184282000	-1.169033000	-0.383044000
H	4.903314000	-2.137434000	-0.169720000
N	-1.184250000	1.169203000	-0.382787000
C	-1.719968000	-0.000132000	1.746019000

H	2.408391000	-2.130430000	-0.259644000
C	0.766048000	0.000040000	-0.341979000
N	0.207956000	-1.207110000	-0.359992000
H	2.408452000	2.130452000	-0.260099000
N	6.487267000	-0.000031000	-0.106516000
H	-0.119302000	3.195596000	-1.649077000
C	2.965089000	-1.205110000	-0.244762000
H	-1.300116000	5.180881000	-2.498936000
C	2.965136000	1.205127000	-0.245048000
C	2.247266000	0.000012000	-0.273195000
H	-3.759064000	5.425223000	-2.185797000
C	-1.871149000	2.266538000	-0.829436000
H	-4.989864000	3.634675000	-0.970192000
H	-3.836721000	1.698810000	-0.089542000
C	-1.182975000	-3.302064000	-1.505833000
C	-1.182952000	3.302165000	-1.505700000
H	-0.119290000	-3.195591000	-1.649013000
C	4.346855000	1.212310000	-0.192296000
H	-1.300127000	-5.180815000	-2.499002000
C	-1.861090000	4.411379000	-1.979466000
H	-3.759162000	-5.424905000	-2.186324000
C	5.032776000	-0.000013000	-0.164982000
H	-4.990023000	-3.634177000	-0.971054000
C	-3.263427000	2.431478000	-0.640334000
H	-3.836874000	-1.698388000	-0.090269000
C	-3.237593000	4.554388000	-1.809711000
H	-1.685928000	-2.137110000	1.917761000
C	4.346816000	-1.212323000	-0.191986000
H	-1.681302000	-2.142922000	4.381451000

C	-1.697329000	-0.000414000	4.548561000
H	-1.685154000	-0.000524000	5.632048000
C	-3.263529000	-2.431140000	-0.640894000
H	-1.680694000	2.142123000	4.381878000
C	-1.706838000	-1.199679000	2.456561000
H	-1.685337000	2.136795000	1.918178000
H	-2.852488000	0.000081000	-0.080773000
C	-1.861128000	-4.411233000	-1.979679000
C	-3.921268000	-3.547742000	-1.133489000
C	-3.921156000	3.548116000	-1.132855000
C	-1.706505000	1.199269000	2.456801000
C	-3.237676000	-4.554106000	-1.810174000
C	-1.697397000	1.199821000	3.847166000
C	-1.697734000	-1.200509000	3.846925000
O	7.071380000	-1.081206000	-0.083275000
O	7.071410000	1.081132000	-0.083460000

12

C	3.564132000	-4.865909000	0.282824000
H	4.073233000	-5.814516000	0.396663000
N	0.174338000	-1.206691000	-0.070928000
C	4.236159000	-3.747154000	-0.199528000
H	5.282470000	-3.821317000	-0.475248000
N	1.567037000	-1.178234000	-0.097136000
C	3.592572000	-2.528140000	-0.355872000
H	4.155362000	-1.700938000	-0.763692000
N	1.567166000	1.178130000	-0.096856000
N	0.174458000	1.206667000	-0.070415000
C	2.230653000	2.376823000	-0.008848000
H	4.155199000	1.700778000	-0.764502000

C	3.592628000	2.527975000	-0.356370000
H	5.282558000	3.821077000	-0.476303000
C	4.236354000	3.746947000	-0.200171000
H	4.073773000	5.814257000	0.396272000
H	1.661792000	5.588355000	0.975113000
C	3.564565000	4.865700000	0.282483000
C	2.214092000	4.731699000	0.603908000
H	0.508300000	3.429005000	0.716018000
H	-2.027160000	2.130663000	-0.059002000
C	1.551717000	3.525572000	0.461686000
C	-1.863582000	0.000069000	-0.053758000
H	-4.522561000	2.137635000	-0.034329000
N	-6.107337000	0.000136000	-0.025762000
C	-2.583465000	1.205194000	-0.048620000
C	-3.965816000	1.212377000	-0.038358000
H	-4.522653000	-2.137393000	-0.035587000
C	-4.653487000	0.000126000	-0.034479000
H	-2.027260000	-2.130515000	-0.060243000
C	-3.965872000	-1.212154000	-0.039075000
H	3.243528000	-0.000092000	-0.385232000
H	2.107665000	0.000090000	-1.755985000
C	-2.583517000	-1.205022000	-0.049327000
C	2.193907000	-0.000032000	-0.655935000
H	0.507835000	-3.429030000	0.715475000
C	-0.382497000	0.000019000	-0.060825000
H	1.661084000	-5.588448000	0.974817000
C	2.230466000	-2.376921000	-0.008845000
C	1.551320000	-3.525642000	0.461439000
C	2.213574000	-4.731828000	0.603812000

O	-6.692884000	-1.081248000	-0.022460000
O	-6.692893000	1.081516000	-0.021716000
13			
C	-4.853319000	-2.701499000	0.312947000
N	-1.204387000	0.699744000	-0.089421000
H	-5.799354000	-3.212163000	0.441581000
C	-3.738305000	-3.372495000	-0.181143000
N	-1.175109000	-0.697500000	-0.121635000
H	-3.813423000	-4.420425000	-0.451579000
C	-2.522853000	-2.727631000	-0.356388000
N	1.174801000	-0.698254000	-0.122851000
H	-1.700104000	-3.291244000	-0.772252000
N	1.205009000	0.698857000	-0.090146000
C	2.366056000	-1.364236000	-0.016779000
H	1.697323000	-3.292872000	-0.771744000
C	2.520580000	-2.729826000	-0.356096000
H	3.809558000	-4.423846000	-0.450338000
C	3.735387000	-3.375717000	-0.180395000
H	5.796518000	-3.217060000	0.442490000
C	4.850969000	-2.705564000	0.313605000
H	5.569029000	-0.799994000	1.004445000
C	4.715354000	-1.352375000	0.625524000
H	3.415973000	0.358680000	0.710059000
C	3.513805000	-0.686724000	0.464269000
H	2.128563000	2.913405000	-0.075968000
C	0.001134000	2.749804000	-0.068527000
H	2.145000000	5.393386000	-0.042165000
H	0.002807000	6.648657000	-0.027528000
C	1.201541000	3.468665000	-0.062295000

H	-2.140501000	5.395186000	-0.039544000
C	1.201607000	4.858355000	-0.046792000
H	-2.126127000	2.915174000	-0.073310000
C	0.002328000	5.564580000	-0.038243000
C	-1.197558000	4.859377000	-0.045334000
H	-0.000715000	-2.369962000	-0.451700000
C	-1.198641000	3.469676000	-0.060826000
H	-0.001164000	-1.200730000	-1.795039000
C	-0.000599000	-1.314245000	-0.696697000
H	-3.415588000	0.361337000	0.710518000
C	0.000529000	1.257687000	-0.079136000
H	-5.569830000	-0.795491000	1.004166000
C	-2.367136000	-1.362383000	-0.016459000
C	-3.514362000	-0.683924000	0.464491000
C	-4.716545000	-1.348519000	0.625320000

14

C	3.788906000	-4.578482000	0.326615000
H	4.384028000	-5.472753000	0.462300000
N	0.066985000	-1.258260000	-0.094910000
C	4.353392000	-3.412310000	-0.182540000
N	1.456064000	-1.103175000	-0.134779000
H	5.402688000	-3.394413000	-0.457583000
C	3.599736000	-2.262666000	-0.367111000
H	4.084045000	-1.396635000	-0.795089000
N	1.247451000	1.235938000	-0.135970000
H	3.776394000	1.993497000	-0.810092000
C	1.807050000	2.478939000	-0.021622000
N	-0.147251000	1.141687000	-0.093727000
C	3.149190000	2.758565000	-0.375373000

H	4.721285000	4.193352000	-0.472714000
C	3.687526000	4.023366000	-0.190853000
H	3.355709000	6.054484000	0.462985000
C	2.928148000	5.069116000	0.326789000
H	0.975850000	5.606618000	1.050189000
C	1.596419000	4.810018000	0.652731000
H	0.007662000	3.363673000	0.739887000
C	1.037035000	3.556631000	0.482804000
H	-2.442951000	1.857115000	-0.075573000
C	-2.081621000	-0.241280000	-0.065524000
H	-4.897251000	1.667815000	-0.038688000
O	-6.246766000	-0.715906000	-0.016552000
C	-2.907280000	0.881248000	-0.059717000
C	-4.296547000	0.768725000	-0.042099000
H	-4.547132000	-2.602447000	-0.029363000
H	-2.066547000	-2.376834000	-0.066711000
C	-4.887066000	-0.491839000	-0.031228000
H	3.013812000	0.214512000	-0.486396000
C	-4.076707000	-1.626691000	-0.037214000
C	-2.697346000	-1.499332000	-0.054767000
H	1.831598000	0.108080000	-1.814655000
C	1.959328000	0.120410000	-0.717947000
H	0.609164000	-3.421807000	0.724267000
C	-0.596334000	-0.107923000	-0.080738000
H	1.958845000	-5.458028000	1.034419000
C	2.227296000	-2.227825000	-0.021362000
C	1.658137000	-3.427266000	0.474257000
C	2.430292000	-4.561990000	0.644045000
C	-7.100665000	0.405162000	-0.004867000

H	-6.968276000	1.027617000	-0.897098000
H	-6.943167000	1.027988000	0.882957000
H	-8.117697000	0.014631000	0.009414000

15

N	-1.136874000	0.523800000	0.159852000
N	-1.123687000	-0.903548000	-0.065882000
C	0.096113000	-1.388135000	0.051804000
N	1.265855000	-0.787988000	0.145470000
N	1.146810000	0.622305000	-0.143882000
C	-0.029099000	1.313964000	-0.013419000
C	-2.446477000	1.087822000	0.014819000
C	2.399491000	1.310970000	-0.045817000
O	-0.087148000	2.551869000	-0.047662000
H	0.146776000	-2.478191000	0.075607000
H	-3.129607000	0.598898000	0.716008000
H	-2.400971000	2.155023000	0.217048000
H	-2.846039000	0.927313000	-0.999841000
H	3.118246000	0.854151000	-0.733116000
H	2.252383000	2.358268000	-0.297749000
H	2.822965000	1.237621000	0.969111000

2.3. The 1-15 cations

1

O	4.219589000	0.004467000	-0.000224000
C	3.021703000	0.002630000	-0.000069000
N	2.226372000	-1.158934000	0.000043000
C	2.936641000	-2.446168000	0.000113000
H	3.570969000	-2.496173000	-0.884270000

H	2.186984000	-3.229038000	0.000130000
H	3.570910000	-2.496112000	0.884581000
N	0.935956000	-1.172691000	0.000072000
C	0.272703000	0.000121000	0.000037000
N	0.933402000	1.174106000	0.000046000
N	2.223601000	1.162983000	0.000020000
C	2.931789000	2.451290000	0.000026000
H	2.180994000	3.233058000	-0.000075000
H	3.566150000	2.502224000	-0.884283000
H	3.565970000	2.502300000	0.884460000
C	-1.181001000	-0.002187000	0.000006000
C	-1.894036000	-1.213696000	-0.000060000
H	-1.363077000	-2.154787000	-0.000117000
C	-3.271052000	-1.220136000	-0.000072000
H	-3.826042000	-2.148083000	-0.000120000
C	-3.975877000	-0.010297000	-0.000019000
C	-3.277424000	1.202365000	0.000041000
H	-3.819357000	2.140494000	0.000075000
C	-1.897174000	1.203955000	0.000054000
H	-1.371660000	2.148144000	0.000103000
O	-5.316348000	-0.084499000	-0.000038000
H	-5.720716000	0.792712000	-0.000002000

2

O	-4.241482000	0.000003000	0.004012000
C	-3.044380000	0.000002000	0.002291000
N	-2.247537000	-1.161707000	0.001177000
C	-2.955872000	-2.450082000	0.002376000
H	-3.588687000	-2.501026000	0.887816000
H	-2.204844000	-3.231675000	0.001414000

H	-3.591217000	-2.501286000	-0.881235000
N	-0.957199000	-1.172437000	-0.000882000
C	-0.297483000	0.000001000	-0.001924000
N	-0.957198000	1.172434000	-0.000873000
N	-2.247537000	1.161702000	0.001187000
C	-2.955876000	2.450083000	0.002360000
H	-2.204840000	3.231669000	0.002200000
H	-3.589331000	2.500677000	0.887352000
H	-3.590572000	2.501628000	-0.881705000
C	1.161520000	0.000002000	-0.003308000
C	1.872156000	-1.207586000	-0.005919000
H	1.344213000	-2.150475000	-0.008091000
C	3.255497000	-1.198957000	-0.009528000
H	3.789435000	-2.140876000	-0.015487000
C	3.976200000	-0.000002000	-0.008508000
C	3.255499000	1.198953000	-0.009508000
H	3.789434000	2.140875000	-0.015456000
C	1.872155000	1.207585000	-0.005898000
H	1.344217000	2.150479000	-0.008046000
C	5.476298000	0.000006000	0.017908000
H	5.836791000	-0.000474000	1.050895000
H	5.884627000	0.885545000	-0.468624000
H	5.884640000	-0.885076000	-0.469449000

3

H	5.457800000	0.000049000	-0.000032000
O	-3.814027000	0.000079000	-0.000045000
C	-2.617803000	-0.000050000	-0.000024000
N	-1.820686000	-1.162584000	0.000136000
C	-2.528679000	-2.451341000	0.000366000

H	-3.162548000	-2.502348000	0.885127000
H	-1.777482000	-3.232790000	0.000326000
H	-3.162878000	-2.502476000	-0.884148000
N	-0.530572000	-1.171770000	0.000185000
C	0.127338000	-0.000070000	0.000017000
N	-0.530562000	1.171766000	-0.000144000
N	-1.820574000	1.162603000	-0.000154000
C	-2.528660000	2.451342000	-0.000328000
H	-3.162339000	2.502413000	-0.885201000
H	-1.777496000	3.232828000	-0.000005000
H	-3.163018000	2.502271000	0.884059000
C	1.590901000	-0.000025000	0.000011000
C	2.294569000	-1.211402000	-0.000480000
H	1.761586000	-2.151206000	-0.000850000
C	3.680591000	-1.205421000	-0.000500000
H	4.219727000	-2.143173000	-0.000906000
C	4.375754000	0.000028000	-0.000018000
C	3.680548000	1.205447000	0.000482000
H	4.219647000	2.143219000	0.000881000
C	2.294521000	1.211378000	0.000488000
H	1.761513000	2.151169000	0.000869000

4

O	-4.468570000	-0.000013000	-0.000199000
C	-3.273863000	-0.000001000	-0.000071000
N	-2.476002000	-1.164630000	0.000191000
C	-3.184782000	-2.453527000	0.000432000
H	-3.818921000	-2.503277000	0.885193000
H	-2.434288000	-3.235697000	0.000697000
H	-3.818790000	-2.503675000	-0.884390000

N	-1.186991000	-1.171900000	0.000249000
C	-0.531782000	0.000014000	0.000047000
N	-1.187001000	1.171902000	-0.000120000
N	-2.476019000	1.164612000	-0.000149000
C	-3.184814000	2.453512000	-0.000341000
H	-2.434328000	3.235697000	-0.000470000
H	-3.818869000	2.503575000	0.884441000
H	-3.818888000	2.503321000	-0.885136000
C	0.934503000	0.000010000	0.000032000
C	1.638400000	-1.210676000	-0.000518000
H	1.107777000	-2.151530000	-0.000936000
C	3.021179000	-1.211310000	-0.000551000
H	3.565315000	-2.145403000	-0.001004000
C	3.722111000	0.000023000	-0.000014000
C	3.021178000	1.211340000	0.000542000
H	3.565289000	2.145446000	0.000970000
C	1.638389000	1.210691000	0.000556000
H	1.107762000	2.151548000	0.000987000
C	5.151089000	-0.000002000	-0.000039000
N	6.302706000	-0.000034000	-0.000058000

5

N	1.644174000	1.163075000	-0.156041000
C	-2.472646000	1.212606000	0.017829000
H	-1.941406000	2.153045000	-0.009062000
O	-5.894143000	0.085299000	0.181957000
H	-6.295490000	-0.792774000	0.202473000
N	0.356414000	1.169760000	-0.128128000
C	-3.848875000	1.219966000	0.083575000
H	-4.402599000	2.148341000	0.109644000

O	3.633672000	-0.003805000	-0.018901000
N	0.354071000	-1.170926000	-0.128519000
C	-4.553154000	0.011297000	0.117667000
H	-4.396990000	-2.138765000	0.111490000
N	1.641743000	-1.166393000	-0.156424000
C	-3.855691000	-1.200542000	0.085124000
C	-2.476157000	-1.202044000	0.019161000
H	-1.950770000	-2.145851000	-0.006552000
C	-1.760199000	0.002437000	-0.016196000
C	-0.304626000	-0.000006000	-0.084354000
C	2.360817000	-2.488997000	-0.189108000
H	3.311368000	-2.249526000	-0.663547000
C	2.436099000	-0.002186000	-0.093842000
H	3.316357000	2.244267000	-0.659458000
C	2.364790000	2.485053000	-0.187770000
C	1.595294000	3.498360000	-1.017902000
H	1.379554000	3.121269000	-2.018042000
H	2.218220000	4.386605000	-1.121800000
H	0.661590000	3.791231000	-0.541649000
C	2.617308000	2.933623000	1.253273000
H	3.190637000	2.194404000	1.811739000
H	1.674785000	3.128238000	1.767233000
H	3.194022000	3.858063000	1.232570000
C	2.617189000	-2.937013000	1.251407000
H	3.192552000	-2.197852000	1.807791000
H	3.193302000	-3.861807000	1.229623000
H	1.676049000	-3.130675000	1.768286000
C	1.588415000	-3.502236000	-1.016533000
H	2.210483000	-4.390919000	-1.121809000

H	0.655919000	-3.794289000	-0.537366000
H	1.369977000	-3.125480000	-2.016212000
6			
C	6.057212000	-0.000940000	0.187177000
H	1.931352000	-2.146441000	-0.029833000
N	-1.660271000	-1.166509000	-0.155256000
C	2.458283000	-1.203679000	0.004073000
C	3.839113000	-1.193734000	0.068546000
O	-3.651333000	-0.002676000	-0.018934000
N	-0.372344000	-1.169383000	-0.127738000
H	4.374150000	-2.135305000	0.085019000
C	4.557996000	0.006781000	0.112393000
N	-0.374824000	1.169717000	-0.129478000
C	3.836620000	1.202624000	0.087958000
N	-1.662186000	1.164418000	-0.156826000
H	4.367945000	2.145352000	0.120253000
C	2.452964000	1.208748000	0.022897000
H	1.923772000	2.150672000	0.004150000
C	1.744988000	0.002744000	-0.020136000
C	0.284462000	0.000711000	-0.086351000
C	-2.382405000	2.486800000	-0.188086000
H	-3.334186000	2.246475000	-0.659602000
C	-2.454497000	-0.002034000	-0.094126000
C	-2.377790000	-2.490340000	-0.183697000
H	-3.330077000	-2.253020000	-0.655728000
C	-1.605821000	-3.503385000	-1.011829000
H	-1.392007000	-3.128205000	-2.013106000
H	-2.226149000	-4.393758000	-1.112981000
H	-0.670876000	-3.792087000	-0.535459000

C	-2.628544000	-2.936275000	1.258483000
H	-3.203130000	-3.862085000	1.240026000
H	-1.685289000	-3.127579000	1.772340000
H	-3.203344000	-2.197299000	1.815773000
C	-2.634109000	2.935230000	1.253160000
H	-3.207330000	2.196228000	1.812033000
H	-3.210677000	3.859764000	1.232671000
H	-1.691285000	3.129705000	1.766621000
C	-1.612383000	3.499568000	-1.018382000
H	-0.677881000	3.790966000	-0.542793000
H	-2.234367000	4.388582000	-1.121288000
H	-1.397995000	3.122711000	-2.018906000
H	6.486710000	-0.553714000	-0.651215000
H	6.397023000	-0.492589000	1.101897000
H	6.465159000	1.008424000	0.174202000

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H	-5.972670000	-0.000054000	0.245768000
N	1.295650000	1.166436000	-0.163288000
C	-2.814001000	1.210068000	0.061284000
H	-2.281144000	2.149288000	0.028471000
O	3.287348000	0.000049000	-0.065339000
C	-4.197854000	1.204771000	0.142163000
N	0.008907000	1.169115000	-0.115285000
H	-4.735801000	2.142798000	0.173099000
C	-4.892437000	-0.000046000	0.182976000
N	0.008936000	-1.169109000	-0.115386000
N	1.295695000	-1.166392000	-0.163378000
C	-4.197781000	-1.204854000	0.143097000
H	-4.735669000	-2.142889000	0.174796000

C	-2.813929000	-1.210127000	0.062205000
H	-2.281013000	-2.149338000	0.030116000
C	-2.110527000	-0.000024000	0.020054000
C	-0.646751000	-0.000015000	-0.064866000
C	2.014555000	-2.489667000	-0.202783000
H	2.954151000	-2.252978000	-0.700101000
C	2.090055000	0.000021000	-0.117185000
C	2.014484000	2.489727000	-0.202605000
H	2.954024000	2.253116000	-0.700066000
C	1.223488000	3.508738000	-1.004841000
H	0.302855000	3.798564000	-0.501974000
H	1.843902000	4.397546000	-1.118387000
H	0.981525000	3.139280000	-2.001811000
C	2.302925000	2.926984000	1.235366000
H	2.891373000	2.184722000	1.773632000
H	1.373627000	3.116697000	1.774599000
H	2.877840000	3.852324000	1.206726000
C	2.302836000	-2.927118000	1.235156000
H	1.373489000	-3.117155000	1.774190000
H	2.877994000	-3.852306000	1.206461000
H	2.891001000	-2.184810000	1.773671000
H	1.844076000	-4.397407000	-1.118758000
H	0.302927000	-3.798402000	-0.502625000
H	0.981948000	-3.139023000	-2.002257000
C	1.223682000	-3.508578000	-1.005268000

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C	-5.467546000	-0.099851000	0.058723000
C	-1.878366000	1.201238000	-0.042894000
H	-1.352233000	2.143118000	-0.096391000

O	-6.148045000	0.959431000	0.543619000
N	2.237563000	1.167632000	-0.174887000
N	0.950733000	1.168249000	-0.147398000
C	-3.263794000	1.191900000	0.008355000
O	4.227841000	0.003691000	-0.031719000
H	-3.788869000	2.138326000	-0.029131000
N	0.953393000	-1.170156000	-0.109000000
C	-3.963655000	-0.013953000	0.057090000
N	2.239828000	-1.168658000	-0.135981000
H	-3.805730000	-2.144868000	0.060089000
C	-3.253286000	-1.215519000	0.046797000
C	-1.871099000	-1.215062000	0.011260000
H	-1.336405000	-2.153622000	0.011632000
C	-1.169401000	-0.003695000	-0.036772000
C	0.298270000	-0.000839000	-0.090737000
C	2.960873000	-2.492382000	-0.139422000
H	3.905070000	-2.264556000	-0.632341000
C	3.032612000	0.001062000	-0.099374000
C	2.957568000	2.490615000	-0.223383000
H	3.899972000	2.247631000	-0.712551000
C	2.172730000	3.501823000	-1.040989000
H	1.934686000	3.122057000	-2.035020000
H	2.796032000	4.387643000	-1.161579000
H	1.250848000	3.800440000	-0.545502000
C	3.238028000	2.942304000	1.211976000
H	3.815071000	3.866050000	1.176223000
H	2.305919000	3.140303000	1.743343000
H	3.821922000	2.205266000	1.762113000
C	3.235093000	-2.896935000	1.311135000

H	3.816895000	-2.142471000	1.839508000
H	3.811968000	-3.821465000	1.307791000
H	2.300581000	-3.077474000	1.844410000
H	1.945572000	-3.182588000	-1.933893000
C	2.179116000	-3.529616000	-0.926911000
H	1.255000000	-3.812000000	-0.426184000
H	2.802823000	-4.418905000	-1.015788000
O	-6.045445000	-1.060547000	-0.360338000
H	-5.567398000	1.600515000	0.972505000

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N	0.457345000	1.153255000	-0.541592000
C	-1.198414000	0.000519000	0.693193000
H	5.215423000	2.138331000	-0.895145000
C	-1.686671000	-2.112414000	-0.633268000
N	-0.774606000	-1.139105000	-0.137997000
H	5.213473000	-2.141391000	-0.906167000
N	-0.773925000	1.139327000	-0.138603000
C	-0.582189000	0.000763000	2.081061000
H	2.773797000	-2.146180000	-0.654624000
C	1.143494000	-0.000547000	-0.488049000
N	0.456493000	-1.153911000	-0.541209000
H	2.775958000	2.144127000	-0.644197000
H	-0.537972000	2.476964000	-2.414811000
C	3.304115000	-1.205564000	-0.716603000
C	6.890497000	-0.000464000	-1.111455000
C	3.305554000	1.203417000	-0.710814000
H	-2.088351000	4.211356000	-3.252619000
C	2.597462000	-0.001086000	-0.649748000
H	-4.108914000	4.804698000	-1.949289000

C	-1.685444000	2.112660000	-0.634836000
H	-4.565179000	3.674377000	0.205234000
H	-3.015159000	1.983894000	1.069687000
C	-1.418776000	-2.749089000	-1.846723000
C	-1.416886000	2.748484000	-1.848601000
H	-0.540048000	-2.478126000	-2.413497000
C	4.682668000	1.196191000	-0.852917000
H	-2.091180000	-4.212733000	-3.249493000
C	-2.290422000	3.718772000	-2.310971000
H	-4.111226000	-4.804854000	-1.944839000
C	5.398386000	-0.001822000	-0.934322000
H	-4.566376000	-3.672941000	0.209086000
C	-2.819952000	2.443519000	0.110106000
H	-3.015636000	-1.982164000	1.071735000
C	-3.427840000	4.050151000	-1.579036000
H	-0.513416000	-2.149134000	2.241810000
C	4.681749000	-1.198999000	-0.858996000
H	0.328941000	-2.140571000	4.546101000
C	0.377656000	0.001546000	4.698075000
H	0.753229000	0.001830000	5.712788000
C	-2.820954000	-2.442500000	0.112379000
H	0.328324000	2.143578000	4.545063000
C	-0.340921000	-1.203873000	2.740331000
H	-0.513974000	2.150755000	2.240745000
H	-2.282677000	0.000830000	0.725405000
C	-2.292718000	-3.719491000	-2.308076000
C	-3.690284000	-3.410349000	-0.368337000
C	-3.688884000	3.411219000	-0.371644000
C	-0.341243000	1.205790000	2.739750000

C	-3.429872000	-4.050155000	-1.575410000
C	0.138251000	1.203914000	4.043516000
C	0.138573000	-1.201208000	4.044097000
H	7.339982000	-0.913474000	-0.721211000
H	7.350671000	0.851649000	-0.610477000
H	7.151557000	0.065899000	-2.171679000

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N	0.679809000	1.153686000	-0.643622000
C	-0.856585000	0.000045000	0.736863000
H	5.372753000	2.142468000	-1.507285000
N	-0.508784000	-1.139810000	-0.129105000
C	-1.460667000	-2.115459000	-0.537302000
H	5.372354000	-2.142869000	-1.508938000
N	-0.508660000	1.139853000	-0.129252000
C	-0.117883000	0.000125000	2.063675000
H	2.963720000	-2.146106000	-0.988025000
C	1.366201000	-0.000123000	-0.657172000
N	0.679722000	-1.153848000	-0.643448000
H	2.964120000	2.145743000	-0.986366000
C	3.489501000	-1.208624000	-1.106624000
H	6.583262000	-0.000235000	-1.775454000
H	-0.489868000	2.467914000	-2.422366000
C	3.489720000	1.208253000	-1.105712000
H	-2.108508000	4.205542000	-3.112447000
C	2.799485000	-0.000171000	-0.966326000
H	-3.989582000	4.811962000	-1.620599000
C	-1.460480000	2.115489000	-0.537606000
H	-4.238653000	3.691868000	0.572839000
C	-1.308635000	-2.745558000	-1.773990000

H	-2.617212000	1.995937000	1.288426000
C	-1.308413000	2.745380000	-1.774398000
H	-0.490081000	-2.468241000	-2.422006000
C	4.844951000	1.204149000	-1.398965000
H	-2.108812000	-4.205883000	-3.111809000
H	-3.989934000	-4.811955000	-1.619866000
C	-2.219232000	3.717257000	-2.153566000
C	5.524975000	-0.000205000	-1.549315000
H	-4.238980000	-3.691445000	0.573364000
C	-2.516019000	2.452812000	0.313124000
H	-2.617409000	-1.995537000	1.288698000
C	-3.278588000	4.055931000	-1.315314000
H	-0.033391000	-2.150021000	2.216402000
C	4.844720000	-1.204542000	-1.399880000
H	1.007943000	-2.141826000	4.437860000
C	1.068469000	0.000244000	4.585954000
H	1.531507000	0.000300000	5.563847000
C	-2.516238000	-2.452566000	0.313469000
H	1.007797000	2.142303000	4.437727000
C	0.181326000	-1.204789000	2.698335000
H	-0.033548000	2.150289000	2.216268000
H	-1.933870000	0.000123000	0.865249000
C	-2.219515000	-3.717439000	-2.153006000
C	-3.424047000	-3.422434000	-0.084955000
C	-3.423761000	3.422678000	-0.085447000
C	0.181241000	1.205104000	2.698261000
C	-3.278902000	-4.055906000	-1.314712000
C	0.773459000	1.202819000	3.954971000
C	0.773546000	-1.202385000	3.955051000

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N	0.051511000	1.156376000	-0.461642000
C	-1.709394000	-0.000023000	0.615154000
H	4.839507000	2.135167000	-0.498943000
C	-2.070550000	-2.131768000	-0.722007000
N	-1.209737000	-1.141941000	-0.172579000
H	4.839527000	-2.135087000	-0.498541000
N	-1.209714000	1.142029000	-0.172402000
C	-1.225192000	-0.000152000	2.054137000
H	2.356693000	-2.147074000	-0.408765000
C	0.723450000	0.000039000	-0.358329000
N	0.051500000	-1.156266000	-0.461797000
H	2.356703000	2.147159000	-0.409131000
N	6.429821000	0.000020000	-0.556652000
H	-0.776648000	2.527221000	-2.392876000
C	2.893652000	-1.209456000	-0.433688000
H	-2.245256000	4.288175000	-3.317514000
C	2.893651000	1.209532000	-0.433897000
C	2.191367000	0.000040000	-0.417062000
H	-4.365310000	4.863017000	-2.174844000
C	-2.070532000	2.131923000	-0.721697000
H	-5.005558000	3.689354000	-0.091507000
H	-3.539465000	1.971736000	0.861954000
C	-1.697875000	-2.791839000	-1.895230000
C	-1.697988000	2.791966000	-1.894971000
H	-0.776437000	-2.527166000	-2.392989000
C	4.277686000	1.213244000	-0.483467000
H	-2.245016000	-4.288011000	-3.317851000
C	-2.526410000	3.776409000	-2.406972000

H	-4.365309000	-4.862692000	-2.175527000
C	4.948656000	0.000032000	-0.509004000
H	-5.005795000	-3.688977000	-0.092284000
C	-3.263117000	2.451392000	-0.067207000
H	-3.539731000	-1.971499000	0.861411000
C	-3.720304000	4.097268000	-1.765116000
H	-1.173883000	-2.151422000	2.222964000
C	4.277685000	-1.213173000	-0.483240000
H	-0.548733000	-2.142496000	4.593260000
C	-0.512336000	-0.000433000	4.749717000
H	-0.231577000	-0.000538000	5.794595000
C	-3.263259000	-2.451153000	-0.067709000
H	-0.547819000	2.141661000	4.593462000
C	-1.047104000	-1.205245000	2.733300000
H	-1.172976000	2.151080000	2.223167000
H	-2.791613000	0.000011000	0.543047000
C	-2.526285000	-3.776221000	-2.407357000
C	-4.084935000	-3.433626000	-0.598798000
C	-4.084801000	3.433925000	-0.598161000
C	-1.046596000	1.204802000	2.733412000
C	-3.720310000	-4.096995000	-1.765693000
C	-0.690148000	1.202135000	4.076159000
C	-0.690656000	-1.202862000	4.076046000
O	6.987180000	-1.083189000	-0.574703000
O	6.987182000	1.083224000	-0.574986000

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C	3.938788000	-4.148488000	0.757356000
H	4.599362000	-4.928855000	1.110797000
N	0.118162000	-1.158838000	-0.268477000

C	4.221944000	-3.486614000	-0.433261000
H	5.092888000	-3.759004000	-1.013706000
N	1.363009000	-1.146958000	-0.621683000
C	3.380798000	-2.485128000	-0.892442000
H	3.590033000	-2.008350000	-1.840612000
N	1.363024000	1.146939000	-0.621735000
N	0.118196000	1.158851000	-0.268515000
C	2.251221000	2.147779000	-0.142573000
H	3.589753000	2.008586000	-1.840947000
C	3.380688000	2.485265000	-0.892689000
H	5.092622000	3.759342000	-1.014142000
C	4.221844000	3.486749000	-0.433544000
H	4.599494000	4.928752000	1.110681000
H	2.589960000	4.319760000	2.422632000
C	3.938872000	4.148425000	0.757237000
C	2.807022000	3.808427000	1.494542000
H	1.085235000	2.527203000	1.624002000
H	-2.187577000	2.148100000	-0.206480000
C	1.959359000	2.806240000	1.053700000
C	-2.021793000	0.000028000	-0.207834000
H	-4.662237000	2.135224000	0.007091000
N	-6.247789000	0.000037000	0.146092000
C	-2.721907000	1.209950000	-0.155704000
C	-4.101784000	1.213351000	-0.036797000
H	-4.662331000	-2.135145000	0.006151000
C	-4.770256000	0.000043000	0.022401000
H	-2.187696000	-2.148036000	-0.207470000
C	-4.101850000	-1.213272000	-0.037340000
H	2.868198000	-0.000036000	-1.546705000

H	1.264277000	-0.000059000	-2.373834000
C	-2.721962000	-1.209872000	-0.156252000
C	1.795654000	-0.000045000	-1.417545000
H	1.084894000	-2.527553000	1.623818000
C	-0.558337000	0.000008000	-0.340200000
H	2.589565000	-4.320117000	2.422477000
C	2.251165000	-2.147814000	-0.142510000
C	1.959136000	-2.806458000	1.053636000
C	2.806768000	-3.808655000	1.494490000
O	-6.802576000	-1.083315000	0.192568000
O	-6.802533000	1.083374000	0.193489000

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C	3.094374000	-4.102323000	0.716169000
N	-0.782607000	-1.156471000	-0.221768000
H	3.772895000	-4.871326000	1.060408000
C	3.331653000	-3.458829000	-0.494194000
N	0.447469000	-1.144386000	-0.626847000
H	4.185114000	-3.733966000	-1.098895000
C	2.466616000	-2.472378000	-0.942326000
N	0.447380000	1.144404000	-0.626759000
H	2.639706000	-2.010134000	-1.904904000
N	-0.782695000	1.156341000	-0.221659000
C	1.360176000	2.130314000	-0.161060000
H	2.639819000	2.010102000	-1.904574000
C	2.466550000	2.472421000	-0.942067000
H	4.185040000	3.734027000	-1.098501000
C	3.331489000	3.458939000	-0.493902000
H	3.772467000	4.871618000	1.060605000
C	3.094019000	4.102554000	0.716356000

H	1.801360000	4.256165000	2.427201000
C	1.984127000	3.758849000	1.484174000
H	0.255777000	2.489564000	1.647503000
C	1.113954000	2.770829000	1.054594000
H	-3.090153000	2.146767000	-0.101003000
C	-2.924001000	-0.000138000	-0.105185000
H	-5.538453000	2.142610000	0.172712000
H	-6.769742000	-0.000145000	0.314825000
C	-3.624394000	1.208775000	-0.035790000
H	-5.538201000	-2.142903000	0.174889000
C	-5.002309000	1.204399000	0.118555000
H	-3.089905000	-2.147060000	-0.098835000
C	-5.693841000	-0.000143000	0.198722000
C	-5.002167000	-1.204685000	0.119766000
H	1.907640000	0.000102000	-1.625051000
C	-3.624251000	-1.209063000	-0.034579000
H	0.264514000	0.000078000	-2.372039000
C	0.842757000	0.000070000	-1.443305000
H	0.256220000	-2.489313000	1.647571000
C	-1.467829000	-0.000094000	-0.275084000
H	1.801989000	-4.255809000	2.427223000
C	1.360353000	-2.130231000	-0.161187000
C	1.114321000	-2.770626000	1.054570000
C	1.984584000	-3.758572000	1.484121000

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C	3.989409000	-3.896678000	0.773985000
H	4.710920000	-4.615670000	1.138298000
N	-0.053860000	-1.211685000	-0.248899000
C	4.200877000	-3.256976000	-0.443118000

N	1.177321000	-1.132414000	-0.647079000
H	5.078171000	-3.485340000	-1.033047000
C	3.280380000	-2.334750000	-0.917063000
H	3.436311000	-1.876181000	-1.884324000
N	1.054065000	1.149392000	-0.649122000
H	3.210261000	2.129624000	-1.899520000
C	1.918110000	2.168944000	-0.162478000
N	-0.177907000	1.096268000	-0.248766000
C	3.012260000	2.570694000	-0.931832000
H	4.675498000	3.907469000	-1.060913000
C	3.831571000	3.587147000	-0.465109000
H	4.202934000	4.995159000	1.111830000
C	3.560406000	4.202447000	0.752641000
H	2.253011000	4.275450000	2.457361000
C	2.462270000	3.800066000	1.508499000
H	0.789221000	2.454324000	1.643331000
C	1.637669000	2.781357000	1.059986000
H	-2.555930000	1.954062000	-0.200251000
C	-2.253657000	-0.174960000	-0.184119000
H	-4.983595000	1.830538000	0.016559000
O	-6.365448000	-0.511735000	0.179675000
C	-3.031845000	0.984488000	-0.139290000
C	-4.409825000	0.916545000	-0.014860000
H	-4.768698000	-2.455317000	0.056405000
H	-2.313997000	-2.331681000	-0.162517000
C	-5.039915000	-0.330843000	0.061616000
H	2.573742000	0.085932000	-1.648111000
C	-4.265348000	-1.499486000	0.005001000
C	-2.896886000	-1.421688000	-0.118523000

H	0.932102000	-0.003391000	-2.393478000
C	1.510609000	0.028937000	-1.465438000
H	1.041039000	-2.455852000	1.643923000
C	-0.804854000	-0.094732000	-0.318430000
H	2.685987000	-4.108119000	2.470177000
C	2.144614000	-2.051619000	-0.155020000
C	1.923901000	-2.689383000	1.066798000
C	2.849662000	-3.613468000	1.522220000
C	-7.227955000	0.623226000	0.244113000
H	-7.160389000	1.220045000	-0.668331000
H	-6.996187000	1.243541000	1.112883000
H	-8.232858000	0.222731000	0.341909000

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N	-1.163193000	0.444680000	0.045296000
N	-1.103105000	-0.843064000	0.077744000
C	0.099789000	-1.408014000	0.051465000
N	1.243399000	-0.733386000	-0.006343000
N	1.180913000	0.554438000	-0.038708000
C	-0.028896000	1.295653000	-0.016181000
C	-2.484073000	1.091273000	0.073421000
C	2.434841000	1.320822000	-0.102887000
O	-0.085720000	2.484408000	-0.045426000
H	0.151072000	-2.485569000	0.078479000
H	-3.227466000	0.303251000	0.119839000
H	-2.534179000	1.745081000	0.943949000
H	-2.594759000	1.698098000	-0.825070000
H	3.249309000	0.605051000	-0.112333000
H	2.424487000	1.932254000	-1.005002000

H	2.486317000	1.979168000	0.764108000
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