Electronic Supplementary Material (ESI) for Energy & Environmental Science


**Supporting Information for**

# Fuel selection for a regenerative organic fuel cell/flow battery: thermodynamic considerations

C. Moyses Araujo,[†,‡] Davide L. Simone,[¶] Steven J. Konezny,[†] Aaron Shim,[†]

Robert H. Crabtree,[†,‡] Grigorii L. Soloveichik,[*,¶] and Victor S. Batista[*,†,‡]

*Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520-8107, Yale Climate and Energy Institute, Yale University, P.O. Box 208109, New Haven, CT 06520-8109, and General Electric Global Research, One Research Circle, Niskayuna, NY 12309*

E-mail: soloveichik@ge.com; victor.batista@yale.edu

[*]To whom correspondence should be addressed
[†]Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520-8107
[‡]Yale Climate and Energy Institute, Yale University, P.O. Box 208109, New Haven, CT 06520-8109
[¶]General Electric Global Research, One Research Circle, Niskayuna, NY 12309

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**Static bomb combustion calorimetry**

The heat capacity of the calorimeter vessel was determined using the following setup: a quartz crucible combustion vessel (C 5010), combustion crucible support (C 5010.4), cotton thread igniter (C 710.4), benzoic acid pellet (CAS 65-85-0, standard reference material (SRM 309j) supplied by National Institute of Standards, C 723, $Q_{standard}$ value = 26434 J/g) and 1 ml deionized water to absorb any acid formed. The calorimeter vessel is purged with pure oxygen three times prior to filling the vessel to the reaction pressure of 35 psi of oxygen. Following the combustion experiment the calorimeter vessel gaseous contents were purged into approximately 15 mL of deionized water and the interior of the vessel, including crucible and ignition apparatus, were rinsed with deionized water. The total amount of deionized rinse/purge water was not allowed to exceed 50 mL as a precaution for unnecessary dilution of acidic species formed during combustion. To this solution is added approximately 1 mL of a 1% w/v aqueous methyl red indicator and is then titrated using the following titration setup: 1) a 10 mL capacity Kimax automatic buret with 0.05 mL subdivisions that is purchased as traceable to standards provided by NIST ; 2) 0.1M NaOH standardized to KHP as the titrant. In the case of benzoic acid, the amount of acid species formed after combustion is negligible relative to the acidity of deionized water. If nitrogen containing organic fuels are used, acid corrections become significant, see above ASTM standard for more details. The heat capacity determination for a calorimeter setup as described above gave the average number of 9974 J/K with a relative standard deviation of 0.07 % (see Supporting Information, Table S1).

The internal calorific values assigned as constant during the calorimetric experiments is 100 J for the ignition wire and 50 J for the cotton thread primary combustor. In the cases of very high and

very low vapour pressure liquids it was found that Scotch Brand tape, #610, was adequate in providing, in conjunction with the cotton thread, a secondary, non-absorbing ignition source for low volatility organic fuels and a combustion crucible cover for high volatility liquids. The acid corrected calorific value for Scotch brand #610 tape used in determining the calorific values of organic fuels was measured with a relative standard deviation 0.36 % (see Supporting Information, Table S2).

**Table S1.** Heat capacity determination of the calorimeter vessel.

| Calibration run | Heat capacity of the calorimeter vessel , W (J/K) |
|---|---|
| 1 | 9978 |
| 2 | 9986 |
| 3 | 9976 |
| 4 | 9968 |
| 5 | 9967 |
| 6 | 9971 |
| Average | 9974 |
| Standard deviation | ±7 |

**Table S2.** Calorific values for Scotch brand #610 tape.

| Tape calibration run | Calorific value Q of the tape (J/g) |
|---|---|
| 1 | 25032 |
| 2 | 24948 |
| 3 | 25130 |
| Average | 25037 |
| Standard deviation | ±91 |

**Table S3**. Combustion enthalpy of select organic fuels.

| Compound | $-\Delta H_{c,298K}$ (MJ/mol)* | $-\Delta H_{c,298K}$ literature (MJ/mol) | % deviation from literature |
|---|---|---|---|
| cyclohexane | 3.891±0.002 | 3.920 | 0.7 |
| benzene | 3.242±0.009 | 3.267 | 0.7 |
| decalin | 6.266±0.006 | 6.280 | 0.2 |
| naphthalene | 5.156±0.003 | 5.154 | 0.04 |
| piperidine | 3.442±0.002 | 3.448 | 0.17 |
| pyridine | 2.777±0.005 | 2.782 | 0.18 |
| pyrrolidine | 2.796±0.001 | 2.819 | 0.8 |
| pyrrole | 2.350±0.001 | 2.352 | 0.09 |
| Indoline** | 4.489±0.001 | 4.492 | 0.07 |
| indole | 4.243±0.007 | 4.273 | 0.7 |
| 2,3-dihydrobenzofuran | 4.164±0.003 | 4.192 | 0.7 |
| 2,3-benzofuran | 3.954±0.0001 | 3.971 | 0.4 |
| decahydroquinoline | 5.741±0.003 | 5.822 | 1.4 |
| quinoline | 4.630±0.005 | 4.698 | 1.5 |
| N-ethyldodecahydrocarbazole** | 8.806±0.02 | NA | NA |
| N-ethylcarbazole | 7.345±0.02 | 7.438 | 1.3 |

* - Values for the enthalpy of combustion for fuels/spent fuels have been corrected to 298K if the enthalpy value has a correction factor associated with it (see ASTM D4809-00 page 845).[1]

** - The dehydrogenation thermodynamic data for these fuels is based on combustion data from 4 combustion measurements (2 runs for each substrate). All other fuels are based on six experiments (3 runs per substrate).

**Table S4.** Thermodynamic parameters of tabulated organic compounds.

| Organic compounds | $\Delta_f H°$ (kJ/mol) | S° (J/mol*K) | $C_p$ (J/mol*K) |
|---|---|---|---|
| Hydrogenated form | | | |
| ethylbenzene | -12.5 | 255.0 | 184.8 |
| cyclooctane | -169.4 | 262.0 | 215.8 |
| cyclohexane | -156.2 | 204.35 | 156 |
| cyclohexene | -38.2 | 214.6 | 148.8 |
| cyclopentane | -105.9 | 204.1 | 126.7 |
| indane | 10.7 | 234.4 | 190.3 |
| cycloheptane | -156.8 | 242.6 | 123.1 |
| tetrahydrofuran | -216.1 | 203.9 | 124.1 |
| tetrahydrothiophene | -72.8 | 207.82 | 140.2 |
| 2,3-dihydrobenzofuran | -99.8 | 226.4 | 188.6 |
| n-propylamine | -101.5 | 324.0 | 162.5 |
| cyclohexanethiol | -140.4 | 255.6 | 192.6 |
| cyclohexanol | -352 | 203.9 | 214.1 |
| N-methylpyrrolidine | -50.0 | 236.4 | 161.1 |
| trans-Decalin | -228.7 | 264.9 | 229.2 |
| tetralin | -32.6 | 251.5 | 217.4 |
| tetrahydroquinoline | 16.7 | 240.4 | 236.0 |
| piperidine | -86.4 | 209.9 | 179.9 |
| cyclohexylamine | -147.6 | 241.0 | n/a |
| 2-methylpiperidine | -124.9 | 243.8 | 213.0 |
| isopropanol | -318.2 | 180.6 | 161.2 |
| 2-butanol | -342.6 | 213.1 | 198.3 |
| piperazine | -41.8 | 301.2 | 237.0 |
| pyrrolidine | -49.5 | 204.1 | 160.2 |
| 1,4-cyclohexadiene | 66.1 | 189.4 | 142.2 |
| 1,3-cyclohexadiene | 71.4 | 197.3 | 141.3 |
| Dehydrogenated form | | | |
| phenylacetylene | 284.3 | 221.2 | 180.1 |
| styrene | 103.4 | 240.5 | 183.2 |
| cyclooctatetraene | 255.0 | 220.3 | 180.0 |
| cyclopentene | 4.3 | 201.3 | 122.4 |
| cyclopentadiene | 24.0 | 250.0 | 198.9 |
| 1H-Indene | 110.4 | 214.2 | 187.0 |
| cycloheptatriene | 143.2 | 214.7 | 162.8 |
| furan | -62.3 | 176.7 | 114.6 |
| thiophene | 80.96 | 181.2 | 122.4 |
| benzofuran | -34.8 | 215.6 | 178.7 |

| | | | |
|---|---|---|---|
| propionitrile | 15.5 | 189.33 | 119.5 |
| benzene | 49.0 | 173.3 | 135.9 |
| thiophenol | 63.7 | 222.8 | 173.2 |
| toluene | 12.0 | 221.0 | 157.1 |
| phenol | -165.1 | 144.0 | 127.2 |
| N-methylpyrrole | 62.4 | 200.5 | 150.1 |
| Naphtalene | 75.4 | 167.4 | 165.7 |
| quinoline | 141.2 | 219.7 | 194.9 |
| pyridine | 100.0 | 177.7 | 134.9 |
| aniline | 31.3 | 191.3 | 194.1 |
| 2-methylpyridine | 56.5 | 217.9 | 158.4 |
| acetone | -249.4 | 200.4 | 125.5 |
| 2-butanone | -273.3 | 239.0 | 159.0 |
| pyrazine | 139.8 | 280.4 | 180.0 |

**Table S5.** Comparison of the electronic energy (E) of the investigated organic molecules computed using Spartan 08 and Gaussian 09 software packages.

| Organic compounds | E (Spartan) (Hartree) | E (Gaussian) (Hartree) | Difference (kcal/mol) |
|---|---|---|---|
| ethylbenzene | -310.9921 | -310.9919 | 0.112 |
| cyclooctane | -314.6024 | -314.6028 | -0.256 |
| cyclohexane | -235.9656 | -235.9655 | 0.098 |
| cyclohexene | -234.7342 | -234.7341 | 0.020 |
| cyclopentane | -196.6292 | -196.6292 | -0.007 |
| indane | -349.1086 | -349.1086 | 0.011 |
| cycloheptane | -275.2826 | -275.2825 | 0.090 |
| tetrahydrofuran | -232.5380 | -232.5379 | 0.043 |
| tetrahydrothiophene | -555.5294 | -555.5293 | 0.080 |
| 2,3-dihydrobenzofuran | -385.0205 | -385.0206 | -0.013 |
| n-propylamine | -174.5590 | -174.5590 | -0.018 |
| cyclohexanethiol | -634.1882 | -634.1880 | 0.109 |
| cyclohexanol | -311.2129 | -311.2128 | 0.084 |
| N-methylpyrrolidine | -251.9869 | -251.9870 | -0.043 |
| trans-Decalin | -392.0697 | -392.0694 | 0.205 |
| tetralin | -388.4404 | -388.4403 | 0.086 |
| tetrahydroquinoline | -404.4830 | -404.4829 | 0.059 |
| piperidine | -251.9991 | -251.9989 | 0.100 |
| cyclohexylamine | -291.3364 | -291.3362 | 0.130 |
| 2-methylpiperidine | -291.3308 | -291.3307 | 0.041 |
| isopropanol | -194.4391 | -194.4391 | 0.001 |

| | | | |
|---|---|---|---|
| 2-butanol | -233.7668 | -233.7668 | 0.018 |
| piperazine | -268.0308 | -268.0315 | -0.430 |
| pyrrolidine | -212.6632 | -212.6630 | 0.110 |
| 1,4-cyclohexadiene | -233.5052 | -233.5053 | -0.029 |
| 1,3-cyclohexadiene | -233.5053 | -233.5051 | 0.110 |
| phenylacetylene | -308.5064 | -308.5064 | 0.031 |
| styrene | -309.7604 | -309.7603 | 0.020 |
| cyclooctatetraene | -309.6811 | -309.6811 | 0.015 |
| cyclopentene | -195.3996 | -195.3996 | -0.023 |
| cyclopentadiene | -194.1740 | -194.1741 | -0.072 |
| 1H-Indene | -347.8835 | -347.8836 | -0.036 |
| cycloheptatriene | -271.6093 | -271.6094 | -0.048 |
| furan | -230.1087 | -230.1087 | -0.029 |
| thiophene | -553.0982 | -553.0982 | -0.005 |
| benzofuran | -383.8095 | -383.8096 | -0.022 |
| propionitrile | -172.1346 | -172.1346 | 0.022 |
| benzene | -232.3334 | -232.3334 | 0.029 |
| thiophenol | -630.5562 | -630.5561 | 0.068 |
| toluene | -271.6645 | -271.6645 | 0.019 |
| phenol | -307.5857 | -307.5857 | 0.027 |
| N-methylpyrrole | -249.5714 | -249.5714 | -0.011 |
| Naphtalene | -386.0256 | -386.0256 | 0.046 |
| quinoline | -402.0676 | -402.0676 | 0.033 |
| pyridine | -248.3732 | -248.3732 | 0.006 |
| aniline | -287.7129 | -287.7129 | 0.013 |
| 2-methylpyridine | -287.7076 | -287.7075 | 0.035 |
| acetone | -193.2332 | -193.2332 | -0.005 |
| 2-butanone | -232.5617 | -232.5617 | 0.016 |
| pyrazine | -264.4095 | -264.4095 | -0.013 |
| hexahydropyrimidine | -268.0346 | -268.0344 | 0.108 |
| hexahydropyridazine | -268.0068 | -268.0067 | 0.059 |
| hexahydro-1,3,5-triazine | | | |
| tetrahydro-1H-imidazole | -228.6997 | -228.6997 | -0.037 |
| pyrazolidine | -228.6718 | -228.6718 | 0.003 |
| 1,2,3-triazolidine | -244.6875 | -244.6875 | 0.009 |
| 1,2,4-triazolidine | -244.7181 | -244.7181 | 0.012 |
| perhydroquinoline | -408.1056 | -408.1053 | 0.195 |
| perhydroisoquinoline | -408.1031 | -408.1028 | 0.184 |
| perhydro-4H-quinolizine | -408.1008 | -408.1005 | 0.187 |
| perhydrocinnoline | -424.1160 | -424.1158 | 0.153 |
| perhydrophthalazine | -424.1139 | -424.1136 | 0.177 |

| | | | |
|---|---|---|---|
| perhydroquinazoline | -424.1414 | -424.1410 | 0.236 |
| perhydroquinoxaline | -424.1399 | -424.1395 | 0.242 |
| perhydro1,8-naphthyridine | -424.1390 | -424.1388 | 0.167 |
| perhydro1,5-naphthyridine | -424.1412 | -424.1409 | 0.184 |
| perhydropteridine | -456.2148 | -456.2144 | 0.245 |
| perhydropyrazino[2,3-b]pyrazine | -456.2110 | -456.2106 | 0.223 |
| perhydropyrimido[4,5-d]pyrimidine | -456.2056 | -456.2053 | 0.227 |
| perhydro-1H-indene | -352.7322 | -352.7319 | 0.171 |
| perhydrobenzofuran | -388.6431 | -388.6429 | 0.092 |
| perhydrobenzothiophene | -711.6320 | -711.6320 | 0.001 |
| perhydro-1H-indole | -368.7671 | -368.7669 | 0.084 |
| perhydro-2H-isoindole | -368.7643 | -368.7641 | 0.101 |
| perhydroindolizine (delta-coniceine) | -368.7675 | -368.7673 | 0.141 |
| perhydrobenzimidazole | -384.8025 | -384.8023 | 0.113 |
| perhydro-1H-indazole | -384.7732 | -384.7731 | 0.065 |
| octahydro-1H-pyrrolo[2,3-b]pyridine | -384.8030 | -384.8029 | 0.047 |
| perhydroimidazo[1,2-a]pyrazine | -400.8349 | -400.8347 | 0.114 |
| octahydro-1H-purine | -416.8730 | -416.8729 | 0.108 |
| perhydropentalene | -313.3873 | -313.3872 | 0.092 |
| perhydropyrrolizine | -329.4261 | -329.4259 | 0.120 |
| perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole | -345.4509 | -345.4509 | 0.016 |
| perhydro-1,4-dihydroimidazo [4,5-d]imidazole | -377.5179 | -377.5181 | -0.098 |
| perhydro-N-ethylindole | -447.4185 | -447.4184 | 0.083 |
| perhydro-N-ethylindazole | -463.4295 | -463.4291 | 0.200 |
| octahydro-1Methylpurine | -456.1950 | -456.1950 | 0.013 |
| N-ethylperhydropurine | -495.5134 | -495.5134 | -0.021 |
| perhydrofluorene | -508.8313 | -508.8313 | -0.010 |
| perhydro-9-ethylfluorene | -587.4825 | -587.4823 | 0.128 |
| perhydro-9H-carbazole | -524.8675 | -524.8675 | 0.016 |
| perhydro-N-ethylcarbazole | -603.5122 | -603.5123 | -0.020 |
| perhydro-1,8-diazacarbazole | -556.9379 | -556.9379 | 0.025 |
| perhydro-N-methyl-1,8-diazacarbazole | -596.2537 | -596.2534 | 0.182 |
| perhydro-N-ethyl-1,8-diazacarbazole | -635.5808 | -635.5807 | 0.071 |
| perhydrodibenzoborole | -494.9567 | -494.9567 | -0.043 |
| perhydro-5Me-dibenzoborole | -534.3038 | -534.3038 | 0.010 |
| perhydro[b,d]dibenzofuran | -544.7452 | -544.7451 | 0.082 |
| perhydrodibenzothiophene | -867.7334 | -867.7333 | 0.035 |
| perhydro-3,6-diazacarbazole | -556.9316 | -556.9314 | 0.081 |
| perhydro-4,5-diazacarbazole | -556.9309 | -556.9308 | 0.019 |
| pyrimidine | -264.4162 | -264.4161 | 0.046 |
| pyridazine | -264.3804 | -264.3804 | 0.038 |

| | | | |
|---|---|---|---|
| 1,3,5-triazine | -280.4619 | -280.4618 | 0.037 |
| 1H-pyrrole | -210.2490 | -210.2490 | -0.022 |
| 1H-imidazole | -226.3014 | -226.3013 | 0.033 |
| 1H-pyrazole | -226.2846 | -226.2846 | 0.008 |
| 1H-1,2,3-triazole | -242.3125 | -242.3125 | 0.016 |
| 1H-1,2,4-triazole | -242.3393 | -242.3393 | 0.009 |
| naphthalene | -386.0256 | -386.0256 | 0.046 |
| isoquinoline | -402.0658 | -402.0657 | 0.056 |
| 4H-quinolizine | -403.2206 | -403.2205 | 0.041 |
| cinnoline | -418.0737 | -418.0736 | 0.043 |
| phtalazine | -418.0756 | -418.0755 | 0.059 |
| quinazoline | -418.1112 | -418.1111 | 0.041 |
| quinoxaline | -418.1061 | -418.1061 | 0.018 |
| 1,8-naphthyridine | -418.1070 | -418.1070 | 0.009 |
| 1,5-naphthyridine | -418.1094 | -418.1094 | 0.011 |
| pteridine | -450.1862 | -450.1861 | 0.004 |
| pyrazino[2,3-b]pyrazine | -450.1815 | -450.1816 | -0.022 |
| pyrimido[4,5-d]pyrimidine | -450.1912 | -450.1912 | 0.026 |
| benzo[b]thiophene | -706.7969 | -706.7969 | -0.008 |
| 1H-indole | -363.9472 | -363.9472 | -0.010 |
| 2H-isoindole | -363.9327 | -363.9327 | -0.004 |
| indolizine(delta-coniceine) | -363.9274 | -363.9274 | -0.006 |
| 1H-benzo[d]imidazole | -380.0006 | -380.0006 | 0.005 |
| 1H-indazole | -379.9774 | -379.9774 | -0.006 |
| 1H-pyrrolo[2,3-b]pyridine | -379.9951 | -379.9951 | -0.041 |
| imidazo[1,2-a]pyrazine | -396.0196 | -396.0195 | 0.045 |
| 7H-purine | -412.0831 | -412.0830 | 0.006 |
| 1,4-dihydropentalene | -309.7163 | -309.7164 | -0.064 |
| 1H-pyrrolizine | -325.7845 | -325.7845 | -0.039 |
| 1,4-dihydropyrrolo [3,2-b]pyrrole | -341.8427 | -341.8428 | -0.023 |
| 1,4-dihydroimidazo[4,5-d]imidazole | -373.9459 | -373.9459 | -0.010 |
| N-ethylindole | -442.6000 | -442.6000 | 0.005 |
| N-ethylindazole | -458.6315 | -458.6314 | 0.034 |
| N-methylpurine | -451.4074 | -451.4074 | 0.023 |
| N-ethylpurine | -490.7377 | -490.7377 | 0.013 |
| 9H-fluorene | -501.5917 | -501.5917 | 0.010 |
| 9-ethylfluorene | -580.2458 | -580.2458 | 0.000 |
| N-ethylcarbazole | -596.3012 | -596.3011 | 0.042 |
| N-methyl-1,8-diazacarbazole | -549.7439 | -549.7439 | 0.009 |
| N-ethyl-1,8-diazacarbazole | -589.0684 | -589.0683 | 0.056 |
| 5H-dibenzoborole | -628.3990 | -628.3989 | 0.050 |

| | | | |
|---|---|---|---|
| dibenzo-5Me-borole | -487.7192 | -487.7192 | -0.018 |
| dibenzo[b,d]furan | -527.0665 | -527.0666 | -0.028 |
| dibenzo[b,d]thiophene | -537.5133 | -537.5132 | 0.026 |
| 9H-carbazole | -517.6488 | -517.6487 | 0.031 |
| 1,8-diazacarbazole | -860.4979 | -860.4979 | -0.006 |
| 3,6-diazacarbazole | -549.7305 | -549.7305 | 0.042 |
| 4,5-diazacarbazole | -549.7252 | -549.7252 | 0.003 |

**Table S6.** The electronic energy (E), enthalpy (H), Entropy (S) and Gibbs free energy (G) of the investigated organic molecules.

| Organic compounds | E (Hartree) | H (Hartree) | S (cal/molK) | G (Hartree) |
|---|---|---|---|---|
| ethylbenzene | -310.9919 | -310.8272 | 85.279 | -310.8678 |
| cyclooctane | -314.6028 | -314.3669 | 87.443 | -314.4084 |
| cyclohexane | -235.9655 | -235.7891 | 72.296 | -235.8234 |
| cyclohexene | -234.7341 | -234.5819 | 72.508 | -234.6164 |
| cyclopentane | -196.6292 | -196.4838 | 66.729 | -196.5155 |
| indane | -349.1086 | -348.9367 | 81.817 | -348.9756 |
| cycloheptane | -275.2825 | -275.0761 | 80.291 | -275.1143 |
| tetrahydrofuran | -232.5379 | -232.4165 | 67.327 | -232.4485 |
| tetrahydrothiophene | -555.5293 | -555.4097 | 71.751 | -555.4438 |
| 2,3-dihydrobenzofuran | -385.0206 | -384.8728 | 81.550 | -384.9116 |
| n-propylamine | -174.5590 | -174.4315 | 72.660 | -174.4660 |
| cyclohexanethiol | -634.1880 | -634.0106 | 84.225 | -634.0506 |
| cyclohexanol | -311.2128 | -311.0309 | 80.510 | -311.0692 |
| N-methylpyrrolidine | -251.9870 | -251.8231 | 77.814 | -251.8601 |
| trans-Decalin | -392.0694 | -391.7965 | 89.095 | -391.8389 |
| tetralin | -388.4403 | -388.2382 | 85.646 | -388.2789 |
| tetrahydroquinoline | -404.4829 | -404.2924 | 86.786 | -404.3336 |
| piperidine | -251.9989 | -251.8339 | 74.057 | -251.8691 |
| cyclohexylamine | -291.3362 | -291.1416 | 81.020 | -291.1801 |
| 2-methylpiperidine | -291.3307 | -291.1366 | 80.773 | -291.1750 |
| isopropanol | -194.4391 | | | -194.3590 |
| 2-butanol | -233.7668 | -233.6232 | 78.810 | -233.6606 |
| piperazine | -268.0315 | -267.8777 | 71.984 | -267.9119 |
| pyrrolidine | -212.6630 | -212.5279 | 74.108 | -212.5631 |
| 1,4-cyclohexadiene | -233.5053 | -233.3772 | 70.288 | -233.4106 |
| 1,3-cyclohexadiene | -233.5051 | -233.3769 | 70.917 | -233.4106 |
| phenylacetylene | -308.5064 | -308.3896 | 78.134 | -308.4267 |
| styrene | -309.7603 | -309.6195 | 82.268 | -309.6586 |
| cyclooctatetraene | -309.6811 | -309.5407 | 74.884 | -309.5762 |

| | | | | |
|---|---|---|---|---|
| cyclopentene | -195.3996 | -195.2776 | 69.503 | -195.3107 |
| cyclopentadiene | -194.1741 | -194.0767 | 65.266 | -194.1077 |
| 1H-Indene | -347.8836 | -347.7360 | 79.504 | -347.7738 |
| cycloheptatriene | -271.6094 | -271.4750 | 75.339 | -271.5108 |
| furan | -230.1087 | -230.0342 | 63.660 | -230.0645 |
| thiophene | -553.0982 | -553.0266 | 66.434 | -553.0582 |
| benzofuran | -383.8096 | -383.6855 | 77.884 | -383.7225 |
| propionitrile | -172.1346 | -172.0548 | 68.065 | -172.0872 |
| benzene | -232.3334 | -232.2276 | 64.037 | -232.2581 |
| thiophenol | -630.5561 | -630.4497 | 79.584 | -630.4875 |
| toluene | -271.6645 | -271.5298 | 80.458 | -271.5680 |
| phenol | -307.5857 | -307.4747 | 74.522 | -307.5101 |
| N-methylpyrrole | -249.5714 | | | -249.4905 |
| Naphtalene | -386.0256 | -385.8706 | 79.176 | -385.9082 |
| quinoline | -402.0676 | -401.9245 | 81.466 | -401.9632 |
| pyridine | -248.3732 | -248.2793 | 67.228 | -248.3113 |
| aniline | -287.7129 | -287.5893 | 75.537 | -287.6252 |
| 2-methylpyridine | -287.7075 | -287.5857 | 73.750 | -287.6208 |
| acetone | -193.2332 | -193.1436 | 73.239 | -193.1784 |
| 2-butanone | -232.5617 | -232.4432 | 74.992 | -232.4788 |
| pyrazine | -264.4095 | -264.3277 | 65.533 | -264.3588 |
| hexahydropyrimidine | -268.0344 | -267.8806 | 73.417 | -267.9155 |
| hexahydropyridazine | -268.0067 | -267.8529 | 73.432 | -267.8878 |
| hexahydro-1,3,5-triazine | -284.0603 | -283.9185 | 70.904 | -283.9521 |
| tetrahydro-1H-imidazole | -228.6997 | -228.5756 | 70.498 | -228.6091 |
| pyrazolidine | -228.6718 | -228.5479 | 71.258 | -228.5818 |
| 1,2,3-triazolidine | -244.6875 | -244.5754 | 70.204 | -244.6087 |
| 1,2,4-triazolidine | -244.7181 | -244.6053 | 69.334 | -244.6383 |
| perhydroquinoline | -408.1053 | -407.8438 | 89.882 | -407.8865 |
| perhydroisoquinoline | -408.1028 | -407.8412 | 89.958 | -407.8839 |
| perhydro-4H-quinolizine | -408.1005 | -407.8396 | 90.177 | -407.8824 |
| perhydrocinnoline | -424.1158 | -423.8659 | 89.243 | -423.9083 |
| perhydrophthalazine | -424.1136 | -423.8636 | 89.245 | -423.9060 |
| perhydroquinazoline | -424.1410 | -423.8906 | 89.510 | -423.9331 |
| perhydroquinoxaline | -424.1395 | -423.8894 | 89.413 | -423.9319 |
| perhydro1,8-naphthyridine | -424.1388 | -423.8888 | 89.560 | -423.9313 |
| perhydro1,5-naphthyridine | -424.1409 | -423.8907 | 89.169 | -423.9330 |
| perhydropteridine | -456.2144 | -455.9866 | 88.020 | -456.0284 |
| perhydropyrazino[2,3-b]pyrazine | -456.2106 | -455.9832 | 88.144 | -456.0251 |
| perhydropyrimido[4,5-d]pyrimidine | -456.2053 | -455.9779 | 88.466 | -456.0200 |
| perhydro-1H-indene | -352.7319 | -352.4891 | 86.351 | -352.5301 |

| | | | | |
|---|---|---|---|---|
| perhydrobenzofuran | -388.6429 | -388.4241 | 86.597 | -388.4653 |
| perhydrobenzothiophene | -711.6320 | -711.4156 | 88.733 | -711.4578 |
| perhydro-1H-indole | -368.7669 | -368.5354 | 87.283 | -368.5769 |
| perhydro-2H-isoindole | -368.7641 | -368.5325 | 86.980 | -368.5738 |
| perhydroindolizine (delta-coniceine) | -368.7673 | -368.5364 | 87.081 | -368.5777 |
| perhydrobenzimidazole | -384.8023 | -384.5820 | 85.843 | -384.6227 |
| perhydro-1H-indazole | -384.7731 | -384.5530 | 85.189 | -384.5935 |
| octahydro-1H-pyrrolo[2,3-b]pyridine | -384.8029 | -384.5824 | 85.545 | -384.6231 |
| perhydroimidazo[1,2-a]pyrazine | -400.8347 | -400.6263 | 85.770 | -400.6670 |
| octahydro-1H-purine | -416.8729 | -416.6750 | 84.696 | -416.7153 |
| perhydropentalene | -313.3872 | -313.1744 | 82.596 | -313.2136 |
| perhydropyrrolizine | -329.4259 | -329.2250 | 83.701 | -329.2648 |
| perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole | -345.4509 | -345.2606 | 82.390 | -345.2998 |
| perhydro-1,4-dihydroimidazo [4,5-d]imidazole | -377.5181 | -377.3504 | 80.870 | -377.3889 |
| perhydro-N-ethylindole | -447.4184 | -447.1284 | 100.652 | -447.1763 |
| perhydro-N-ethylindazole | -463.4291 | -463.1507 | 98.855 | -463.1977 |
| octahydro-1Methylpurine | -456.1950 | -455.9684 | 91.697 | -456.0120 |
| N-ethylperhydropurine | -495.5134 | -495.2576 | 98.861 | -495.3046 |
| perhydrofluorene | -508.8313 | -508.4917 | 100.435 | -508.5394 |
| perhydro-9-ethylfluorene | -587.4823 | -587.0837 | 116.025 | -587.1388 |
| perhydro-9H-carbazole | -524.8675 | -524.5393 | 101.296 | -524.5874 |
| perhydro-N-ethylcarbazole | -603.5123 | -603.1258 | 116.157 | -603.1810 |
| perhydro-1,8-diazacarbazole | -556.9379 | -556.6323 | 99.882 | -556.6797 |
| perhydro-N-methyl-1,8-diazacarbazole | -596.2534 | -595.9194 | 108.035 | -595.9707 |
| perhydro-N-ethyl-1,8-diazacarbazole | -635.5807 | -635.2170 | 115.498 | -635.2719 |
| perhydrodibenzoborole | -494.9567 | -494.6348 | 101.542 | -494.6830 |
| perhydro-5Me-dibenzoborole | -534.3038 | -533.9519 | 113.627 | -534.0059 |
| perhydro[b,d]dibenzofuran | -544.7451 | -544.4296 | 99.223 | -544.4768 |
| perhydrodibenzothiophene | -867.7333 | -867.4203 | 102.982 | -867.4692 |
| perhydro-3,6-diazacarbazole | -556.9314 | -556.6259 | 100.227 | -556.6735 |
| perhydro-4,5-diazacarbazole | -556.9308 | -556.6257 | 100.778 | -556.6736 |
| pyrimidine | -264.4161 | -264.3341 | 66.960 | -264.3659 |
| pyridazine | -264.3804 | -264.2991 | 67.112 | -264.3310 |
| 1,3,5-triazine | -280.4618 | -280.3916 | 64.582 | -280.4222 |
| 1H-pyrrole | -210.2490 | -210.1618 | 65.853 | -210.1930 |
| 1H-imidazole | -226.3013 | -226.2256 | 65.136 | -226.2565 |
| 1H-pyrazole | -226.2846 | -226.2088 | 65.091 | -226.2397 |
| 1H-1,2,3-triazole | -242.3125 | -242.2490 | 64.588 | -242.2797 |
| 1H-1,2,4-triazole | -242.3393 | -242.2751 | 64.475 | -242.3057 |
| naphthalene | -386.0256 | -385.8706 | 79.180 | -385.9082 |
| isoquinoline | -402.0657 | -401.9226 | 81.603 | -401.9613 |

| | | | | |
|---|---|---|---|---|
| 4H-quinolizine | -403.2205 | -403.0549 | 86.214 | -403.0959 |
| cinnoline | -418.0736 | -417.9431 | 81.339 | -417.9817 |
| phtalazine | -418.0755 | -417.9448 | 80.224 | -417.9830 |
| quinazoline | -418.1111 | -417.9798 | 81.224 | -418.0184 |
| quinoxaline | -418.1061 | -417.9751 | 79.656 | -418.0129 |
| 1,8-naphthyridine | -418.1070 | -417.9760 | 79.753 | -418.0139 |
| 1,5-naphthyridine | -418.1094 | -417.9782 | 81.003 | -418.0167 |
| pteridine | -450.1861 | -450.0791 | 80.428 | -450.1173 |
| pyrazino[2,3-b]pyrazine | -450.1816 | -450.0748 | 77.538 | -450.1116 |
| pyrimido[4,5-d]pyrimidine | -450.1912 | -450.0838 | 79.319 | -450.1215 |
| benzo[b]thiophene | -706.7969 | -706.6755 | 80.858 | -706.7139 |
| 1H-indole | -363.9472 | -363.8105 | 79.060 | -363.8481 |
| 2H-isoindole | -363.9327 | -363.7961 | 78.791 | -363.8335 |
| indolizine(delta-coniceine) | -363.9274 | -363.7913 | 78.551 | -363.8286 |
| 1H-benzo[d]imidazole | -380.0006 | -379.8755 | 78.145 | -379.9126 |
| 1H-indazole | -379.9774 | -379.8523 | 78.433 | -379.8896 |
| 1H-pyrrolo[2,3-b]pyridine | -379.9951 | -379.8701 | 78.193 | -379.9073 |
| imidazo[1,2-a]pyrazine | -396.0195 | -395.9068 | 77.410 | -395.9436 |
| 7H-purine | -412.0830 | -411.9816 | 77.246 | -412.0183 |
| 1,4-dihydropentalene | -309.7164 | -309.5769 | 76.387 | -309.6132 |
| 1H-pyrrolizine | -325.7845 | -325.6555 | 76.560 | -325.6919 |
| 1,4-dihydropyrrolo [3,2-b]pyrrole | -341.8428 | -341.7245 | 75.867 | -341.7606 |
| 1,4-dihydroimidazo[4,5-d]imidazole | -373.9459 | -373.8507 | 75.019 | -373.8863 |
| N-ethylindole | -442.6000 | -442.4042 | 93.778 | -442.4488 |
| N-ethylindazole | -458.6314 | -458.4483 | 88.763 | -458.4905 |
| N-methylpurine | -451.4074 | -451.2764 | 85.738 | -451.3172 |
| N-ethylpurine | -490.7377 | -490.5771 | 92.578 | -490.6211 |
| 9H-fluorene | -501.5917 | -501.3942 | 91.063 | -501.4374 |
| 9-Ethylfluorene | -580.2458 | -579.9890 | 106.396 | -580.0395 |
| N-ethylcarbazole | -596.3011 | -596.0557 | 106.452 | -596.1063 |
| N-methyl-1,8-diazacarbazole | -589.0683 | -588.8770 | 95.460 | -588.9224 |
| N-ethyl-1,8-diazacarbazole | -628.3989 | -628.1770 | 105.661 | -628.2272 |
| 5H-dibenzoborole | -487.7192 | -487.5366 | 91.777 | -487.5802 |
| dibenzo-5Me-borole | -527.0666 | -526.8552 | 99.286 | -526.9023 |
| dibenzo[b,d]furan | -537.5132 | -537.3396 | 89.299 | -537.3821 |
| dibenzo[b,d]thiophene | -860.4979 | -860.3267 | 92.538 | -860.3707 |
| 9H-carbazole | -517.6487 | -517.4626 | 90.815 | -517.5058 |
| 1,8-diazacarbazole | -549.7439 | -549.5811 | 89.097 | -549.6235 |
| 3,6-diazacarbazole | -549.7305 | -549.5678 | 89.680 | -549.6104 |
| 4,5-diazacarbazole | -549.7252 | -549.5630 | 89.977 | -549.6058 |

**Table S7.** The electronic energy (E), enthalpy (H), Entropy (S) and Gibbs free energy (G) of the molecules used for the analysis of correlation with Hammett constant.

| Organic compounds | E(Hartree) | H(Hartree) | S(cal/mol-Kelvin) | G(Hartree) |
|---|---|---|---|---|
| 4-aminopiperidine | -307.3692 | -307.1859 | 80.508 | -307.2242 |
| 4-chloropiperidine | -711.6345 | -711.4773 | 81.278 | -711.5160 |
| 4-dimethylaminopiperidine | -386.0028 | -385.7611 | 93.938 | -385.8057 |
| 4-fluoropiperidine | -351.2767 | -351.1186 | 78.595 | -351.1559 |
| 4-methylpiperidine | -291.3282 | -291.1341 | 80.935 | -291.1725 |
| 4-trifluoromethylpiperidine | -589.1781 | -589.0045 | 92.858 | -589.0486 |
| chlorocyclohexane | -695.6015 | -695.4330 | 81.832 | -695.4719 |
| dimethylaminocyclohexane | -369.9697 | -369.7168 | 94.515 | -369.7617 |
| fluorocyclohexane | -335.2439 | -335.0743 | 79.064 | -335.1119 |
| methylcyclohexane | -275.2947 | -275.0892 | 81.480 | -275.1279 |
| trifluoromethylcyclohexane | -573.1449 | -572.9599 | 93.332 | -573.0042 |
| aminocyclohexane | -291.3362 | -291.1416 | 81.024 | -291.1800 |
| 4-aminopyridine | -303.7576 | -303.6457 | 74.985 | -303.6814 |
| 4-chloropyridine | -708.0049 | -707.9195 | 74.428 | -707.9548 |
| 4-dimethylaminopyridine | -382.3933 | -382.2224 | 91.170 | -382.2657 |
| 4-fluoropyridine | -347.6491 | -347.5626 | 71.643 | -347.5966 |
| 4-methylpyridine | -287.7060 | -287.5831 | 80.498 | -287.6213 |
| 4-trifluoromethylpyridine | -585.5452 | -585.4441 | 83.596 | -585.4839 |
| chlorobenzene | -691.9653 | -691.8680 | 74.798 | -691.9035 |
| dimethylaminobenzene | -366.3475 | -366.1650 | 90.705 | -366.2081 |
| fluorobenzene | -331.6087 | -331.5103 | 72.016 | -331.5446 |
| methylbenzene | -271.6645 | -271.5298 | 80.456 | -271.5680 |
| trifluoromethylbenzene | -569.5078 | -569.3939 | 92.463 | -569.4378 |
| aminobenzene | -287.7129 | -287.5893 | 75.510 | -287.6252 |

**Table S8.** Calculated enthalpy and entropy of the dehydrogenation reaction $LQ*nH_2$ -> $LQ + nH_2$. The dissociation temperature is estimated as $T_d = \Delta H / \Delta S$.

| $LQ*H_2$ | LQ | number of realeased molecules | $\Delta H$ (kcal/mol $H_2$) | $\Delta S$ (cal/molK) | $T_d$ (Kelvin) |
|---|---|---|---|---|---|
| ethylbenzene | phenylacetylene | 2 | 32.748 | 27.560 | 1188.213 |
| ethylbenzene | styrene | 1 | 25.811 | 28.121 | 917.861 |
| cyclooctane | cyclooctatetraene | 4 | 25.051 | 27.993 | 894.896 |
| cyclohexane | cyclohexene | 1 | 25.431 | 31.346 | 811.313 |
| cyclohexene | cyclohexadiene | 1 | 24.051 | 29.542 | 814.139 |
| cyclopentane | cyclopentene | 1 | 24.807 | 33.907 | 731.611 |
| cyclopentane | cyclopentadiene | 2 | 23.162 | 30.402 | 761.878 |
| indane | 1H-indene | 1 | 21.364 | 28.820 | 741.277 |
| cycloheptane | cycloheptatriene | 3 | 21.187 | 29.482 | 718.623 |
| tetrahydrofuran | furan | 2 | 15.381 | 29.300 | 524.948 |

| | | | | | |
|---|---|---|---|---|---|
| tetrahydrothiophene | thiophene | 2 | 15.624 | 28.475 | 548.686 |
| 2,3-dihydrobenzofuran | benzofuran | 1 | 12.974 | 27.467 | 472.346 |
| n-propylamine | propionitrile | 2 | 13.625 | 28.836 | 472.508 |
| chlorocyclohexane | chlorobenzene | 3 | 13.638 | 28.788 | 473.743 |
| cyclohexane | benzene | 3 | 12.874 | 28.380 | 453.642 |
| cyclohexanethio | thiophenol | 3 | 12.767 | 29.586 | 431.524 |
| methylcyclohexane | toluene | 3 | 12.452 | 30.792 | 404.380 |
| cyclohexanol | phenol | 3 | 11.779 | 29.137 | 404.247 |
| trans-decalin | naphtalene | 5 | 11.651 | 29.149 | 399.711 |
| tetralin | naphtalene | 2 | 10.791 | 27.898 | 386.811 |
| tetrahydroquinoline | quinoline | 2 | 10.870 | 28.473 | 381.771 |
| piperidine | pyridine | 3 | 11.429 | 28.856 | 396.073 |
| cyclohexylamine | aniline | 3 | 10.956 | 29.305 | 373.845 |
| 2-methylpiperidine | 2-methylpyridine | 3 | 10.665 | 28.792 | 370.408 |
| 2-butanol | 2-butanone | 1 | 8.387 | 27.315 | 307.034 |
| piperazine | pyrazine | 3 | 10.480 | 28.983 | 361.603 |
| pyrrolidine | pyrrole | 2 | 10.306 | 27.006 | 381.631 |
| cyclohexane | benzene | 3 | 12.874 | 28.380 | 453.642 |
| piperidine | pyridine | 3 | 11.429 | 28.856 | 396.073 |
| hexahydropyrimidine | pyrimidine | 3 | 9.748 | 28.981 | 336.346 |
| hexahydropyridazine | pyridazine | 3 | 11.280 | 29.026 | 388.604 |
| hexahydro-1,3,5-triazine | 1,3,5-triazine | 3 | 5.650 | 29.026 | 194.652 |
| cyclopentane | cyclopentadiene | 2 | 23.162 | 30.402 | 761.878 |
| tetrahydrofuran | furan | 2 | 15.381 | 29.300 | 524.948 |
| pyrrolidine | 1H-pyrrole | 2 | 10.306 | 27.006 | 381.631 |
| tetrahydro-1H-imidazole | 1H-imidazole | 2 | 5.252 | 28.452 | 184.581 |
| pyrazolidine | 1H-pyrazole | 2 | 1.836 | 28.050 | 65.470 |
| decalin | naphthalene | 5 | 11.651 | 29.149 | 399.717 |
| perhydroquinoline | quinoline | 5 | 10.813 | 29.452 | 367.142 |
| perhydroisoquinoline | isoquinoline | 5 | 10.731 | 29.462 | 364.239 |
| perhydro-4H-quinolizine | 4H-quinolizine | 4 | 18.537 | 30.142 | 614.993 |
| perhydrocinnoline | cinnoline | 5 | 11.254 | 29.552 | 380.803 |
| perhydrophthalazine | phtalazine | 5 | 10.743 | 29.329 | 366.285 |
| perhydroquinazoline | quinazoline | 5 | 9.744 | 29.476 | 330.588 |
| perhydroquinoxaline | quinoxaline | 5 | 10.184 | 29.182 | 348.987 |
| perhydro1,8-naphthyridine | 1,8-naphthyridine | 5 | 9.993 | 29.171 | 342.551 |
| perhydro1,5-naphthyridine | 1,5-naphthyridine | 5 | 9.951 | 29.500 | 337.322 |
| perhydropteridine | pteridine | 5 | 9.339 | 29.615 | 315.349 |
| perhydropyrazino [2,3-b]pyrazine | pyrazino[2,3-b]pyrazine | 5 | 9.449 | 29.012 | 325.708 |
| perhydropyrimido [4,5-d]pyrimidine | pyrimido [4,5-d]pyrimidine | 5 | 7.655 | 29.304 | 261.247 |
| perhydro-1H-indene | 1H-indene | 4 | 13.577 | 29.421 | 461.471 |
| perhydrobenzofuran | benzofuran | 4 | 11.313 | 28.954 | 390.725 |

| | | | | | |
|---|---|---|---|---|---|
| perhydrobenzothiophene | benzo[b]thiophene | 4 | 11.548 | 29.164 | 395.979 |
| perhydro-1H-indole | 1H-indole | 4 | 9.156 | 29.077 | 314.880 |
| perhydro-2H-isoindole | 2H-isoindole | 4 | 10.972 | 29.086 | 377.220 |
| perhydroindolizine (delta-coniceine) | indolizine(delta-coniceine) | 4 | 12.328 | 29.000 | 425.104 |
| perhydrobenzimidazole | 1H-benzo[d]imidazole | 4 | 6.275 | 29.208 | 214.834 |
| perhydro-1H-indazole | 1H-indazole | 4 | 5.366 | 29.444 | 182.228 |
| octahydro-1H-pyrrolo[2,3-b]pyridine | 1H-pyrrolo[2,3-b]pyridine | 4 | 7.185 | 29.295 | 245.257 |
| perhydroimidazo[1,2-a]pyrazine | imidazo[1,2-a]pyrazine | 4 | 8.301 | 29.043 | 285.812 |
| octahydro-1H-purine | 7H-purine | 4 | 4.224 | 29.270 | 144.307 |
| perhydropentalene | 1,4-dihydropentalene | 3 | 20.414 | 29.063 | 702.386 |
| perhydropyrrolizine | 1H-pyrrolizine | 3 | 14.568 | 28.753 | 506.669 |
| perhydro-1,4-dihydropyrrolo [3,2-b]pyrrole | 1,4-dihydropyrrolo [3,2-b]pyrrole | 3 | 7.573 | 28.959 | 261.509 |
| perhydro-1H-indole | 1H-indole | 4 | 9.156 | 29.077 | 314.880 |
| perhydro-N-ethylindole | N-ethylindole | 4 | 9.051 | 29.415 | 307.690 |
| perhydro-1H-indazole | 1H-indazole | 4 | 5.366 | 29.444 | 182.228 |
| perhydro-N-ethylindazole | N-ethylindazole | 4 | 5.639 | 28.610 | 197.092 |
| octahydro-1H-purine | 7H-purine | 4 | 4.224 | 29.270 | 144.307 |
| octahydro-1Methylpurine | N-methylpurine | 4 | 4.000 | 29.643 | 134.934 |
| N-ethylperhydropurine | N-ethylpurine | 4 | 2.193 | 29.562 | 74.187 |
| perhydrofluorene | 9H-fluorene | 6 | 10.224 | 29.571 | 345.752 |
| perhydro-9-ethylfluorene | 9-ethylfluorene | 6 | 9.933 | 29.528 | 336.389 |
| perhydro-9H-carbazole | 9H-carbazole | 6 | 8.045 | 29.386 | 273.758 |
| perhydro-N-ethylcarbazole | N-ethylcarbazole | 6 | 7.355 | 29.516 | 249.178 |
| perhydro-1,8-diazacarbazole | 1,8-diazacarbazole | 6 | 5.372 | 29.336 | 183.115 |
| perhydro-N-methyl-1,8-diazacarbazole | N-methyl-1,8-diazacarbazole | 6 | 4.458 | 29.037 | 153.515 |
| perhydro-N-ethyl-1,8-diazacarbazole | N-ethyl-1,8-diazacarbazole | 6 | 4.216 | 29.493 | 142.951 |
| perhydrodibenzoborole | 5H-dibenzoborole | 6 | 10.298 | 29.505 | 349.037 |
| Perhydro-5Me-dibenzoborole | dibenzo-5Me-borole | 6 | 10.146 | 28.743 | 352.996 |
| perhydrofluorene | 9H-fluorene | 6 | 10.224 | 29.571 | 345.752 |
| perhydro[b,d] dibenzofuran | dibenzo[b,d]furan | 6 | 9.439 | 29.479 | 320.207 |
| perhydro dibenzothiophene | dibenzo[b,d]thiophene | 6 | 9.815 | 29.392 | 333.936 |
| perhydrodibenzoborole | 5H-dibenzoborole | 6 | 10.298 | 29.505 | 349.037 |
| perhydro-9H-carbazole | 9H-carbazole | 6 | 8.045 | 29.386 | 273.758 |
| perhydro-1,8-diazacarbazole | 1,8-diazacarbazole | 6 | 5.372 | 29.336 | 183.115 |
| perhydro-3,6-diazacarbazole | 3,6-diazacarbazole | 6 | 6.109 | 29.375 | 207.972 |

| | | | | | |
|---|---|---|---|---|---|
| perhydro-4,5-diazacarbazole | 4,5-diazacarbazole | 6 | 6.579 | 29.333 | 224.285 |
| 4-aminopiperidine | 4-aminopyridine | 3 | 8.434 | 29.292 | 287.940 |
| 4-chloropiperidine | 4-chloropyridine | 3 | 12.134 | 28.849 | 420.588 |
| 4-dimethyl aminopiperidine | 4-dimethyl aminopyridine | 3 | 8.122 | 30.210 | 268.856 |
| 4-fluoropiperidine | 4-fluoropyridine | 3 | 11.740 | 28.816 | 407.411 |
| 4-methylpiperidine | 4-methylpyridine | 3 | 10.693 | 30.987 | 345.065 |
| 4-trifluoro methylpiperidine | 4-trifluoro methylpyridine | 3 | 12.653 | 28.045 | 451.149 |
| chlorocyclohexane | chlorobenzene | 3 | 13.638 | 28.788 | 473.743 |
| dimethyl aminocyclohexane | Dimethyl aminobenzene | 3 | 10.871 | 29.863 | 364.019 |
| fluorocyclohexane | fluorobenzene | 3 | 13.407 | 28.783 | 465.801 |
| methylcyclohexane | methylbenzene | 3 | 12.451 | 30.791 | 404.382 |
| trifluoro methylcyclohexane | trifluoro methylbenzene | 3 | 13.833 | 30.843 | 448.508 |
| aminocyclohexane | aminobenzene | 3 | 10.955 | 29.295 | 373.958 |

**Table S9** : Minimum energy geometries of the investigated organic molecules obtained at the DFT/UB3LYP/cc-pVTZ level of theory using Gaussian 09.

**ethylbenzene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 0.2517881447 | -0.2964369076 | 2.1379612813 |
| C | -0.2731748854 | -0.1835491438 | 1.1970273033 |
| C | -1.6349931385 | 0.0921227386 | -1.2001953284 |
| C | 0.4298423456 | -0.3238711013 | 0.0000000000 |
| C | -1.6349931385 | 0.0921227386 | 1.2001953284 |
| C | -2.3213077396 | 0.2321523043 | 0.0000000000 |
| C | -0.2731748854 | -0.1835491438 | -1.1970273033 |
| H | -2.1611421810 | 0.1931553725 | 2.1403873224 |
| H | -3.3821679504 | 0.4434031807 | 0.0000000000 |
| H | 0.2517881447 | -0.2964369076 | -2.1379612813 |
| H | -2.1611421810 | 0.1931553725 | -2.1403873224 |
| C | 1.9168420734 | -0.5850722901 | 0.0000000000 |
| H | 2.1793185785 | -1.1832580765 | -0.8753922980 |
| H | 2.1793185785 | -1.1832580765 | 0.8753922980 |
| C | 2.7532942078 | 0.7016973358 | 0.0000000000 |
| H | 2.5372029332 | 1.3083654008 | -0.8804392500 |
| H | 3.8203241608 | 0.4729378027 | 0.0000000000 |
| H | 2.5372029332 | 1.3083654008 | 0.8804392500 |

**cyclooctane**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | -1.7240319605 | 0.7141101673 | -0.2817976852 |
| H | -1.6270720850 | 0.6739520474 | -1.3722722916 |
| H | -2.7188518682 | 1.1263002751 | -0.0926845111 |
| C | -0.7140274627 | 1.7237498069 | 0.2820222276 |
| H | -0.6735762527 | 1.6264098356 | 1.3724545242 |
| H | -1.1261037450 | 2.7187047399 | 0.0933947276 |
| C | 0.7140274627 | 1.7237498069 | -0.2820222276 |
| H | 0.6735762527 | 1.6264098356 | -1.3724545242 |

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.1261037450 | 2.7187047399 | -0.0933947276 |
| C | 1.7240319605 | 0.7141101673 | 0.2817976852 |
| H | 1.6270720850 | 0.6739520474 | 1.3722722916 |
| H | 2.7188518682 | 1.1263002751 | 0.0926845111 |
| C | 1.7240319605 | -0.7141101673 | -0.2817976852 |
| H | 1.6270720850 | -0.6739520474 | -1.3722722916 |
| H | 2.7188518682 | -1.1263002751 | -0.0926845111 |
| C | 0.7140274627 | -1.7237498069 | 0.2820222276 |
| H | 0.6735762527 | -1.6264098356 | 1.3724545242 |
| H | 1.1261037450 | -2.7187047399 | 0.0933947276 |
| C | -0.7140274627 | -1.7237498069 | -0.2820222276 |
| H | -0.6735762527 | -1.6264098356 | -1.3724545242 |
| H | -1.1261037450 | -2.7187047399 | -0.0933947276 |
| C | -1.7240319605 | -0.7141101673 | 0.2817976852 |
| H | -2.7188518682 | -1.1263002751 | 0.0926845111 |
| H | -1.6270720850 | -0.6739520474 | 1.3722722916 |

**cyclohexane**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.4886263291 | 0.0001925385 | -0.1501101969 |
| C | 1.4634555345 | -0.0001452610 | 0.2273043307 |
| C | -0.7316019676 | 1.2674623007 | 0.2273043307 |
| C | -0.7318535669 | -1.2673170397 | 0.2273043307 |
| C | -1.4634555345 | 0.0001452610 | -0.2273043307 |
| C | 0.7316019676 | -1.2674623007 | -0.2273043307 |
| C | 0.7318535669 | 1.2673170397 | -0.2273043307 |
| H | -0.7676302445 | 1.3299228070 | 1.3203219753 |
| H | -0.7679318137 | -1.3297486960 | 1.3203219753 |
| H | -1.5355620582 | 0.0001741110 | -1.3203219753 |
| H | 0.7676302445 | -1.3299228070 | -1.3203219753 |
| H | 0.7679318137 | 1.3297486960 | -1.3203219753 |
| H | 1.5355620582 | -0.0001741110 | 1.3203219753 |
| H | -1.2444799078 | 2.1551173523 | -0.1501101969 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2441464214 | -2.1553098908 | -0.1501101969 |
| H | -2.4886263291 | -0.0001925385 | 0.1501101969 |
| H | 1.2444799078 | -2.1551173523 | 0.1501101969 |
| H | 1.2441464214 | 2.1553098908 | 0.1501101969 |

**cyclohexene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.3732234956 | 0.5362080273 | 0.1679747349 |
| C | -1.4937295544 | -0.1031934276 | 0.0504195185 |
| C | 0.6957285927 | -0.3186695774 | -1.1881512322 |
| C | 0.6628464287 | 0.0536369824 | 1.3041731717 |
| C | 1.4937295544 | 0.1031934276 | 0.0504195185 |
| C | -0.6628464287 | -0.0536369824 | 1.3041731717 |
| C | -0.6957285927 | 0.3186695774 | -1.1881512322 |
| H | 0.5892918680 | -1.4076120773 | -1.1920824261 |
| H | 1.8880802310 | 1.1178568245 | -0.0837195085 |
| H | -1.1926309648 | -0.1065072781 | 2.2492055867 |
| H | -0.5892918680 | 1.4076120773 | -1.1920824261 |
| H | -1.8880802310 | -1.1178568245 | -0.0837195085 |
| H | 1.2405246591 | -0.0534865033 | -2.0962558449 |
| H | 1.1926309648 | 0.1065072781 | 2.2492055867 |
| H | 2.3732234956 | -0.5362080273 | 0.1679747349 |
| H | -1.2405246591 | 0.0534865033 | -2.0962558449 |

**cyclopentane**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.1866956584 | -1.3275244843 | -1.8297946401 |
| C | 0.2444556836 | -0.7259256781 | -1.0289735658 |
| C | -0.2444556836 | 0.7259256781 | -1.0289735658 |
| C | 0.1384382327 | 1.2322251124 | 0.3712623373 |
| C | 0.0000000000 | 0.0000000000 | 1.3044595533 |
| C | -0.1384382327 | -1.2322251124 | 0.3712623373 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.3307411936 | -0.7475663053 | -1.1538431224 |
| H | -1.3307411936 | 0.7475663053 | -1.1538431224 |
| H | 0.1866956584 | 1.3275244843 | -1.8297946401 |
| H | 1.1734591176 | 1.5799725131 | 0.3621226347 |
| H | -0.4750102386 | 2.0727519539 | 0.6955630206 |
| H | -0.8689507626 | 0.0917842415 | 1.9561890590 |
| H | 0.8689507626 | -0.0917842415 | 1.9561890590 |
| H | -1.1734591176 | -1.5799725131 | 0.3621226347 |
| H | 0.4750102386 | -2.0727519539 | 0.6955630206 |

**indane**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0558451038 | -0.0063366532 | 2.4834747342 |
| C | -1.0507729386 | -0.0094133550 | 1.4004105961 |
| C | -1.0507729386 | -0.0094133550 | -1.4004105961 |
| C | 0.1460079950 | -0.0492258596 | 0.6981837102 |
| C | -2.2514729510 | 0.0347257042 | 0.6959961540 |
| C | -2.2514729510 | 0.0347257042 | -0.6959961540 |
| C | 0.1460079950 | -0.0492258596 | -0.6981837102 |
| H | -3.1898531879 | 0.0746290766 | 1.2333744184 |
| H | -3.1898531879 | 0.0746290766 | -1.2333744184 |
| H | -1.0558451038 | -0.0063366532 | -2.4834747342 |
| C | 1.5593681430 | -0.1184479173 | 1.2273576998 |
| H | 1.7895178091 | -1.1378022423 | 1.5551019282 |
| H | 1.7290883148 | 0.5335495743 | 2.0850855431 |
| C | 2.4144469968 | 0.2717697318 | 0.0000000000 |
| H | 3.3960527416 | -0.2004572242 | 0.0000000000 |
| H | 2.5713450993 | 1.3519348269 | 0.0000000000 |
| C | 1.5593681430 | -0.1184479173 | -1.2273576998 |
| H | 1.7895178091 | -1.1378022423 | -1.5551019282 |
| H | 1.7290883148 | 0.5335495743 | -2.0850855431 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**cycloheptane**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | -0.3966952997 | 1.2514098729 | 0.9698880680 |
| H | -1.4547287465 | 1.1900976375 | 0.6990360712 |
| H | -0.3164462257 | 2.1132555284 | 1.6366697249 |
| C | 0.4018812806 | 1.5250623647 | -0.3134184751 |
| H | 1.4647518325 | 1.3154125268 | -0.1545855473 |
| H | 0.3387966868 | 2.5926873890 | -0.5382263874 |
| C | -0.1136734595 | 0.7572411823 | -1.5382913572 |
| H | -1.1861864694 | 0.9574179056 | -1.6358738585 |
| H | 0.3510574689 | 1.1701865240 | -2.4379986473 |
| C | 0.1136734595 | -0.7572411823 | -1.5382913572 |
| H | 1.1861864694 | -0.9574179056 | -1.6358738585 |
| H | -0.3510574689 | -1.1701865240 | -2.4379986473 |
| C | -0.4018812806 | -1.5250623647 | -0.3134184751 |
| H | -0.3387966868 | -2.5926873890 | -0.5382263874 |
| H | -1.4647518325 | -1.3154125268 | -0.1545855473 |
| C | 0.3966952997 | -1.2514098729 | 0.9698880680 |
| H | 1.4547287465 | -1.1900976375 | 0.6990360712 |
| H | 0.3164462257 | -2.1132555284 | 1.6366697249 |
| C | 0.0000000000 | 0.0000000000 | 1.7732710491 |
| H | 0.8340970965 | 0.2506961624 | 2.4343048840 |
| H | -0.8340970965 | -0.2506961624 | 2.4343048840 |

**tetrahydrofuran**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| O | -0.0009684610 | -1.1942165994 | -0.2248456032 |
| C | -1.1258693343 | -0.4416608528 | 0.2108455906 |
| C | -0.7825007661 | 1.0163352788 | -0.1150544170 |
| C | 0.7627778677 | 1.0462046066 | -0.0118592644 |
| C | 1.1466311038 | -0.4405434765 | 0.1536385237 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2771662165 | -0.5755225958 | 1.2910504036 |
| H | -2.0040421673 | -0.8182778855 | -0.3106689664 |
| H | -1.1035853710 | 1.2603336397 | -1.1269512131 |
| H | -1.2649892701 | 1.7168766419 | 0.5653861640 |
| H | 1.1059437462 | 1.6378118828 | 0.8359491181 |
| H | 1.2067096977 | 1.4730814174 | -0.9095506647 |
| H | 1.4094386504 | -0.6590057215 | 1.1965718502 |
| H | 1.9732945207 | -0.7539593358 | -0.4814945213 |

**tetrahydrothiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.1178641750 | 1.2973261063 | -2.1146077329 |
| C | 0.2679586740 | 0.7164497694 | -1.2747261252 |
| C | -0.1398815463 | 1.3420792171 | 0.0584088508 |
| S | 0.0000000000 | 0.0000000000 | 1.3220527180 |
| C | 0.1398815463 | -1.3420792171 | 0.0584088508 |
| C | -0.2679586740 | -0.7164497694 | -1.2747261252 |
| H | 1.3570064016 | 0.7014731003 | -1.3557501153 |
| H | -1.1694058817 | 1.6965704867 | 0.0332522692 |
| H | 0.5059660533 | 2.1671954508 | 0.3499544944 |
| H | -0.5059660533 | -2.1671954508 | 0.3499544944 |
| H | 1.1694058817 | -1.6965704867 | 0.0332522692 |
| H | -1.3570064016 | -0.7014731003 | -1.3557501153 |
| H | 0.1178641750 | -1.2973261063 | -2.1146077329 |

**2,3-dihydrobenzofuran**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0250996870 | -2.5004169255 | 0.0133347235 |
| C | -1.0166099391 | -1.4177698140 | 0.0095539178 |
| C | -1.0093019289 | 1.4002114729 | -0.0109365900 |
| C | 0.1782243274 | -0.7209265546 | -0.0155283493 |
| C | -2.2169888688 | -0.7051317839 | 0.0286622791 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.2065546202 | 0.6863844319 | 0.0151990209 |
| C | 0.1677453312 | 0.6707380252 | -0.0237905518 |
| H | -3.1584288190 | -1.2363138272 | 0.0536741621 |
| H | -3.1431286112 | 1.2279261440 | 0.0300006146 |
| H | -0.9911373109 | 2.4806594896 | -0.0176937613 |
| C | 1.6150671394 | -1.1765545811 | -0.0926734284 |
| H | 1.8431693115 | -1.5909194319 | -1.0779517712 |
| H | 1.8714766860 | -1.9329412147 | 0.6487599650 |
| C | 2.3682770927 | 0.1469652036 | 0.1559159781 |
| H | 3.2055365039 | 0.3109347047 | -0.5182801538 |
| H | 2.7227179083 | 0.2181954081 | 1.1865441904 |
| O | 1.4157874847 | 1.2198572529 | -0.0597842457 |

**n-propylamine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.0495192685 | -0.6794062047 | 0.9727495776 |
| C | -1.9237203709 | -0.1434408600 | 0.0296010865 |
| H | -2.0702557640 | -0.8619726934 | -0.7796003118 |
| H | -2.7220983727 | 0.5963188997 | -0.0382241163 |
| C | -0.5486505000 | 0.5150266616 | -0.0587013700 |
| H | -0.4461587186 | 1.2558367216 | 0.7413083438 |
| H | -0.4482877573 | 1.0628756739 | -0.9980316961 |
| C | 0.5989412274 | -0.4840738259 | 0.0422458095 |
| H | 0.5178108413 | -1.2060222105 | -0.7747847166 |
| H | 0.4937140573 | -1.0563482917 | 0.9763536397 |
| N | 1.8934823120 | 0.1916358536 | -0.0889950552 |
| H | 2.0469119426 | 0.8096663727 | 0.6999488366 |
| H | 2.6494793714 | -0.4822760972 | -0.0759190277 |

**cyclohexanethiol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.6126501855 | -0.0136967204 | 0.3695118388 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.5655470100 | 1.2603990937 | 0.2132176816 |
| C | -1.5756112936 | -1.2674524401 | 0.1834156792 |
| C | -2.2698434372 | 0.0051803489 | -0.3089130721 |
| C | -0.0815781043 | -1.2661398062 | -0.1677956423 |
| C | -0.0714159541 | 1.2606066082 | -0.1335496102 |
| H | -1.6831425721 | 1.3152599424 | 1.3003077094 |
| H | -1.6934416949 | -1.3469490115 | 1.2691509788 |
| H | -2.2650573747 | 0.0178216351 | -1.4037247674 |
| H | 0.0444603352 | -1.2991195831 | -1.2534511930 |
| H | 0.0510529944 | 1.3245007984 | -1.2193996524 |
| H | 0.5781376020 | -0.0202535053 | 1.4606634440 |
| H | -2.0355538449 | 2.1578824712 | -0.1941517197 |
| H | -2.0524898849 | -2.1517507987 | -0.2444924487 |
| H | -3.3181898033 | 0.0065978648 | -0.0031129256 |
| H | 0.4004763858 | -2.1612807933 | 0.2307396055 |
| H | 0.4164324168 | 2.1392426787 | 0.2919496230 |
| S | 2.3965205015 | 0.0747616826 | -0.1071860353 |
| H | 2.7788225528 | -1.0787724656 | 0.4714455064 |

**cyclohexanol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.0322435902 | 0.0366751246 | 0.3237494067 |
| C | -1.1901314609 | 1.2333627163 | 0.2122224972 |
| C | -1.1180240426 | -1.2961848452 | 0.2071380148 |
| C | -1.8659991049 | -0.0507589776 | -0.2786230951 |
| C | 0.3646674144 | -1.2428577496 | -0.1798875901 |
| C | 0.2934156607 | 1.2734451324 | -0.1700739767 |
| H | -1.2868955182 | 1.2968168407 | 1.3011067372 |
| H | -1.2069041878 | -1.3678768458 | 1.2961585895 |
| H | -1.8899903698 | -0.0496931019 | -1.3731614623 |
| H | 0.4693845141 | -1.2739753277 | -1.2684291443 |
| H | 0.3989967975 | 1.3184971825 | -1.2580701362 |
| H | 1.0104094900 | 0.0340500984 | 1.4232774975 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.7005139034 | 2.1093034685 | -0.1927870223 |
| H | -1.5773046960 | -2.1995774213 | -0.1990791398 |
| H | -2.9054293099 | -0.0818768094 | 0.0551259423 |
| H | 0.8920449163 | -2.1164108008 | 0.2159343220 |
| H | 0.7763853772 | 2.1654507884 | 0.2322428693 |
| O | 2.3857235081 | 0.1458270871 | -0.1230110994 |
| H | 2.8707823252 | -0.6279125597 | 0.1797507898 |

**N-methylpyrrolidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 0.7131508942 | 0.3411011254 | 0.0000000000 |
| C | -0.0218817271 | -0.1593387705 | -1.1559742785 |
| C | -1.4939232323 | 0.0563645097 | -0.7766565937 |
| C | -1.4939232323 | 0.0563645097 | 0.7766565937 |
| C | -0.0218817271 | -0.1593387705 | 1.1559742785 |
| H | 0.1774819607 | -1.2341489491 | -1.3209977525 |
| H | 0.2745892229 | 0.3712127649 | -2.0619887434 |
| H | -1.8511515421 | 1.0116748906 | -1.1584445174 |
| H | -2.1327514131 | -0.7209773327 | -1.1936415317 |
| H | -2.1327514131 | -0.7209773327 | 1.1936415317 |
| H | -1.8511515421 | 1.0116748906 | 1.1584445174 |
| H | 0.1774819607 | -1.2341489491 | 1.3209977525 |
| H | 0.2745892229 | 0.3712127649 | 2.0619887434 |
| C | 2.1239070300 | 0.0224596665 | 0.0000000000 |
| H | 2.6034510754 | 0.4492951897 | -0.8818529828 |
| H | 2.3156833854 | -1.0654493973 | 0.0000000000 |
| H | 2.6034510754 | 0.4492951897 | 0.8818529828 |

**trans-Decalin**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.2568879574 | -0.7265983644 | 0.0000000000 |
| C | 0.2509200852 | -0.7234202294 | -2.5436044753 |

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.2568879574 | 0.7265983644 | 0.0000000000 |
| C | -0.1747642462 | -1.4638216716 | -1.2729443040 |
| H | 1.3440399454 | -0.7248249008 | -2.6112005580 |
| H | -1.3551015132 | 0.6798726483 | 0.0000000000 |
| H | -1.2650813557 | -1.5753296086 | -1.2666141339 |
| H | 1.3551015132 | -0.6798726483 | 0.0000000000 |
| H | -0.1138532310 | -1.2507041545 | -3.4281248859 |
| H | 0.2374405883 | -2.4766021242 | -1.2702349602 |
| C | -0.1747642462 | -1.4638216716 | 1.2729443040 |
| H | 0.2374405883 | -2.4766021242 | 1.2702349602 |
| H | -1.2650813557 | -1.5753296086 | 1.2666141339 |
| C | 0.2509200852 | -0.7234202294 | 2.5436044753 |
| H | 1.3440399454 | -0.7248249008 | 2.6112005580 |
| H | -0.1138532310 | -1.2507041545 | 3.4281248859 |
| C | -0.2509200852 | 0.7234202294 | 2.5436044753 |
| H | 0.1138532310 | 1.2507041545 | 3.4281248859 |
| H | -1.3440399454 | 0.7248249008 | 2.6112005580 |
| C | 0.1747642462 | 1.4638216716 | 1.2729443040 |
| H | 1.2650813557 | 1.5753296086 | 1.2666141339 |
| H | -0.2374405883 | 2.4766021242 | 1.2702349602 |
| C | 0.1747642462 | 1.4638216716 | -1.2729443040 |
| H | -0.2374405883 | 2.4766021242 | -1.2702349602 |
| H | 1.2650813557 | 1.5753296086 | -1.2666141339 |
| C | -0.2509200852 | 0.7234202294 | -2.5436044753 |
| H | -1.3440399454 | 0.7248249008 | -2.6112005580 |
| H | 0.1138532310 | 1.2507041545 | -3.4281248859 |

**tetralin**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0745347705 | -2.4604550481 | -1.3588140495 |
| C | 0.0424667491 | -1.3770916121 | -1.3606382808 |
| C | -0.0424667491 | 1.3770916121 | -1.3606382808 |
| C | 0.0230581948 | -0.6999103901 | -0.1386251793 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0206321149 | -0.6952855265 | -2.5672462836 |
| C | -0.0206321149 | 0.6952855265 | -2.5672462836 |
| C | -0.0230581948 | 0.6999103901 | -0.1386251793 |
| H | 0.0352078573 | -1.2423811689 | -3.5006430610 |
| H | -0.0352078573 | 1.2423811689 | -3.5006430610 |
| H | -0.0745347705 | 2.4604550481 | -1.3588140495 |
| C | 0.0814330694 | -1.4903335976 | 1.1531780229 |
| H | 1.1080336394 | -1.8450635245 | 1.2992402671 |
| H | -0.5328786434 | -2.3882799436 | 1.0568655764 |
| C | -0.3419333747 | -0.6831252717 | 2.3806044810 |
| H | -0.1022509380 | -1.2374048500 | 3.2899996881 |
| H | -1.4274143119 | -0.5430525161 | 2.3749008188 |
| C | 0.3419333747 | 0.6831252717 | 2.3806044810 |
| H | 1.4274143119 | 0.5430525161 | 2.3749008188 |
| H | 0.1022509380 | 1.2374048500 | 3.2899996881 |
| C | -0.0814330694 | 1.4903335976 | 1.1531780229 |
| H | 0.5328786434 | 2.3882799436 | 1.0568655764 |
| H | -1.1080336394 | 1.8450635245 | 1.2992402671 |

**tetrahydroquinoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.3430252239 | -1.3750787854 | -0.0470570175 |
| C | -2.5512005475 | 0.7058448844 | 0.0028744186 |
| C | -0.1190919449 | 0.7141952032 | 0.0414566398 |
| C | -1.3395402493 | 1.3834915571 | 0.0391088986 |
| C | -0.1195458830 | -0.6921567891 | -0.0092959783 |
| C | -2.5433168092 | -0.6847592703 | -0.0385427412 |
| H | -3.4842816688 | 1.2519448415 | 0.0043258029 |
| H | -1.3342684936 | 2.4671171595 | 0.0697124512 |
| H | -1.3404146122 | -2.4579903242 | -0.0915417331 |
| N | 1.0754159765 | -1.4023524260 | -0.0723540221 |
| C | 1.1886536882 | 1.4748267174 | 0.1113455046 |
| C | 2.3765418034 | 0.6281368409 | -0.3518218779 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 2.3211636935 | -0.7507010256 | 0.2968056735 |
| H | 2.4235419150 | -0.6437325954 | 1.3870546546 |
| H | 3.1486917332 | -1.3721072035 | -0.0480198816 |
| H | -3.4748153334 | -1.2349077648 | -0.0671903201 |
| H | 1.3633505307 | 1.8033202548 | 1.1415376984 |
| H | 1.1182673196 | 2.3853143575 | -0.4872716418 |
| H | 2.3490823164 | 0.5056342096 | -1.4367874135 |
| H | 3.3177878637 | 1.1194433856 | -0.1012435557 |
| H | 1.0012959257 | -2.3714212273 | 0.1894104406 |

**piperidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.2307253240 | -1.4547154664 | 0.0000000000 |
| C | 0.2031434253 | 0.7512463561 | -1.2149516240 |
| C | 0.2031434253 | 0.7512463561 | 1.2149516240 |
| N | -0.3149977258 | 1.3769847122 | 0.0000000000 |
| C | -0.2236955750 | -0.7150337827 | 1.2627248712 |
| C | -0.2236955750 | -0.7150337827 | -1.2627248712 |
| H | 1.3049158737 | 0.8022064849 | -1.2731078093 |
| H | 1.3049158737 | 0.8022064849 | 1.2731078093 |
| H | -1.3128602342 | -0.7588796704 | 1.3425218145 |
| H | -1.3128602342 | -0.7588796704 | -1.3425218145 |
| H | 1.3236210251 | -1.5259361224 | 0.0000000000 |
| H | -0.1911640571 | 1.2898930798 | -2.0781491588 |
| H | -0.1911640571 | 1.2898930798 | 2.0781491588 |
| H | 0.1884073492 | -1.1914698627 | 2.1550302198 |
| H | 0.1884073492 | -1.1914698627 | -2.1550302198 |
| H | -0.1099463841 | 2.3673897017 | 0.0000000000 |
| H | -0.1475678029 | -2.4789650350 | 0.0000000000 |

**cyclohexylamine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.8111326387 | -0.2098025732 | -2.1475837704 |
| C | 0.3102684130 | 0.1834088365 | -1.2577860553 |
| C | -1.8849829971 | 0.2702629104 | 0.0000000000 |
| C | 0.3102684130 | 0.1834088365 | 1.2577860553 |
| C | -1.1693697906 | -0.2124146056 | 1.2655616019 |
| C | 1.0274340213 | -0.3123825421 | 0.0000000000 |
| C | -1.1693697906 | -0.2124146056 | -1.2655616019 |
| H | -1.9145966614 | 1.3647802746 | 0.0000000000 |
| H | 0.4080824746 | 1.2722616734 | 1.2984742846 |
| H | -1.2544065176 | -1.3019987805 | 1.3344120432 |
| H | 0.9727666330 | -1.4134883094 | 0.0000000000 |
| H | -1.2544065176 | -1.3019987805 | -1.3344120432 |
| H | 0.4080824746 | 1.2722616734 | -1.2984742846 |
| H | -2.9232986390 | -0.0688767234 | 0.0000000000 |
| H | 0.8111326387 | -0.2098025732 | 2.1475837704 |
| H | -1.6581485159 | 0.1910479616 | 2.1549586092 |
| H | -1.6581485159 | 0.1910479616 | -2.1549586092 |
| N | 2.4121618842 | 0.1722180995 | 0.0000000000 |
| H | 2.9080716774 | -0.1767763671 | 0.8126628644 |
| H | 2.9080716774 | -0.1767763671 | -0.8126628644 |

**2-methylpiperidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.2372048972 | -1.2271123941 | 0.2133182893 |
| C | 1.0807154320 | 1.2803631584 | 0.1787592712 |
| C | -0.9865641619 | -0.0171751819 | 0.3205411592 |
| N | -0.3117384445 | 1.1532142438 | -0.2456023737 |
| C | -0.2515869737 | -1.2778430213 | -0.1440216293 |
| C | 1.8785438533 | 0.0674079458 | -0.2937616175 |
| H | 1.1766689398 | 1.3635068124 | 1.2757011749 |
| H | -0.9422943128 | 0.0016144277 | 1.4253383770 |
| H | -0.3676278749 | -1.3625111541 | -1.2285834976 |
| H | 1.8978668271 | 0.0649539040 | -1.3866276324 |

Continued on Next Page...

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.3483003841 | -1.2808032795 | 1.3015041988 |
| H | 1.4903715508 | 2.1961636573 | -0.2506130930 |
| H | -0.7203109660 | -2.1577849111 | 0.3029334515 |
| H | 2.9117892373 | 0.1456587683 | 0.0515318967 |
| H | -0.8268872467 | 1.9934170807 | -0.0141306467 |
| H | 1.7554747948 | -2.0972455606 | -0.1948654057 |
| C | -2.4509690250 | -0.0168604735 | -0.0981341035 |
| H | -2.9730924578 | -0.8822048329 | 0.3123556463 |
| H | -2.5350379341 | -0.0423683685 | -1.1855107951 |
| H | -2.9632255190 | 0.8794891790 | 0.2593713294 |

**isopropanol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8882230642 | -1.9377437164 | 0.3055820827 |
| C | -1.0698471014 | -0.9398201020 | -0.0975740805 |
| H | -1.0810538773 | -1.0016290565 | -1.1867292024 |
| H | -2.0608425571 | -0.6239971434 | 0.2366994174 |
| C | 0.0015436654 | 0.0409487739 | 0.3653059598 |
| H | -0.0094046286 | 0.0849306902 | 1.4623720683 |
| C | 1.3947598878 | -0.3554564241 | -0.0915181256 |
| H | 1.4343859548 | -0.4041004015 | -1.1807191974 |
| H | 1.6710926640 | -1.3307458134 | 0.3105377373 |
| H | 2.1268754848 | 0.3781466352 | 0.2442486465 |
| O | -0.2372931499 | 1.3525025725 | -0.1596455705 |
| H | -1.1192392783 | 1.6314049855 | 0.1039012644 |

**2-butanol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.7482603131 | -1.7270975915 | 0.4464255883 |
| C | -1.7655623487 | -0.7271715555 | 0.0090625292 |
| H | -1.9038016125 | -0.8208933921 | -1.0690927963 |
| H | -2.6318574739 | -0.2020997548 | 0.4182161032 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.4764124566 | 0.0267185951 | 0.3151129181 |
| H | -0.3558286122 | 0.0993958097 | 1.4051821292 |
| C | 0.7546003682 | -0.6636011798 | -0.2606740777 |
| H | 0.6469125567 | -0.6912647157 | -1.3486013893 |
| H | 0.7568031808 | -1.7011126421 | 0.0833046427 |
| C | 2.0698712438 | 0.0143112455 | 0.1167830583 |
| H | 2.9195666258 | -0.5024206552 | -0.3312286705 |
| H | 2.2156888463 | 0.0145098733 | 1.1993920234 |
| H | 2.0824662196 | 1.0489952085 | -0.2222828780 |
| O | -0.5102335099 | 1.3460029762 | -0.2433101630 |
| H | -1.2573867142 | 1.8197287783 | 0.1331089823 |

**piperazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.7360312745 | -0.1968461037 | 1.2105015678 |
| C | -0.7360312745 | -0.1968461037 | -1.2105015678 |
| N | -1.3688348986 | 0.3251796456 | 0.0000000000 |
| C | 0.7360312745 | 0.1968461037 | -1.2105015678 |
| C | 0.7360312745 | 0.1968461037 | 1.2105015678 |
| H | -0.8014820421 | -1.2938403583 | 1.2828866620 |
| H | -0.8014820421 | -1.2938403583 | -1.2828866620 |
| H | 0.8014820421 | 1.2938403583 | -1.2828866620 |
| H | 0.8014820421 | 1.2938403583 | 1.2828866620 |
| H | -1.2343555841 | 0.2315090685 | 2.0815346274 |
| H | -1.2343555841 | 0.2315090685 | -2.0815346274 |
| H | 1.2343555841 | -0.2315090685 | -2.0815346274 |
| H | 1.2343555841 | -0.2315090685 | 2.0815346274 |
| H | -2.3581897834 | 0.1156066265 | 0.0000000000 |
| N | 1.3688348986 | -0.3251796456 | 0.0000000000 |
| H | 2.3581897834 | -0.1156066265 | 0.0000000000 |

**pyrrolidine**

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
| H | 0.6883486848 | 1.6976095340 | -1.1905816149 |
| C | -0.0686484200 | 1.0321224726 | -0.7756494401 |
| C | 0.1903525579 | -0.4464394852 | -1.1587106802 |
| N | -0.1902869122 | -1.2632348799 | 0.0000000000 |
| C | 0.1903525579 | -0.4464394852 | 1.1587106802 |
| C | -0.0686484200 | 1.0321224726 | 0.7756494401 |
| H | -1.0329765853 | 1.3646663178 | -1.1610538588 |
| H | 1.2550831528 | -0.6022312414 | -1.3523327239 |
| H | -0.3520369333 | -0.7648634794 | -2.0479875607 |
| H | 1.2550831528 | -0.6022312414 | 1.3523327239 |
| H | -0.3520369333 | -0.7648634794 | 2.0479875607 |
| H | 0.6883486848 | 1.6976095340 | 1.1905816149 |
| H | -1.0329765853 | 1.3646663178 | 1.1610538588 |
| H | -1.1968050010 | -1.3876403574 | 0.0000000000 |

**1,4-cyclohexadiene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.1989887646 | -2.1937305513 | 0.0000000000 |
| C | 0.6637668338 | -1.2509265536 | 0.0000000000 |
| C | 0.6637668338 | 1.2509265536 | 0.0000000000 |
| C | -1.4937173443 | 0.0000000000 | 0.0000000000 |
| C | -0.6637668338 | 1.2509265536 | 0.0000000000 |
| C | -0.6637668338 | -1.2509265536 | 0.0000000000 |
| C | 1.4937173443 | 0.0000000000 | 0.0000000000 |
| H | -2.1670178280 | 0.0000000000 | 0.8671295391 |
| H | -1.1989887646 | 2.1937305513 | 0.0000000000 |
| H | -1.1989887646 | -2.1937305513 | 0.0000000000 |
| H | 2.1670178280 | 0.0000000000 | -0.8671295391 |
| H | 1.1989887646 | 2.1937305513 | 0.0000000000 |
| H | -2.1670178280 | 0.0000000000 | -0.8671295391 |
| H | 2.1670178280 | 0.0000000000 | 0.8671295391 |

Continued on Next Page. . .

**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**1,3-cyclohexadiene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 0.1411388927 | 2.4982727723 | 0.1218285664 |
| C | 0.0391099210 | 1.4202129181 | 0.1186695850 |
| C | -0.0940240577 | -0.7253381423 | 1.2590092830 |
| C | 0.2537220015 | -0.7240973772 | -1.1853873415 |
| C | -0.0391099210 | -1.4202129181 | 0.1186695850 |
| C | -0.2537220015 | 0.7240973772 | -1.1853873415 |
| C | 0.0940240577 | 0.7253381423 | 1.2590092830 |
| H | 1.3408783371 | -0.7336635943 | -1.3458447718 |
| H | -0.1411388927 | -2.4982727723 | 0.1218285664 |
| H | -1.3408783371 | 0.7336635943 | -1.3458447718 |
| H | 0.2570177693 | 1.2276904327 | 2.2041817733 |
| H | -0.2570177693 | -1.2276904327 | 2.2041817733 |
| H | -0.1786760180 | -1.2728281368 | -2.0233950945 |
| H | 0.1786760180 | 1.2728281368 | -2.0233950945 |

**phenylacetylene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -2.1405488515 | 0.0000000000 | 0.4241814977 |
| C | -1.2072602094 | 0.0000000000 | -0.1208836474 |
| C | 1.2029059614 | 0.0000000000 | -1.5073517745 |
| C | 0.0000000000 | 0.0000000000 | 0.5903530696 |
| C | -1.2029059614 | 0.0000000000 | -1.5073517745 |
| C | 0.0000000000 | 0.0000000000 | -2.2048507426 |
| C | 1.2072602094 | 0.0000000000 | -0.1208836474 |
| H | -2.1412475628 | 0.0000000000 | -2.0453594751 |
| H | 0.0000000000 | 0.0000000000 | -3.2863903239 |
| H | 2.1405488515 | 0.0000000000 | 0.4241814977 |
| H | 2.1412475628 | 0.0000000000 | -2.0453594751 |
| C | 0.0000000000 | 0.0000000000 | 2.0160300472 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | 4.2787393243 |
| C | 0.0000000000 | 0.0000000000 | 3.2177754335 |

**styrene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.0087190604 | -2.2938267147 | 0.0760561603 |
| C | -0.3919172165 | -1.2815962439 | 0.0375772941 |
| C | -1.3782658031 | 1.3034466323 | -0.0606692440 |
| C | 0.5118368645 | -0.2139879969 | -0.0052043009 |
| C | -1.7640158774 | -1.0655961769 | 0.0315448555 |
| C | -2.2636553682 | 0.2290558952 | -0.0176564852 |
| C | -0.0100557683 | 1.0857497767 | -0.0545603572 |
| H | -2.4413571594 | -1.9086711207 | 0.0652706211 |
| H | -3.3313216274 | 0.4026898211 | -0.0225708631 |
| H | 0.6595393358 | 1.9341908636 | -0.0884773242 |
| H | -1.7591867298 | 2.3155576488 | -0.0991446319 |
| C | 1.9517958152 | -0.5022900185 | 0.0035242051 |
| H | 2.1974536505 | -1.5589647326 | 0.0439355797 |
| C | 2.9575096192 | 0.3707643140 | -0.0319369118 |
| H | 3.9841257205 | 0.0329150646 | -0.0206498006 |
| H | 2.8041856050 | 1.4409329878 | -0.0730757968 |

**cyclooctatetraene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.8363190000 | -0.0004380000 | 0.0000000000 |
| H | 2.9200100000 | 0.0436790000 | 0.0000000000 |
| C | 1.2471120000 | 1.3478950000 | 0.0000000000 |
| H | 2.0156710000 | 2.1133910000 | 0.0000000000 |
| C | 0.0004380000 | 1.8363190000 | 0.0000000000 |
| H | -0.0436790000 | 2.9200100000 | 0.0000000000 |
| C | -1.3478950000 | 1.2471120000 | 0.0000000000 |
| H | -2.1133910000 | 2.0156710000 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.8363190000 | 0.0004380000 | 0.0000000000 |
| H | -2.9200100000 | -0.0436790000 | 0.0000000000 |
| C | -1.2471120000 | -1.3478950000 | 0.0000000000 |
| H | -2.0156710000 | -2.1133910000 | 0.0000000000 |
| C | -0.0004380000 | -1.8363190000 | 0.0000000000 |
| H | 0.0436790000 | -2.9200100000 | 0.0000000000 |
| C | 1.3478950000 | -1.2471120000 | 0.0000000000 |
| H | 2.1133910000 | -2.0156710000 | 0.0000000000 |

**cyclopentene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.6187220329 | -0.5210508503 | -2.0343483531 |
| C | 0.0956589228 | -0.3163542994 | -1.2340665788 |
| C | -0.0447743786 | 1.0729340099 | -0.6642592352 |
| C | -0.0447743786 | 1.0729340099 | 0.6642592352 |
| C | 0.0956589228 | -0.3163542994 | 1.2340665788 |
| C | -0.1240102354 | -1.2267728091 | 0.0000000000 |
| H | 1.0914467409 | -0.4525662182 | -1.6703816681 |
| H | -0.0988870397 | 1.9580324397 | -1.2841287939 |
| H | -0.0988870397 | 1.9580324397 | 1.2841287939 |
| H | -0.6187220329 | -0.5210508503 | 2.0343483531 |
| H | 1.0914467409 | -0.4525662182 | 1.6703816681 |
| H | -1.1510853857 | -1.5936398967 | 0.0000000000 |
| H | 0.5290941941 | -2.0983814574 | 0.0000000000 |

**cyclopentadiene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0000000000 | -0.8745420000 | -1.8740230000 |
| C | 0.0000000000 | 0.0000000000 | -1.2131040000 |
| C | -1.1764710000 | 0.0000000000 | -0.2804370000 |
| C | -0.7326670000 | 0.0000000000 | 0.9874400000 |
| C | 0.7326670000 | 0.0000000000 | 0.9874400000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.1764710000 | 0.0000000000 | -0.2804370000 |
| H | 0.0000000000 | 0.8745420000 | -1.8740230000 |
| H | -2.2051550000 | 0.0000000000 | -0.6065400000 |
| H | -1.3449970000 | 0.0000000000 | 1.8773900000 |
| H | 1.3449970000 | 0.0000000000 | 1.8773900000 |
| H | 2.2051550000 | 0.0000000000 | -0.6065400000 |

**1H-Indene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0173629051 | -2.4927465096 | 0.0000000000 |
| C | -0.9968241556 | -1.4104370475 | 0.0000000000 |
| C | -0.9536835618 | 1.4044903961 | 0.0000000000 |
| C | 0.2106413356 | -0.7200239533 | 0.0000000000 |
| C | -2.1834073952 | -0.6824471737 | 0.0000000000 |
| C | -2.1642942941 | 0.7103194196 | 0.0000000000 |
| C | 0.2284599372 | 0.6865242967 | 0.0000000000 |
| H | -3.1319783646 | -1.2030884901 | 0.0000000000 |
| H | -3.0970204263 | 1.2584710609 | 0.0000000000 |
| H | -0.9482297305 | 2.4875083584 | 0.0000000000 |
| C | 1.5946639467 | -1.1923913392 | 0.0000000000 |
| H | 1.8834703188 | -2.2336777016 | 0.0000000000 |
| C | 2.4315747317 | -0.1441369522 | 0.0000000000 |
| H | 3.5101673959 | -0.1929349395 | 0.0000000000 |
| C | 1.6626474406 | 1.1518638080 | 0.0000000000 |
| H | 1.8983708634 | 1.7657423835 | -0.8755062363 |
| H | 1.8983708634 | 1.7657423835 | 0.8755062363 |

**cycloheptatriene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.4449098910 | -0.5483215419 | 0.0000000000 |
| H | -1.0407630778 | -1.5667321107 | 0.0000000000 |
| H | -2.5307602285 | -0.6232748604 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.9568098003 | 0.1857129079 | -1.2192227614 |
| H | -1.6886180512 | 0.6423821547 | -1.8749166565 |
| C | 0.3494809254 | 0.2726284549 | -1.5240019676 |
| H | 0.6277876977 | 0.7203147074 | -2.4722742153 |
| C | 1.4371663659 | -0.1558801029 | -0.6792125404 |
| H | 2.3769949621 | -0.3723473596 | -1.1750468874 |
| C | 1.4371663659 | -0.1558801029 | 0.6792125404 |
| H | 2.3769949621 | -0.3723473596 | 1.1750468874 |
| C | 0.3494809254 | 0.2726284549 | 1.5240019676 |
| H | 0.6277876977 | 0.7203147074 | 2.4722742153 |
| C | -0.9568098003 | 0.1857129079 | 1.2192227614 |
| H | -1.6886180512 | 0.6423821547 | 1.8749166565 |

**furan**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| O | 0.0000000000 | 0.0000000000 | 1.1442281287 |
| C | -1.0924803539 | 0.0000000000 | 0.3321217199 |
| C | -0.7157282071 | 0.0000000000 | -0.9688402113 |
| C | 0.7157282071 | 0.0000000000 | -0.9688402113 |
| C | 1.0924803539 | 0.0000000000 | 0.3321217199 |
| H | -2.0460975609 | 0.0000000000 | 0.8273893811 |
| H | -1.3692847517 | 0.0000000000 | -1.8235719540 |
| H | 1.3692847517 | 0.0000000000 | -1.8235719540 |
| H | 2.0460975609 | 0.0000000000 | 0.8273893811 |

**thiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.7116343007 | 0.0000000000 | 1.2864597402 |
| C | 1.2380227027 | 0.0000000000 | 0.0296321230 |
| S | 0.0000000000 | 0.0000000000 | -1.1733660218 |
| C | -1.2380227027 | 0.0000000000 | 0.0296321230 |
| C | -0.7116343007 | 0.0000000000 | 1.2864597402 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.3141691752 | 0.0000000000 | 2.1825696932 |
| H | 2.2742672461 | 0.0000000000 | -0.2619375455 |
| H | -2.2742672461 | 0.0000000000 | -0.2619375455 |
| H | -1.3141691752 | 0.0000000000 | 2.1825696932 |

**benzofuran**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0052439508 | -2.5094483084 | 0.0000000000 |
| C | -0.9695982465 | -1.4283013126 | 0.0000000000 |
| C | -0.9050253856 | 1.4149592664 | 0.0000000000 |
| C | 0.2533161199 | -0.7508832718 | 0.0000000000 |
| C | -2.1373459588 | -0.6818818317 | 0.0000000000 |
| C | -2.1070006138 | 0.7199897139 | 0.0000000000 |
| C | 0.2491794420 | 0.6513109953 | 0.0000000000 |
| H | -3.0935814466 | -1.1873877561 | 0.0000000000 |
| H | -3.0376970977 | 1.2707220218 | 0.0000000000 |
| H | -0.8657993110 | 2.4947477016 | 0.0000000000 |
| C | 1.6433529460 | -1.1287867846 | 0.0000000000 |
| H | 2.0563325604 | -2.1227270084 | 0.0000000000 |
| C | 2.3447615523 | 0.0239003446 | 0.0000000000 |
| H | 3.3998914692 | 0.2321668705 | 0.0000000000 |
| O | 1.5310389211 | 1.1272513593 | 0.0000000000 |

**propionitrile**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.4484779024 | -1.0989818575 | 0.8819533216 |
| C | -1.5479322770 | -0.4683643126 | 0.0000000000 |
| H | -1.4484779024 | -1.0989818575 | -0.8819533216 |
| H | -2.5453619971 | -0.0306972945 | 0.0000000000 |
| C | -0.4920979986 | 0.6461376351 | 0.0000000000 |
| H | -0.6117159341 | 1.2865615391 | 0.8760658444 |
| H | -0.6117159341 | 1.2865615391 | -0.8760658444 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.8737429985 | 0.1295866427 | 0.0000000000 |
| N | 1.9434119471 | -0.2934160337 | 0.0000000000 |

**benzene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.4722869898 | 0.0000000050 | 0.0000000000 |
| C | 1.3903488329 | 0.0000000028 | 0.0000000000 |
| C | -1.3903488329 | -0.0000000028 | 0.0000000000 |
| C | 0.6951744140 | 1.2040774108 | 0.0000000000 |
| C | 0.6951744189 | -1.2040774080 | 0.0000000000 |
| C | -0.6951744140 | -1.2040774108 | 0.0000000000 |
| C | -0.6951744189 | 1.2040774080 | 0.0000000000 |
| H | 1.2361434906 | 2.1410633411 | 0.0000000000 |
| H | 1.2361434992 | -2.1410633361 | 0.0000000000 |
| H | -1.2361434906 | -2.1410633411 | 0.0000000000 |
| H | -1.2361434992 | 2.1410633361 | 0.0000000000 |
| H | -2.4722869898 | -0.0000000050 | 0.0000000000 |

**thiophenol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.3359707659 | -2.1435163359 | 0.0000000000 |
| C | -0.2001056255 | -1.2036478289 | 0.0000000000 |
| C | -1.5853045039 | 1.2021633295 | 0.0000000000 |
| C | 0.5049198886 | 0.0006982957 | 0.0000000000 |
| C | -1.5883171488 | -1.1972430756 | 0.0000000000 |
| C | -2.2887649100 | 0.0036931902 | 0.0000000000 |
| C | -0.1960577026 | 1.2061312161 | 0.0000000000 |
| H | -2.1230618597 | -2.1377859058 | 0.0000000000 |
| H | -3.3699592342 | 0.0053542939 | 0.0000000000 |
| H | 0.3378930972 | 2.1468819764 | 0.0000000000 |
| H | -2.1174961017 | 2.1442634344 | 0.0000000000 |
| S | 2.2846558396 | -0.0830870120 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.5114154949 | 1.2415094219 | 0.0000000000 |

**toluene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.7270783779 | 0.0214702041 | 2.1380684607 |
| C | 0.1903262312 | 0.0112647374 | 1.1971773779 |
| C | -1.1994107665 | -0.0023802006 | -1.2000835751 |
| C | 0.9073434211 | 0.0152270143 | 0.0000000000 |
| C | -1.1994107665 | -0.0023802006 | 1.2000835751 |
| C | -1.9005219792 | -0.0103258574 | 0.0000000000 |
| C | 0.1903262312 | 0.0112647374 | -1.1971773779 |
| H | -1.7347267409 | -0.0029950331 | 2.1406363647 |
| H | -2.9822732756 | -0.0181556282 | 0.0000000000 |
| H | 0.7270783779 | 0.0214702041 | -2.1380684607 |
| H | -1.7347267409 | -0.0029950331 | -2.1406363647 |
| C | 2.4142023062 | -0.0021686660 | 0.0000000000 |
| H | 2.7944906683 | -1.0270718370 | 0.0000000000 |
| H | 2.8182543279 | 0.4938877793 | 0.8825663818 |
| H | 2.8182543279 | 0.4938877793 | -0.8825663818 |

**phenol**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.7421868417 | -2.1589962596 | 0.0000000000 |
| C | 0.2075281219 | -1.2194963767 | 0.0000000000 |
| C | -1.1228987899 | 1.2224937282 | 0.0000000000 |
| C | 0.9330851076 | -0.0303533250 | 0.0000000000 |
| C | -1.1791040678 | -1.1763956598 | 0.0000000000 |
| C | -1.8535935064 | 0.0411681646 | 0.0000000000 |
| C | 0.2669396896 | 1.1926977729 | 0.0000000000 |
| H | -1.7373883270 | -2.1032597897 | 0.0000000000 |
| H | -2.9342705209 | 0.0674439626 | 0.0000000000 |
| H | 0.8331809236 | 2.1170580165 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.6328312703 | 2.1767607135 | 0.0000000000 |
| O | 2.2970757943 | -0.1240260662 | 0.0000000000 |
| H | 2.6783770037 | 0.7595021185 | 0.0000000000 |

**N-methylpyrrole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 0.6229332789 | 0.0344213123 | 0.0000000000 |
| C | -0.1742341251 | 0.0121562035 | -1.1157170913 |
| C | -1.4870612565 | -0.0143102931 | -0.7093426876 |
| C | -1.4870612565 | -0.0143102931 | 0.7093426876 |
| C | -0.1742341251 | 0.0121562035 | 1.1157170913 |
| H | 0.2580677877 | 0.0205749960 | -2.1013534040 |
| H | -2.3470865861 | -0.0202389974 | -1.3569518857 |
| H | -2.3470865861 | -0.0202389974 | 1.3569518857 |
| H | 0.2580677877 | 0.0205749960 | 2.1013534040 |
| C | 2.0696170322 | -0.0262879142 | 0.0000000000 |
| H | 2.4576314929 | 0.4793681763 | -0.8824761073 |
| H | 2.4302990625 | -1.0573145631 | 0.0000000000 |
| H | 2.4576314929 | 0.4793681763 | 0.8824761073 |

**Naphtalene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.3645215766 | -1.2402275820 | 0.0000000000 |
| C | 2.4238428070 | -0.7058025573 | 0.0000000000 |
| H | 1.2392614266 | -2.4798275384 | 0.0000000000 |
| C | 1.2406174149 | -1.3969645822 | 0.0000000000 |
| C | 1.2406174149 | 1.3969645822 | 0.0000000000 |
| C | 0.0000000000 | -0.7139541915 | 0.0000000000 |
| C | 2.4238428070 | 0.7058025573 | 0.0000000000 |
| C | 0.0000000000 | 0.7139541915 | 0.0000000000 |
| C | -1.2406174149 | -1.3969645822 | 0.0000000000 |
| H | 3.3645215766 | 1.2402275820 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2392614266 | 2.4798275384 | 0.0000000000 |
| H | 1.2392614266 | 2.4798275384 | 0.0000000000 |
| C | -2.4238428070 | -0.7058025573 | 0.0000000000 |
| H | -1.2392614266 | -2.4798275384 | 0.0000000000 |
| H | -3.3645215766 | -1.2402275820 | 0.0000000000 |
| C | -2.4238428070 | 0.7058025573 | 0.0000000000 |
| H | -3.3645215766 | 1.2402275820 | 0.0000000000 |
| C | -1.2406174149 | 1.3969645822 | 0.0000000000 |

**quinoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.3873072013 | -1.1179926599 | 0.0000000000 |
| C | 2.4143649698 | -0.6463802819 | 0.0000000000 |
| H | 1.2920685416 | -2.4676109287 | 0.0000000000 |
| C | 1.2628296026 | -1.3849404065 | 0.0000000000 |
| N | 1.1842448776 | 1.4227266132 | 0.0000000000 |
| C | 0.0148341359 | -0.7223225077 | 0.0000000000 |
| C | 2.3177610657 | 0.7630979763 | 0.0000000000 |
| C | 0.0276884848 | 0.7040505525 | 0.0000000000 |
| C | -1.2264167478 | -1.4016900451 | 0.0000000000 |
| H | 3.2240431270 | 1.3605712145 | 0.0000000000 |
| H | -1.1714050850 | 2.4801686399 | 0.0000000000 |
| C | -2.4029573656 | -0.6994172037 | 0.0000000000 |
| H | -1.2313343094 | -2.4846283466 | 0.0000000000 |
| H | -3.3485105341 | -1.2248441822 | 0.0000000000 |
| C | -2.3901776781 | 0.7127741445 | 0.0000000000 |
| H | -3.3277285981 | 1.2526849728 | 0.0000000000 |
| C | -1.2044236881 | 1.3996914485 | 0.0000000000 |

**pyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | 2.4619988193 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0000000000 | 0.0000000000 | 1.3801000078 |
| N | 0.0000000000 | 0.0000000000 | -1.4122818073 |
| C | -1.1929662580 | 0.0000000000 | 0.6709682817 |
| C | 1.1929662580 | 0.0000000000 | 0.6709682817 |
| C | 1.1386362604 | 0.0000000000 | -0.7178839481 |
| C | -1.1386362604 | 0.0000000000 | -0.7178839481 |
| H | 2.1476133087 | 0.0000000000 | 1.1787001075 |
| H | 2.0526762455 | 0.0000000000 | -1.3011004510 |
| H | -2.0526762455 | 0.0000000000 | -1.3011004510 |
| H | -2.1476133087 | 0.0000000000 | 1.1787001075 |

**aniline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.7554882075 | -0.0201250997 | 2.1429252173 |
| C | 0.2171898734 | -0.0123285244 | 1.2028579787 |
| C | -1.1701110877 | -0.0050361554 | -1.1974416586 |
| C | 0.9328981934 | -0.0158433343 | 0.0000000000 |
| C | -1.1701110877 | -0.0050361554 | 1.1974416586 |
| C | -1.8772114457 | -0.0014958664 | 0.0000000000 |
| C | 0.2171898734 | -0.0123285244 | -1.2028579787 |
| H | -1.7023017738 | -0.0011792137 | 2.1398843622 |
| H | -2.9581497564 | 0.0048514909 | 0.0000000000 |
| H | 0.7554882075 | -0.0201250997 | -2.1429252173 |
| H | -1.7023017738 | -0.0011792137 | -2.1398843622 |
| N | 2.3258806105 | -0.0830209295 | 0.0000000000 |
| H | 2.7724569798 | 0.2611973130 | -0.8344684103 |
| H | 2.7724569798 | 0.2611973130 | 0.8344684103 |

**2-methylpyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.5635436207 | -2.1690155812 | 0.0000000000 |
| C | -1.0931657851 | -1.1917634217 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.1728658810 | 1.2010354079 | 0.0000000000 |
| N | 0.2417092133 | -1.1871029506 | 0.0000000000 |
| C | -1.8668177866 | -0.0409343189 | 0.0000000000 |
| C | -1.2116752650 | 1.1847821236 | 0.0000000000 |
| C | 0.8732666343 | -0.0091274593 | 0.0000000000 |
| H | -2.9459888967 | -0.1045839513 | 0.0000000000 |
| H | -1.7717961683 | 2.1107245015 | 0.0000000000 |
| H | 0.7141698946 | 2.1381049553 | 0.0000000000 |
| C | 2.3781072528 | -0.0360071334 | 0.0000000000 |
| H | 2.7811036470 | 0.4714184269 | -0.8789017473 |
| H | 2.7261493525 | -1.0656500258 | 0.0000000000 |
| H | 2.7811036470 | 0.4714184269 | 0.8789017473 |

**acetone**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0000000000 | 0.0000000000 | 0.1918834177 |
| C | -1.2878322568 | 0.0000000000 | -0.6045693086 |
| H | -1.3313963417 | 0.8770948024 | -1.2542217104 |
| H | -2.1405331971 | 0.0000000000 | 0.0689793627 |
| H | -1.3313963417 | -0.8770948024 | -1.2542217104 |
| C | 1.2878322568 | 0.0000000000 | -0.6045693086 |
| H | 1.3313963417 | 0.8770948024 | -1.2542217104 |
| H | 1.3313963417 | -0.8770948024 | -1.2542217104 |
| H | 2.1405331971 | 0.0000000000 | 0.0689793627 |
| O | 0.0000000000 | 0.0000000000 | 1.4011933159 |

**2-butanone**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.9843732517 | -1.1501657752 | 0.8770907045 |
| C | -1.8812017858 | -0.5075658654 | 0.0000000000 |
| H | -1.9843732517 | -1.1501657752 | -0.8770907045 |
| H | -2.6703210328 | 0.2396057625 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.5271451792 | 0.1718627988 | 0.0000000000 |
| C | 0.6877834794 | -0.7418499481 | 0.0000000000 |
| H | 0.6028176872 | -1.4043252250 | -0.8680762356 |
| H | 0.6028176872 | -1.4043252250 | 0.8680762356 |
| C | 2.0202389644 | -0.0053925020 | 0.0000000000 |
| H | 2.8503196806 | -0.7120076641 | 0.0000000000 |
| H | 2.1128110118 | 0.6341616267 | 0.8767039111 |
| H | 2.1128110118 | 0.6341616267 | -0.8767039111 |
| O | -0.4228310212 | 1.3770171653 | 0.0000000000 |

**pyrazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 0.0000000000 | -1.4008270976 | 0.0000000000 |
| N | 0.0000000000 | 1.4008270976 | 0.0000000000 |
| C | -1.1295929741 | -0.6952812212 | 0.0000000000 |
| C | 1.1295929741 | -0.6952812212 | 0.0000000000 |
| C | 1.1295929741 | 0.6952812212 | 0.0000000000 |
| C | -1.1295929741 | 0.6952812212 | 0.0000000000 |
| H | -2.0598784152 | -1.2512162047 | 0.0000000000 |
| H | 2.0598784152 | -1.2512162047 | 0.0000000000 |
| H | 2.0598784152 | 1.2512162047 | 0.0000000000 |
| H | -2.0598784152 | 1.2512162047 | 0.0000000000 |

**hexahydropyrimidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.0048906344 | -1.3853422897 | 0.1592098004 |
| C | -1.1705843229 | -0.8010501278 | -0.2307808003 |
| C | -0.0154769723 | 1.4286834301 | -0.2089708244 |
| C | 1.2310369916 | -0.6438683682 | -0.2054508822 |
| N | 1.1577154249 | 0.7258467973 | 0.3122542142 |
| N | 0.0832472111 | -1.4375355850 | 0.1859691904 |
| C | -1.2770725668 | 0.6673464712 | 0.2010707767 |

Continued on Next Page...

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0062017848 | 1.5145521948 | -1.3093949699 |
| H | 1.2747555065 | -0.6650802055 | -1.3067480493 |
| H | -1.3852038072 | 0.7208185385 | 1.2873301874 |
| H | -1.2240402888 | -0.8639994671 | -1.3224957889 |
| H | -0.0299681752 | 2.4422981667 | 0.1939078385 |
| H | 2.1396594569 | -1.1113219745 | 0.1746736735 |
| H | -2.1602876695 | 1.1334994069 | -0.2430034450 |
| H | 0.0881362529 | -1.5359448320 | 1.1953996263 |
| H | 2.0061848084 | 1.2323558443 | 0.0899514526 |

**hexahydropyridazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.2392610334 | -0.6975447202 | 0.1688187533 |
| N | 0.0564938977 | 1.3548492316 | 0.3222647784 |
| N | 1.1741859296 | 0.6715028385 | -0.3537273895 |
| C | -1.1915219699 | 0.7678917724 | -0.1776563837 |
| C | -0.0254058148 | -1.4522566239 | -0.2331559667 |
| H | 1.3367993039 | -0.7069895119 | 1.2639779284 |
| H | -1.2572378340 | 0.8325334829 | -1.2733359273 |
| H | -0.0489949820 | -1.5428590362 | -1.3222106376 |
| H | 2.1251464295 | -1.1694408117 | -0.2592440240 |
| H | -2.0163741670 | 1.3398672988 | 0.2503578235 |
| H | -0.0036738039 | -2.4629872161 | 0.1789938748 |
| H | 2.0009385633 | 1.1615019089 | -0.0278613706 |
| C | -1.2677861736 | -0.6963766729 | 0.2482459862 |
| H | -2.1766113838 | -1.1533911906 | -0.1479836663 |
| H | -1.3263018001 | -0.7422730133 | 1.3388102850 |
| H | 0.1025097718 | 2.3090242638 | -0.0201190638 |

**hexahydro-1,3,5-triazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 1.3626676559 | -0.0000001582 | 0.3089233473 |

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | -0.6813334722 | 1.1801047597 | 0.3089233473 |
| C | 0.6923522953 | 1.1991887782 | -0.1770086770 |
| C | -1.3847038747 | 0.0000001607 | -0.1770086770 |
| C | 0.6923520169 | -1.1991889389 | -0.1770086770 |
| H | 0.7247323414 | 1.2552726480 | -1.2876250550 |
| H | 0.7247320499 | -1.2552728163 | -1.2876250550 |
| H | -2.3993106527 | 0.0000002785 | 0.2214355852 |
| H | 2.3291381430 | -0.0000002704 | 0.0087947995 |
| H | -1.1645686186 | 2.0170928096 | 0.0087947995 |
| H | 1.1996553039 | -2.0778642424 | 0.2214355852 |
| H | -1.4494639538 | 0.0000001683 | -1.2876250550 |
| H | 1.1996557863 | 2.0778639639 | 0.2214355852 |
| N | -0.6813337462 | -1.1801046015 | 0.3089233473 |
| H | -1.1645690869 | -2.0170925393 | 0.0087947995 |

**tetrahydro-1H-imidazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.3412486099 | 1.0308090814 | -1.1614194496 |
| C | -0.9813989481 | 0.0723890958 | -0.7837101642 |
| N | 0.4220679449 | -0.1261558826 | -1.1884976608 |
| C | 1.1884501458 | 0.2645860673 | 0.0000000000 |
| N | 0.4220679449 | -0.1261558826 | 1.1884976608 |
| C | -0.9813989481 | 0.0723890958 | 0.7837101642 |
| H | -1.6134263534 | -0.7067345871 | -1.2075252712 |
| H | 2.1825568029 | -0.1787637923 | 0.0000000000 |
| H | 1.2953349735 | 1.3527463307 | 0.0000000000 |
| H | -1.3412486099 | 1.0308090814 | 1.1614194496 |
| H | -1.6134263534 | -0.7067345871 | 1.2075252712 |
| H | 0.5786035053 | -1.1122455114 | -1.3617754947 |
| H | 0.5786035053 | -1.1122455114 | 1.3617754947 |

**pyrazolidine**

Continued on Next Page. . .

**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
| N | 0.6809042857 | -0.9497872594 | -0.3194670559 |
| N | -0.6438353248 | -0.9730138607 | 0.3378330096 |
| C | -1.2162099033 | 0.3115595766 | -0.0964449731 |
| C | -0.0286504141 | 1.2911309358 | -0.0068701808 |
| C | 1.1987026918 | 0.3635157294 | 0.0970350532 |
| H | -1.5834369932 | 0.2712370696 | -1.1279024605 |
| H | -2.0439637730 | 0.5816023843 | 0.5573965068 |
| H | -0.0990620911 | 1.9376793627 | 0.8657343247 |
| H | 0.0149964741 | 1.9266931208 | -0.8892393812 |
| H | 1.5660876786 | 0.3529234552 | 1.1291683654 |
| H | 2.0151720866 | 0.6587437682 | -0.5600905344 |
| H | 1.2202299265 | -1.6744482323 | 0.1440217767 |
| H | -1.1521986438 | -1.7259860503 | -0.1153934505 |

**1,2,3-triazolidine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | -0.8076153928 | -1.0016247605 | 0.1024582541 |
| N | -1.1859830989 | 0.4344657193 | 0.1836299181 |
| N | -0.0089128331 | 1.2310010884 | -0.1501260594 |
| C | 1.1033328061 | 0.3752478663 | 0.2541420590 |
| C | 0.6342351813 | -1.0230692099 | -0.1779259551 |
| H | 1.2243065432 | 0.4281690391 | 1.3379711577 |
| H | 2.0232313678 | 0.7091399606 | -0.2224054275 |
| H | 1.1085951048 | -1.8426278835 | 0.3605146436 |
| H | 0.8142997868 | -1.1680558585 | -1.2467793156 |
| H | -0.9395882799 | -1.3251724750 | 1.0532472753 |
| H | 0.0439439806 | 1.3067106279 | -1.1659102175 |
| H | -1.8438231658 | 0.5909208858 | -0.5725823328 |

**1,2,4-triazolidine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 0.7642080664 | -1.0166167744 | 0.0863504082 |
| N | -0.6541552689 | -1.0922037562 | -0.1536007608 |
| C | -1.1544035054 | 0.2292257486 | 0.2386380084 |
| N | -0.1035653040 | 1.1969699368 | -0.0885758667 |
| C | 1.1384046538 | 0.4329800296 | 0.0742817340 |
| H | -2.0923567253 | 0.4698359345 | -0.2596094614 |
| H | -1.3175222261 | 0.2269289575 | 1.3191161926 |
| H | 1.6392925077 | 0.6832851774 | 1.0125173917 |
| H | 1.8188530709 | 0.6547765925 | -0.7488102581 |
| H | 0.9050137865 | -1.3852880889 | 1.0181034367 |
| H | -0.7684389081 | -1.2097327751 | -1.1552716272 |
| H | -0.1983701475 | 1.4670930177 | -1.0597431973 |

**perhydroquinoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.2352476276 | -1.4564978152 | -0.2043378944 |
| C | -2.5299171910 | 0.7198060032 | -0.2314540641 |
| C | 0.0075801778 | 0.7446333891 | -0.2614582214 |
| C | -1.2631739520 | 1.4657805721 | 0.1982295930 |
| C | 0.0193731191 | -0.7078502304 | 0.2421838110 |
| C | -2.5115320158 | -0.7374731989 | 0.2417000252 |
| H | -2.6062848883 | 0.7419861651 | -1.3233774700 |
| H | -0.0037893646 | 0.6926739512 | -1.3567556665 |
| H | -1.2494643547 | 1.5614244271 | 1.2897254589 |
| H | 0.0141669944 | -0.6652550574 | 1.3486073526 |
| H | -2.5780333178 | -0.7616272115 | 1.3343120071 |
| H | -1.2141506138 | -1.5451181649 | -1.2943507919 |
| H | -3.4171093092 | 1.2288949765 | 0.1518021931 |
| N | 1.2225820441 | -1.3804325104 | -0.2461907501 |
| C | 1.2911857178 | 1.4648402799 | 0.1638630458 |
| C | 2.5375778276 | 0.6800240780 | -0.2549268201 |
| C | 2.4567819044 | -0.7633739413 | 0.2355697006 |
| H | 2.5219427798 | -0.7678551175 | 1.3377925666 |

Continued on Next Page...

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.3030383312 | -1.3410201113 | -0.1399655832 |
| H | -3.3896486996 | -1.2680179215 | -0.1324149708 |
| H | -1.2710472002 | 2.4841181569 | -0.1989116434 |
| H | 1.2876965737 | 1.5863265645 | 1.2530963165 |
| H | 1.3135851325 | 2.4719704003 | -0.2600078446 |
| H | 2.6197610527 | 0.6756453094 | -1.3447025055 |
| H | 3.4396686313 | 1.1543383599 | 0.1378733504 |
| H | -1.2180565191 | -2.4757010670 | 0.1938642220 |
| H | 1.1969047676 | -2.3599342858 | 0.0100055833 |

**perhydroisoquinoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.2442718316 | -1.4722354362 | -0.1794311250 |
| C | -2.5382200163 | 0.7060652493 | -0.2558210078 |
| C | -0.0009492877 | 0.7321453422 | -0.2547522686 |
| C | -1.2773391354 | 1.4612099782 | 0.1756136267 |
| C | 0.0090194862 | -0.7158760750 | 0.2705182642 |
| C | -2.5252731463 | -0.7439690458 | 0.2389868944 |
| H | -2.6029394526 | 0.7119320159 | -1.3490430790 |
| H | -0.0045988714 | 0.6756926963 | -1.3525557007 |
| H | -1.2738034461 | 1.5719372659 | 1.2657045962 |
| H | 0.0078073415 | -0.6695694497 | 1.3661180152 |
| H | -2.6002207109 | -0.7514791120 | 1.3313689974 |
| H | -1.2287860367 | -1.5815378220 | -1.2696238496 |
| H | -3.4301091064 | 1.2205713224 | 0.1089901386 |
| C | 1.3014187526 | -1.4200603723 | -0.1428313517 |
| C | 1.2779017880 | 1.4644258552 | 0.1649351691 |
| C | 2.5231933472 | 0.6762213389 | -0.2356001849 |
| N | 2.4588966444 | -0.6674104244 | 0.3339713310 |
| H | -3.4019769504 | -1.2777776789 | -0.1347558100 |
| H | -1.2840824364 | 2.4736045067 | -0.2374914539 |
| H | 1.2802716682 | 1.6015101651 | 1.2500336231 |
| H | 1.3075864490 | 2.4587743333 | -0.2883904246 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.5939793828 | 0.6599487879 | -1.3375851179 |
| H | 3.4219808810 | 1.1695573564 | 0.1380771040 |
| H | -1.2364233646 | -2.4849341539 | 0.2330542542 |
| H | 3.3125026859 | -1.1738478449 | 0.1393075539 |
| H | 1.3359996453 | -2.4216688514 | 0.2911341513 |
| H | 1.3018757207 | -1.5412209470 | -1.2411253456 |

**perhydro-4H-quinolizine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.2974374738 | -0.7044167880 | 0.0000000000 |
| C | 0.2085665210 | -0.7042479524 | -2.5419033996 |
| N | -0.2184157534 | 0.6727829784 | 0.0000000000 |
| C | -0.1570186505 | -1.4481091781 | -1.2592396482 |
| H | 1.2968920743 | -0.6901742264 | -2.6606687002 |
| H | -1.2424483641 | -1.5746107042 | -1.2095104967 |
| H | 1.4060875159 | -0.6788046231 | 0.0000000000 |
| H | -0.1946726952 | -1.2241290516 | -3.4133834695 |
| H | 0.2832011214 | -2.4479398309 | -1.2547251690 |
| C | -0.1570186505 | -1.4481091781 | 1.2592396482 |
| H | 0.2832011214 | -2.4479398309 | 1.2547251690 |
| H | -1.2424483641 | -1.5746107042 | 1.2095104967 |
| C | 0.2085665210 | -0.7042479524 | 2.5419033996 |
| H | 1.2968920743 | -0.6901742264 | 2.6606687002 |
| H | -0.1946726952 | -1.2241290516 | 3.4133834695 |
| C | -0.3124906377 | 0.7299090391 | 2.4754336760 |
| H | 0.0181823484 | 1.3063833469 | 3.3421322911 |
| H | -1.4055436204 | 0.7258360071 | 2.4851811041 |
| C | 0.1681480164 | 1.4117198089 | 1.2001893916 |
| H | 1.2668902656 | 1.5353920213 | 1.2487940097 |
| H | -0.2563309976 | 2.4149794367 | 1.1271789372 |
| C | 0.1681480164 | 1.4117198089 | -1.2001893916 |
| H | -0.2563309976 | 2.4149794367 | -1.1271789372 |
| H | 1.2668902656 | 1.5353920213 | -1.2487940097 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.3124906377 | 0.7299090391 | -2.4754336760 |
| H | -1.4055436204 | 0.7258360071 | -2.4851811041 |
| H | 0.0181823484 | 1.3063833469 | -3.3421322911 |

**perhydrocinnoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0179955540 | -0.7103259513 | -0.2709516087 |
| C | -2.5037875600 | -0.7319219357 | -0.2430692445 |
| C | 0.0122345161 | 0.7372360890 | 0.2618530474 |
| C | -1.2276051741 | -1.4668207681 | 0.1821559857 |
| H | -2.5754938783 | -0.7480505478 | -1.3353437258 |
| H | -0.0146386836 | 0.6647567543 | 1.3587208353 |
| H | -1.2124228377 | -1.5695040364 | 1.2734681723 |
| H | 0.0294326338 | -0.6744736567 | -1.3647812313 |
| H | -3.3827442482 | -1.2610246446 | 0.1309954639 |
| H | -1.2064266698 | -2.4774255397 | -0.2288679612 |
| N | 1.2356695267 | -1.4339620615 | 0.1112512285 |
| N | 2.3706166747 | -0.7165793430 | -0.3845330107 |
| C | 2.5286386460 | 0.5978747731 | 0.2335189820 |
| C | 1.3119382361 | 1.4523006021 | -0.1238425105 |
| H | 1.3212024011 | 1.6380104326 | -1.2013410986 |
| H | 1.3722906168 | 2.4231592231 | 0.3746412172 |
| C | -1.2524076277 | 1.4746822257 | -0.1862135028 |
| H | -1.2588092607 | 2.4894533255 | 0.2208413264 |
| H | -1.2381693709 | 1.5795744446 | -1.2766384884 |
| C | -2.5178907811 | 0.7230421097 | 0.2397510018 |
| H | -2.5921155774 | 0.7388980524 | 1.3321450986 |
| H | -3.4063156739 | 1.2343379406 | -0.1374136287 |
| H | 1.2703871442 | -1.4619370992 | 1.1349438809 |
| H | 3.1842974222 | -1.3019407295 | -0.2558082184 |
| H | 2.6229176248 | 0.5323109082 | 1.3316012059 |
| H | 3.4462793468 | 1.0489184326 | -0.1494712165 |

Continued on Next Page. . .

**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**perhydrophthalazine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | 0.0186408545 | -0.7263157287 | -0.2578016483 |
| C | -2.5090230482 | -0.7561664832 | -0.2202601046 |
| C | 0.0077908533 | 0.7275303693 | 0.2492130785 |
| C | -1.2282457000 | -1.4769198214 | 0.2148632550 |
| H | -2.5846810872 | -0.7939319911 | -1.3118333437 |
| H | -0.0091489158 | 0.6875952403 | 1.3481356958 |
| H | -1.2100069431 | -1.5617348752 | 1.3070800811 |
| H | 0.0025814886 | -0.6925032878 | -1.3535366937 |
| H | -3.3863532847 | -1.2778719615 | 0.1683434055 |
| H | -1.2213955640 | -2.4982906014 | -0.1756455030 |
| C | 1.3315914744 | -1.4060286952 | 0.1343298717 |
| N | 2.4418971982 | -0.6014962699 | -0.3708589898 |
| N | 2.5085539432 | 0.6978749869 | 0.2242244184 |
| C | 1.3055711426 | 1.4429577286 | -0.1517796802 |
| H | 1.3383986943 | 1.5900512870 | -1.2336288126 |
| H | 1.3608502055 | 2.4269944195 | 0.3198783046 |
| C | -1.2591938898 | 1.4541861800 | -0.2077709845 |
| H | -1.2689012935 | 2.4749278070 | 0.1843442287 |
| H | -1.2483995005 | 1.5414862394 | -1.2996705464 |
| C | -2.5230072704 | 0.7079217832 | 0.2339906809 |
| H | -2.5946029668 | 0.7442108014 | 1.3260490546 |
| H | -3.4129036729 | 1.2112531840 | -0.1504061243 |
| H | 3.3369877728 | -1.0496143238 | -0.2324653515 |
| H | 1.3694372103 | -1.5319955813 | 1.2310697181 |
| H | 1.3964532775 | -2.4005985165 | -0.3137501358 |
| H | 2.5097340216 | 0.6049991103 | 1.2438811255 |

**perhydroquinazoline**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0280345117 | -0.7180434165 | -0.2606145031 |
| C | -2.4988266351 | -0.7515230536 | -0.2454368129 |
| C | 0.0106352724 | 0.7310963849 | 0.2669206693 |
| C | -1.2191909583 | -1.4808369805 | 0.1772997774 |
| H | -2.5712790918 | -0.7634362729 | -1.3378345344 |
| H | 0.0024428245 | 0.6745340753 | 1.3646445574 |
| H | -1.2043441485 | -1.5895734188 | 1.2683378429 |
| H | 0.0217835335 | -0.6646940604 | -1.3579894471 |
| H | -3.3752159398 | -1.2864348014 | 0.1264781439 |
| H | -1.1897168751 | -2.4894715823 | -0.2387907789 |
| N | 1.2518102678 | -1.4391102849 | 0.1019204244 |
| C | 2.4521350641 | -0.6870856445 | -0.2579030232 |
| H | 2.5140329459 | -0.6783367853 | -1.3499185253 |
| H | 3.3253358446 | -1.2197688519 | 0.1178965176 |
| N | 2.5204003696 | 0.7014502820 | 0.1924193931 |
| C | 1.3051421884 | 1.4424468304 | -0.1522741980 |
| H | 1.2987095322 | 1.5862580961 | -1.2388219568 |
| H | 1.3609167731 | 2.4381459928 | 0.2928567893 |
| C | -1.2581131578 | 1.4599790286 | -0.1816543884 |
| H | -1.2717126066 | 2.4755740185 | 0.2237626918 |
| H | -1.2463956290 | 1.5643806285 | -1.2724653864 |
| C | -2.5198821776 | 0.7014380056 | 0.2434851403 |
| H | -2.5920888685 | 0.7125001718 | 1.3360426914 |
| H | -3.4113686831 | 1.2101325227 | -0.1300833957 |
| H | 1.2505505833 | -1.6288950746 | 1.0994337482 |
| H | 2.6624930602 | 0.7277231903 | 1.1960975635 |

**perhydroquinoxaline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0223692713 | -0.7307200522 | -0.2629148687 |
| C | -2.5042044873 | -0.7173221735 | -0.2223690811 |
| C | 0.0320816597 | 0.7224632551 | 0.2425990691 |
| C | -1.2339104904 | -1.4609904385 | 0.2030434807 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.5869015215 | -0.7476859684 | -1.3133974845 |
| H | 0.0217803590 | 0.6738355251 | 1.3490850039 |
| H | -1.2126458116 | -1.5523691249 | 1.2954118589 |
| H | 0.0130231446 | -0.6822074436 | -1.3581183384 |
| H | -3.3866925872 | -1.2280745448 | 0.1685072118 |
| H | -1.2238745128 | -2.4766212065 | -0.1956233701 |
| N | 1.2328497313 | -1.4677452955 | 0.1087401679 |
| C | 2.4492446473 | -0.7416570273 | -0.2603911267 |
| H | 2.5260334154 | -0.7471716885 | -1.3507639300 |
| H | 3.3131603851 | -1.2795666061 | 0.1333703490 |
| C | 2.4591645501 | 0.7084473649 | 0.2255736701 |
| H | 3.3301447799 | 1.2338313609 | -0.1719643240 |
| H | 2.5433142035 | 0.7114007612 | 1.3268734146 |
| N | 1.2465549046 | 1.3771521650 | -0.2405175823 |
| C | -1.2199039322 | 1.4676362900 | -0.2132801072 |
| H | -1.2056438643 | 2.4906918687 | 0.1747803904 |
| H | -1.1988138533 | 1.5467000110 | -1.3039908151 |
| C | -2.4919078159 | 0.7444688735 | 0.2400068983 |
| H | -2.5571333623 | 0.7773959525 | 1.3323767870 |
| H | -3.3737950868 | 1.2660986414 | -0.1374036694 |
| H | 1.2278590418 | -1.6357733226 | 1.1101582622 |
| H | 1.2498632320 | 2.3521738232 | 0.0329271335 |

**perhydro1,8-naphthyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0014322290 | -0.7682175051 | -0.2733443804 |
| C | -2.5237886048 | -0.6993596350 | -0.2338435011 |
| C | -0.0059978528 | 0.6876787064 | 0.2115782463 |
| C | -1.2744258100 | -1.4809507566 | 0.1824933335 |
| H | -2.6205306457 | -0.7135606091 | -1.3220235171 |
| H | -0.0052322871 | 0.6603855276 | 1.3266852884 |
| H | -1.2589737992 | -1.5883708890 | 1.2728526590 |
| H | 0.0007474861 | -0.7125425947 | -1.3660824735 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -3.4222698682 | -1.1621236397 | 0.1801927345 |
| H | -1.3014769667 | -2.4933200032 | -0.2274457299 |
| C | 1.2850864033 | -1.4674420574 | 0.1816004525 |
| C | 2.5259162706 | -0.6727996754 | -0.2355753312 |
| H | 2.6221723627 | -0.6861448889 | -1.3238084764 |
| H | 3.4294297858 | -1.1260816219 | 0.1780043623 |
| C | 2.4182205177 | 0.7774892292 | 0.2291905417 |
| H | 3.2592014786 | 1.3619084657 | -0.1462365052 |
| H | 2.4698084977 | 0.8019221759 | 1.3315665371 |
| N | 1.1826227818 | 1.3709135390 | -0.2822928606 |
| N | -1.2021288036 | 1.3585153241 | -0.2810378904 |
| C | -2.4310458771 | 0.7518909361 | 0.2311087234 |
| H | -2.4821670351 | 0.7755484396 | 1.3335216504 |
| H | -3.2783893602 | 1.3274927874 | -0.1436376644 |
| H | 1.1432902708 | 2.3533972341 | -0.0366065921 |
| H | 1.2714792848 | -1.5749984553 | 1.2719692371 |
| H | 1.3225341275 | -2.4794797016 | -0.2283434713 |
| H | -1.1730245857 | 2.3411986680 | -0.0347033724 |

**perhydro1,5-naphthyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.0174747920 | -0.7264307470 | -0.2485925557 |
| C | -2.4483498127 | -0.7460621770 | -0.2161826333 |
| C | 0.0174747920 | 0.7264307470 | 0.2485925557 |
| N | -1.2204976494 | -1.3728097127 | 0.2706279750 |
| H | -2.5207992281 | -0.7722660047 | -1.3171021044 |
| H | 0.0271981419 | 0.6786017691 | 1.3513869929 |
| H | -0.0271981419 | -0.6786017691 | -1.3513869929 |
| H | -3.3016711234 | -1.2999917246 | 0.1782247608 |
| C | 1.2437526607 | -1.4666080465 | 0.1898459144 |
| C | 2.5020843168 | -0.7091442252 | -0.2458620279 |
| H | 2.5858790125 | -0.7278937436 | -1.3351385231 |
| H | 3.3942578932 | -1.1926664741 | 0.1571294677 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 2.4483498127 | 0.7460621770 | 0.2161826333 |
| H | 3.3016711234 | 1.2999917246 | -0.1782247608 |
| H | 2.5207992281 | 0.7722660047 | 1.3171021044 |
| N | 1.2204976494 | 1.3728097127 | -0.2706279750 |
| C | -1.2437526607 | 1.4666080465 | -0.1898459144 |
| C | -2.5020843168 | 0.7091442252 | 0.2458620279 |
| H | -2.5858790125 | 0.7278937436 | 1.3351385231 |
| H | -3.3942578932 | 1.1926664741 | -0.1571294677 |
| H | 1.2105883686 | 2.3582548933 | -0.0385919665 |
| H | 1.2229647029 | -1.5675940468 | 1.2788909330 |
| H | 1.2470149546 | -2.4798503789 | -0.2222577366 |
| H | -1.2470149546 | 2.4798503789 | 0.2222577366 |
| H | -1.2229647029 | 1.5675940468 | -1.2788909330 |
| H | -1.2105883686 | -2.3582548933 | 0.0385919665 |

**perhydropteridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0089650200 | -0.7197824407 | -0.2506627440 |
| C | -2.4025023526 | -0.7829374393 | -0.2353675973 |
| C | -0.0298123048 | 0.7302399061 | 0.2522420347 |
| N | -1.1687701900 | -1.4215931927 | 0.2291730193 |
| H | -2.4901636768 | -0.7931352083 | -1.3321609684 |
| H | -0.0142990505 | 0.6781287728 | 1.3558266717 |
| H | 0.0413154900 | -0.6722646485 | -1.3527834068 |
| H | -3.2545716548 | -1.3251963124 | 0.1764627043 |
| N | 1.2102740114 | -1.4231417487 | 0.1750039064 |
| C | 2.4121404068 | -0.6824116060 | -0.2115198567 |
| H | 2.4901423630 | -0.7326850013 | -1.3005406477 |
| H | 3.2823759577 | -1.1856129462 | 0.2073296941 |
| N | 2.4611727889 | 0.7297743505 | 0.1668859815 |
| C | 1.2421408767 | 1.4444756223 | -0.2167214293 |
| H | 1.2161081736 | 1.5335168854 | -1.3063968274 |
| H | 1.2857219582 | 2.4599597134 | 0.1834498157 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.1235877157 | -2.3867626181 | -0.0767136113 |
| N | -1.2446637684 | 1.3632238486 | -0.2435494805 |
| C | -2.4398919190 | 0.6668274522 | 0.2352610331 |
| H | -2.5167229651 | 0.6754879405 | 1.3334126217 |
| H | -3.3243272090 | 1.1605470190 | -0.1698524517 |
| H | -1.2734740282 | 2.3409717468 | 0.0195535487 |
| H | 1.1748700450 | -1.5432404702 | 1.1829644788 |
| H | 2.6047107437 | 0.8098493747 | 1.1670665111 |

**perhydropyrazino[2,3-b]pyrazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.0032913814 | -0.7293174579 | -0.2629945502 |
| C | -2.4155757521 | -0.7256141455 | -0.2139692263 |
| C | -0.0006323626 | 0.7294953995 | 0.2170672637 |
| N | -1.1934489231 | -1.3871275178 | 0.2464341291 |
| H | -2.5182984366 | -0.7494059303 | -1.3089515701 |
| H | 0.0098728598 | 0.6918613643 | 1.3287978082 |
| H | 0.0254887276 | -0.6866108874 | -1.3623984214 |
| H | -3.2760494458 | -1.2377309273 | 0.2185321220 |
| N | 1.1768297491 | -1.4587340882 | 0.1753894507 |
| C | 2.4038915048 | -0.7564630884 | -0.2095245495 |
| H | 2.5014002107 | -0.8162816110 | -1.2959262661 |
| H | 3.2567785797 | -1.2765569152 | 0.2282324599 |
| C | 2.4100809662 | 0.7168650279 | 0.2083441079 |
| H | 3.2826475742 | 1.2227856050 | -0.2087898881 |
| H | 2.4870688016 | 0.7712437417 | 1.3079389772 |
| N | 1.2016527759 | 1.3678506730 | -0.3003128938 |
| N | -1.1999635225 | 1.3861784744 | -0.2767895429 |
| C | -2.4047094435 | 0.7305260356 | 0.2366152393 |
| H | -2.4639011875 | 0.7562763697 | 1.3355433293 |
| H | -3.2791665571 | 1.2459942982 | -0.1618037196 |
| H | -1.1983380275 | 2.3677308305 | -0.0242521344 |
| H | 1.2056550786 | 2.3531943974 | -0.0652841684 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 1.1309311015 | -1.5589534600 | 1.1852087368 |
| H | -1.1761178899 | -2.3598131885 | -0.0360136933 |

**perhydropyrimido[4,5-d]pyrimidine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | 0.0068979466 | -0.7455843286 | -0.2738883447 |
| N | -2.4892863605 | -0.7085411660 | -0.1756136597 |
| C | -0.0086880150 | 0.7091760822 | 0.2100675573 |
| C | -1.2753002262 | -1.4486024467 | 0.1849410883 |
| H | 0.0002926997 | 0.6828686406 | 1.3248215130 |
| H | -1.2675996958 | -1.5675930697 | 1.2735342477 |
| H | 0.0193083961 | -0.7029962355 | -1.3651518910 |
| H | -1.3383764294 | -2.4517794254 | -0.2399509037 |
| C | 1.2959376482 | -1.4194191655 | 0.1892336596 |
| H | 1.3677296131 | -2.4266033650 | -0.2252894652 |
| H | 1.2794007176 | -1.5183215629 | 1.2887681994 |
| N | 2.4352665119 | -0.6337087320 | -0.2858206979 |
| C | 2.3924165601 | 0.7364839998 | 0.2038730994 |
| H | 3.2577106849 | 1.2757495258 | -0.1816806055 |
| H | 2.4365191228 | 0.7683491543 | 1.3143950213 |
| N | 1.1817010511 | 1.3824487734 | -0.2916463095 |
| N | -1.2215798289 | 1.3547427936 | -0.2727677646 |
| C | -2.4141377978 | 0.6733215996 | 0.2516008666 |
| H | -2.4350051826 | 0.6718887507 | 1.3529807883 |
| H | -3.2960733542 | 1.2084504243 | -0.0992648601 |
| H | -1.2342740324 | 2.3323213901 | 0.0003420485 |
| H | 1.1803925285 | 2.3554903102 | -0.0064075684 |
| H | 3.3074073915 | -1.0668942811 | -0.0113904932 |
| H | -2.6043379494 | -0.7298926662 | -1.1827535258 |

**perhydro-1H-indene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.2984068525 | -2.4910291240 | -0.9708188503 |
| C | 0.1447521165 | -1.4918001132 | -0.9608850109 |
| C | 0.2560952711 | 0.7242235571 | -2.2308913655 |
| C | 0.2856916478 | 0.7121650700 | 0.2759750826 |
| C | -0.1447521165 | 1.4918001132 | -0.9608850109 |
| C | -0.2856916478 | -0.7121650700 | 0.2759750826 |
| C | -0.2560952711 | -0.7242235571 | -2.2308913655 |
| H | 1.3484369231 | 0.7163150206 | -2.3080296387 |
| H | 1.3804841266 | 0.6196871971 | 0.2499694878 |
| H | -1.2313986590 | 1.6309163915 | -0.9406159344 |
| H | -1.3804841266 | -0.6196871971 | 0.2499694878 |
| H | -1.3484369231 | -0.7163150206 | -2.3080296387 |
| H | 1.2313986590 | -1.6309163915 | -0.9406159344 |
| H | -0.1100912830 | 1.2458823502 | -3.1180183497 |
| H | 0.2984068525 | 2.4910291240 | -0.9708188503 |
| H | 0.1100912830 | -1.2458823502 | -3.1180183497 |
| C | 0.1108382392 | -1.2382151483 | 1.6590074106 |
| C | 0.0000000000 | 0.0000000000 | 2.5941149561 |
| H | 0.8702325902 | 0.0737973508 | 3.2462220705 |
| H | -0.8702325902 | -0.0737973508 | 3.2462220705 |
| C | -0.1108382392 | 1.2382151483 | 1.6590074106 |
| H | 0.5109353713 | 2.0701656233 | 1.9913257966 |
| H | -1.1411739013 | 1.6020304517 | 1.6300023234 |
| H | -0.5109353713 | -2.0701656233 | 1.9913257966 |
| H | 1.1411739013 | -1.6020304517 | 1.6300023234 |

**perhydrobenzofuran**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 2.5029355226 | -0.1308514160 | -0.0547298669 |
| C | 1.6992463713 | 1.1881450107 | 0.0711263434 |
| H | 3.1016096691 | -0.1666380134 | -0.9660174670 |
| H | 1.7305293899 | 1.5650541511 | 1.0955274977 |
| C | 0.2828023928 | 0.7356043456 | -0.2893296371 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.9020418561 | -1.4845786561 | -0.2097767296 |
| C | -2.2051143623 | 0.7308888557 | -0.2227143209 |
| C | -2.1822380331 | -0.7428784181 | 0.2197258295 |
| C | -0.9398721209 | 1.5042687328 | 0.1923672170 |
| C | 0.2874874963 | -0.6813630813 | 0.2705707203 |
| H | -0.8567939873 | -1.5787021145 | -1.2982647225 |
| H | -2.2976729861 | 0.7739210363 | -1.3125458260 |
| H | -2.2665362659 | -0.7885652569 | 1.3101416871 |
| H | -0.9058440470 | 1.6108036654 | 1.2817636861 |
| H | 0.2435701018 | -0.6228087205 | 1.3717660668 |
| H | 0.2216034745 | 0.6415668640 | -1.3799154334 |
| H | -0.8873131797 | -2.4944221265 | 0.2040991645 |
| H | -3.0941534217 | 1.2199400429 | 0.1809535030 |
| H | -3.0593264968 | -1.2582676599 | -0.1758167439 |
| H | -0.9641709361 | 2.5150092032 | -0.2212454640 |
| O | 1.5499304440 | -1.2087136182 | -0.1186637168 |
| H | 3.1709293966 | -0.2809793577 | 0.7978122653 |
| H | 2.0847554343 | 1.9698325314 | -0.5824460525 |

**perhydrobenzothiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 2.4294891494 | 0.6119827984 | -0.1920389033 |
| C | 1.2676227924 | 1.5406762414 | 0.1869596568 |
| H | 2.7375088121 | 0.7633552804 | -1.2251648108 |
| H | 1.2605998821 | 1.7114055561 | 1.2666396872 |
| C | -0.0168688708 | 0.8285881523 | -0.2277960468 |
| C | -1.0228165900 | -1.4864070220 | -0.1718883865 |
| C | -2.5159507777 | 0.5848811961 | -0.2908618254 |
| C | -2.3854181400 | -0.8678379254 | 0.1867256508 |
| C | -1.3464051881 | 1.4659766761 | 0.1755778489 |
| C | 0.0856565351 | -0.5828289505 | 0.3513124645 |
| H | -0.9250425547 | -1.5889143397 | -1.2560841468 |
| H | -2.5522915977 | 0.5995307080 | -1.3848113077 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.5154312762 | -0.9029951493 | 1.2730725033 |
| H | -1.3802318590 | 1.5854518596 | 1.2637800728 |
| H | -0.0042227359 | -0.5194503761 | 1.4394890344 |
| H | -0.0069343779 | 0.7316740217 | -1.3205319643 |
| H | -0.9432566960 | -2.4896410742 | 0.2508435017 |
| H | -3.4631835030 | 1.0044207171 | 0.0542902558 |
| H | -3.1888861521 | -1.4726004941 | -0.2386649656 |
| H | -1.4369376211 | 2.4673308440 | -0.2524004510 |
| S | 1.8079065580 | -1.1288972589 | -0.0215590515 |
| H | 3.2973766707 | 0.7458072792 | 0.4493153562 |
| H | 1.3754305404 | 2.5135932599 | -0.2968391728 |

**perhydro-1H-indole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.9349634604 | -2.4948696380 | 0.2310084683 |
| C | -0.9336118300 | -1.4844713766 | -0.1865959242 |
| C | -2.2193074912 | 0.7313441817 | -0.2235308250 |
| C | 0.2763870377 | 0.7209735724 | -0.2859870674 |
| C | -0.9474271599 | 1.4963326076 | 0.1821388434 |
| C | 0.2831351215 | -0.6983913094 | 0.2772861290 |
| C | -2.2069970264 | -0.7344566626 | 0.2408139664 |
| H | -2.3103206780 | 0.7580698239 | -1.3141280266 |
| H | 0.2232179493 | 0.6221757064 | -1.3762008488 |
| H | -0.9153208680 | 1.6174084488 | 1.2703045036 |
| H | 0.2300924921 | -0.6191481491 | 1.3793870942 |
| H | -2.2854570039 | -0.7629039326 | 1.3325576684 |
| H | -0.8932627362 | -1.5891073879 | -1.2744005647 |
| H | -3.1042620968 | 1.2349447379 | 0.1716677651 |
| H | -0.9630277647 | 2.5022535719 | -0.2445235226 |
| H | -3.0902779966 | -1.2493587707 | -0.1424949217 |
| N | 1.5851728029 | -1.1878995508 | -0.1692044230 |
| H | 1.8798813742 | -2.0173463458 | 0.3279325549 |
| C | 2.5487263729 | -0.0733609136 | -0.0007328158 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.2343112317 | -0.0467629718 | -0.8499404834 |
| H | 3.1581237055 | -0.1803662464 | 0.9029566320 |
| C | 1.6811054760 | 1.2116482278 | 0.0796650181 |
| H | 2.0434930394 | 1.9983062949 | -0.5813968565 |
| H | 1.6850515090 | 1.6124820819 | 1.0956896362 |

**perhydro-2H-isoindole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.9578652761 | -2.4937876953 | 0.2650828092 |
| C | -0.9453630596 | -1.4900148838 | -0.1670387356 |
| C | -2.2152437320 | 0.7321494458 | -0.2482988058 |
| C | 0.2848265544 | 0.7123847187 | -0.2912893034 |
| C | -0.9423113722 | 1.4957887160 | 0.1549406591 |
| C | 0.2808311503 | -0.7089823438 | 0.2839579658 |
| C | -2.2162966512 | -0.7253705054 | 0.2400195839 |
| H | -2.2991417315 | 0.7419365910 | -1.3400351333 |
| H | 0.2508386533 | 0.6190210644 | -1.3849366951 |
| H | -0.9151615164 | 1.6265583040 | 1.2420709846 |
| H | 0.2455834934 | -0.6201206184 | 1.3773652669 |
| H | -2.2972984364 | -0.7358718073 | 1.3318484923 |
| H | -0.9201141986 | -1.6153381625 | -1.2549798020 |
| H | -3.0996775967 | 1.2479831225 | 0.1318809499 |
| H | -0.9543198008 | 2.4979442730 | -0.2812562530 |
| H | -3.1022782429 | -1.2395734974 | -0.1386583189 |
| C | 1.6732518156 | -1.2065793975 | -0.0938450519 |
| H | 1.6737195052 | -1.5632202311 | -1.1327177547 |
| H | 2.0099162650 | -2.0321851336 | 0.5374567019 |
| C | 1.6816083500 | 1.2002918880 | 0.0969426248 |
| H | 2.0718442722 | 1.9572472258 | -0.5862646670 |
| H | 1.6642689897 | 1.6472519054 | 1.0977101255 |
| N | 2.5302684071 | -0.0157693228 | 0.0987705527 |
| H | 3.2531631580 | 0.0371693444 | -0.6020431961 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**perhydroindolizine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -0.9927804481 | -2.4575515734 | 0.3137961973 |
| C | -0.9669830337 | -1.4650450950 | -0.1421502528 |
| C | -2.1590320338 | 0.7592323850 | -0.3160701631 |
| N | 0.2785511030 | 0.6458613143 | -0.2330345594 |
| C | -0.8711684801 | 1.4465598859 | 0.1410846131 |
| C | 0.2620291409 | -0.7023206849 | 0.3327461962 |
| C | -2.2393730126 | -0.6810499953 | 0.2019667624 |
| H | -2.1818569128 | 0.7557731187 | -1.4088099842 |
| H | -0.9048113198 | 1.6075631607 | 1.2360217837 |
| H | 0.2202130363 | -0.6414154987 | 1.4397261643 |
| H | -2.3679185005 | -0.6663903940 | 1.2892577405 |
| H | -0.8956807878 | -1.6035054054 | -1.2247267471 |
| H | -3.0223329224 | 1.3351853079 | 0.0239744299 |
| H | -0.7827800790 | 2.4318328900 | -0.3217448311 |
| H | -3.1188077695 | -1.1818170302 | -0.2078302077 |
| C | 1.5847783633 | 1.1917057291 | 0.1034369505 |
| H | 1.8181267857 | 2.0546577404 | -0.5219849539 |
| H | 1.6205373564 | 1.5266716917 | 1.1553809348 |
| C | 1.6336290019 | -1.2495079762 | -0.0731629751 |
| H | 1.5692384952 | -1.7068961347 | -1.0611230323 |
| H | 1.9905706124 | -2.0101672339 | 0.6204922615 |
| C | 2.5465400268 | 0.0050620753 | -0.1114157779 |
| H | 3.0547999511 | 0.0842713714 | -1.0711146690 |
| H | 3.3146964270 | -0.0217586487 | 0.6602171194 |

**perhydrobenzimidazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -0.9169654628 | -2.5216486056 | 0.2055655051 |
| C | -0.8988592580 | -1.5066068289 | -0.1977812309 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.1826297174 | 0.7198245907 | -0.2444767469 |
| C | 0.2946274826 | 0.7020313682 | -0.2397568592 |
| C | -0.9236075729 | 1.4849875204 | 0.2068900915 |
| C | 0.2896641802 | -0.7169432982 | 0.3320492804 |
| C | -2.1865515964 | -0.7568025089 | 0.1908255852 |
| H | -2.2448143777 | 0.7689423964 | -1.3359004254 |
| H | 0.2640137638 | 0.6144351028 | -1.3331155207 |
| H | -0.9190930916 | 1.5919224305 | 1.2972664561 |
| H | 0.1661006751 | -0.6264251556 | 1.4245865959 |
| H | -2.3072445895 | -0.8063418258 | 1.2779596231 |
| H | -0.8136011146 | -1.5984953327 | -1.2840195556 |
| H | -3.0770467783 | 1.2168255981 | 0.1362557127 |
| H | -0.9168994434 | 2.4918579955 | -0.2143761445 |
| H | -3.0568082927 | -1.2595990548 | -0.2355794214 |
| N | 1.6368003425 | -1.1837764444 | -0.0143137145 |
| H | 2.0084256897 | -1.7994701548 | 0.6949380371 |
| C | 2.4800490194 | 0.0451412390 | -0.1547293274 |
| N | 1.6270248282 | 1.2159882685 | 0.0957281092 |
| H | 3.3379295745 | 0.0404348397 | 0.5194892801 |
| H | 2.8563435676 | 0.0982530863 | -1.1785274638 |
| H | 1.6459251718 | 1.4361907735 | 1.0871191341 |

**perhydro-1H-indazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8975354969 | -2.5105690787 | 0.1146330238 |
| C | -0.9019655125 | -1.4832329853 | -0.2585185881 |
| C | -2.1863076604 | 0.7440914093 | -0.1327295942 |
| C | 0.2912873242 | 0.7236159492 | -0.3114833275 |
| C | -0.8954029056 | 1.4908044773 | 0.2549617322 |
| C | 0.3141898824 | -0.7102162602 | 0.2186453059 |
| C | -2.1616843238 | -0.7489783452 | 0.2413358057 |
| H | -2.3260595636 | 0.8365828417 | -1.2142882860 |
| H | 0.1508384017 | 0.6472072750 | -1.3937837766 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8128360668 | 1.5634038910 | 1.3445509364 |
| H | 0.2820427365 | -0.6696666253 | 1.3245832056 |
| H | -2.2117402428 | -0.8436158833 | 1.3306707294 |
| H | -0.8923652992 | -1.5363882141 | -1.3502976491 |
| H | -3.0525187153 | 1.2207508603 | 0.3310799806 |
| H | -0.9292492922 | 2.5135749360 | -0.1276979771 |
| H | -3.0564771103 | -1.2376883327 | -0.1490294704 |
| N | 1.6405829199 | -1.1247408855 | -0.2369056362 |
| H | 1.9663671179 | -1.9908211268 | 0.1758000095 |
| N | 2.5205379858 | -0.0562214785 | 0.2296692924 |
| C | 1.7469340775 | 1.1822888108 | -0.0660618328 |
| H | 2.1591576529 | 1.6702526034 | -0.9492224268 |
| H | 1.8390456931 | 1.8726389976 | 0.7737192120 |
| H | 2.5568943975 | -0.1220998361 | 1.2485923315 |

**octahydro-1H-pyrrolo[2,3-b]pyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0167798184 | -2.5087405923 | 0.2602719608 |
| C | -0.9681109546 | -1.5053934002 | -0.1684906754 |
| C | -2.1236861049 | 0.7690973404 | -0.2277865988 |
| C | 0.2643834097 | 0.6779829353 | -0.2604787441 |
| N | -0.8813837136 | 1.4125490374 | 0.2279249326 |
| C | 0.2677750540 | -0.7475237092 | 0.2942892150 |
| C | -2.2062719030 | -0.6877342127 | 0.2416274204 |
| H | -2.2081158701 | 0.7875457219 | -1.3270684914 |
| H | 0.2618969529 | 0.6103439479 | -1.3657390068 |
| H | 0.2110735155 | -0.6395344642 | 1.3834410235 |
| H | -2.2974945445 | -0.7011770120 | 1.3307415190 |
| H | -0.9433337694 | -1.6276782308 | -1.2566632446 |
| H | -2.9676324757 | 1.3347048434 | 0.1688123554 |
| H | -3.1154890200 | -1.1379536719 | -0.1620931512 |
| C | 1.6805372224 | -1.2073758792 | -0.0768021089 |
| H | 1.6981406146 | -1.6392733717 | -1.0797200349 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.0726392013 | -1.9596670090 | 0.6070782047 |
| C | 2.5067711963 | 0.1227896814 | -0.0392704095 |
| H | 3.0618123807 | 0.2528479192 | -0.9693509320 |
| H | 3.2331362683 | 0.1364667023 | 0.7720898610 |
| N | 1.5502903919 | 1.2481603212 | 0.1282774035 |
| H | 1.4810537768 | 1.4837384631 | 1.1135417060 |
| H | -0.8457058105 | 2.3689156397 | -0.1063002043 |

**perhydroimidazo[1,2-a]pyrazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.7826988146 | 2.4438241201 | -0.3570300426 |
| C | -0.8404044164 | 1.4748969111 | 0.1427999066 |
| N | -2.1370778483 | -0.5910464831 | 0.3057005749 |
| C | 0.2613167004 | -0.6880995537 | 0.3303971500 |
| C | -0.9977942847 | -1.4058821559 | -0.1145385285 |
| N | 0.2906992397 | 0.6574993421 | -0.2514739824 |
| C | -2.1205708652 | 0.7528151849 | -0.2725399227 |
| H | 0.2499689451 | -0.6298129321 | 1.4328379308 |
| H | -0.9483327272 | -1.5506359807 | -1.2067672793 |
| H | -2.1660648039 | 0.7405101774 | -1.3726711905 |
| H | -0.8566837425 | 1.6576217382 | 1.2310141360 |
| H | -1.0620799948 | -2.3846757317 | 0.3609169126 |
| H | -2.9897981545 | 1.2993610089 | 0.0958727269 |
| C | 1.6310126006 | 1.1446914838 | 0.0393642411 |
| H | 1.6956472449 | 1.6018771301 | 1.0395741477 |
| H | 1.9443010289 | 1.8931573072 | -0.6901407133 |
| C | 2.4842236508 | -0.1562801932 | -0.0116221201 |
| H | 3.0990138509 | -0.2454091012 | 0.8844183450 |
| H | 3.1497588100 | -0.1822776152 | -0.8726818831 |
| N | 1.5214149664 | -1.2832564281 | -0.0793811153 |
| H | 1.4265604274 | -1.5569059041 | -1.0512325987 |
| H | -3.0074868130 | -1.0593513250 | 0.0949303051 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**octahydro-1H-purine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | -0.2467321443 | -0.7075114838 | -0.3279445765 |
| C | -2.4533336757 | -0.0181550636 | 0.1147972071 |
| C | -0.2927457499 | 0.7071445720 | 0.2509342846 |
| N | -1.5584301973 | -1.2152654483 | 0.0380471908 |
| H | -3.2702792759 | -0.0635007117 | -0.6068590967 |
| H | -0.2710514509 | 0.6149058099 | 1.3441926460 |
| H | -0.1243580231 | -0.6128159032 | -1.4209632527 |
| H | -2.8874164636 | 0.0359805552 | 1.1149874032 |
| N | 0.8966457784 | -1.4816057255 | 0.1233824856 |
| C | 2.1117752266 | -0.7121632812 | -0.1894866349 |
| H | 2.2388564407 | -0.7474915280 | -1.2746172036 |
| H | 2.9678395264 | -1.2131262303 | 0.2589569646 |
| N | 2.1487270325 | 0.6995252460 | 0.2082848136 |
| C | 0.9533561631 | 1.4660686117 | -0.1781277153 |
| H | 0.9616081883 | 1.5997855672 | -1.2653807993 |
| H | 1.0067743920 | 2.4591891605 | 0.2682121514 |
| N | -1.6283994003 | 1.1851090014 | -0.1123561787 |
| H | -1.8992337488 | -1.9008886882 | -0.6207863495 |
| H | 0.8145162951 | -1.6453029554 | 1.1224736943 |
| H | 2.2829307649 | 0.7703229901 | 1.2098095816 |
| H | -1.6383796781 | 1.4148195052 | -1.1012666159 |

**perhydropentalene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 0.5726933028 | 2.0624944308 | 1.7089818716 |
| C | -0.0710799888 | 1.2543028264 | 1.3617942812 |
| C | 0.3231300865 | 0.6916401211 | 0.0000000000 |
| C | -0.3231300865 | -0.6916401211 | 0.0000000000 |
| C | 0.0710799888 | -1.2543028264 | 1.3617942812 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0000000000 | 0.0000000000 | 2.2955834504 |
| H | -1.0906837897 | 1.6457826104 | 1.3251075042 |
| H | 1.4107268019 | 0.5350468372 | 0.0000000000 |
| H | -1.4107268019 | -0.5350468372 | 0.0000000000 |
| H | 1.0906837897 | -1.6457826104 | 1.3251075042 |
| H | -0.5726933028 | -2.0624944308 | 1.7089818716 |
| H | 0.8720361109 | 0.0448127385 | 2.9480216934 |
| H | -0.8720361109 | -0.0448127385 | 2.9480216934 |
| C | -0.0710799888 | 1.2543028264 | -1.3617942812 |
| H | 0.5726933028 | 2.0624944308 | -1.7089818716 |
| H | -1.0906837897 | 1.6457826104 | -1.3251075042 |
| C | 0.0000000000 | 0.0000000000 | -2.2955834504 |
| H | -0.8720361109 | -0.0448127385 | -2.9480216934 |
| H | 0.8720361109 | 0.0448127385 | -2.9480216934 |
| C | 0.0710799888 | -1.2543028264 | -1.3617942812 |
| H | 1.0906837897 | -1.6457826104 | -1.3251075042 |
| H | -0.5726933028 | -2.0624944308 | -1.7089818716 |

**perhydropyrrolizine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.6064452069 | 2.0131912739 | 1.7294088868 |
| C | -0.0655627989 | 1.2440155843 | 1.3505287403 |
| C | 0.3671942159 | 0.6844512362 | 0.0000000000 |
| N | -0.2597394717 | -0.6276104882 | 0.0000000000 |
| C | 0.0539120940 | -1.2277293649 | 1.2779177633 |
| C | -0.0882674636 | -0.0273521445 | 2.2552048541 |
| H | -1.0635457349 | 1.6764391245 | 1.2715675302 |
| H | 1.4726142784 | 0.5808628562 | 0.0000000000 |
| H | 1.0843950236 | -1.6239462994 | 1.3038049199 |
| H | -0.6219023336 | -2.0505954527 | 1.5140806628 |
| H | 0.7237821160 | -0.0214457144 | 2.9813859841 |
| H | -1.0200216209 | -0.0864263090 | 2.8154598007 |
| C | -0.0655627989 | 1.2440155843 | -1.3505287403 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.6064452069 | 2.0131912739 | -1.7294088868 |
| H | -1.0635457349 | 1.6764391245 | -1.2715675302 |
| C | -0.0882674636 | -0.0273521445 | -2.2552048541 |
| H | -1.0200216209 | -0.0864263090 | -2.8154598007 |
| H | 0.7237821160 | -0.0214457144 | -2.9813859841 |
| C | 0.0539120940 | -1.2277293649 | -1.2779177633 |
| H | 1.0843950236 | -1.6239462994 | -1.3038049199 |
| H | -0.6219023336 | -2.0505954527 | -1.5140806628 |

**perhydro-1,4-dihydropyrrolo[3,2-b]pyrrole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 1.2756439462 | -1.2154058855 | 0.1442525157 |
| C | 2.2272519489 | -0.0606974520 | 0.0523285843 |
| C | 1.3507692374 | 1.2287716175 | -0.0799234722 |
| C | -0.0157152957 | 0.6857816071 | 0.2984993448 |
| C | 0.0060184084 | -0.6943703457 | -0.3342384430 |
| H | 2.9041637791 | -0.1519743917 | -0.8018940690 |
| H | 2.8438290575 | -0.0274853819 | 0.9518281525 |
| H | -0.0300551283 | 0.5347867102 | 1.3841445722 |
| H | 0.0027822812 | -0.5507753429 | -1.4299616421 |
| C | -1.3614040050 | -1.2282545282 | 0.0707185428 |
| C | -2.2276526286 | 0.0895851020 | 0.0377117554 |
| H | -2.8107699966 | 0.1765590807 | 0.9549880894 |
| H | -2.9320853185 | 0.0992973497 | -0.7933401906 |
| N | -1.3023409033 | 1.2629992322 | -0.0726244944 |
| H | 1.6109899421 | -2.0057043892 | -0.3885229967 |
| H | -1.2642892838 | 1.5594831082 | -1.0419075170 |
| H | -1.7573500618 | -1.9962429829 | -0.5930497106 |
| H | -1.3190728910 | -1.6402394156 | 1.0797665579 |
| H | 1.7074495477 | 2.0349671455 | 0.5585500199 |
| H | 1.3496013641 | 1.5913971626 | -1.1105145992 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**perhydro-1,4-dihydroimidazo[4,5-d]imidazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | 1.2637701088 | -1.1668487473 | 0.2992298979 |
| C | 2.1617507258 | -0.0125088036 | -0.0116653016 |
| N | 1.2786351738 | 1.1949101772 | -0.0961220353 |
| C | -0.0246250223 | 0.6912548982 | 0.2714143633 |
| C | 0.0124777035 | -0.7078629434 | -0.2923564548 |
| H | 2.6783895431 | -0.1434618202 | -0.9703135855 |
| H | 2.9179705939 | 0.0941783094 | 0.7688795161 |
| H | -0.1419634487 | 0.5961005994 | 1.3586649051 |
| H | 0.1186352042 | -0.6356255297 | -1.3912127302 |
| N | -1.3037226340 | -1.1940889022 | 0.0724047291 |
| C | -2.1572855143 | 0.0644584466 | 0.0794546675 |
| H | -2.5784068814 | 0.1841756304 | 1.0775212135 |
| H | -2.9776276965 | 0.0064766021 | -0.6354553118 |
| N | -1.2905362307 | 1.2325028655 | -0.2126673670 |
| H | 1.6221099340 | -2.0085238375 | -0.1344767863 |
| H | -1.2216281001 | 1.3662839294 | -1.2179681740 |
| H | -1.6588263983 | -1.8517206126 | -0.6069532703 |
| H | 1.6002899392 | 1.9124507384 | 0.5378967241 |

**perhydro-N-ethylindole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -0.2693751625 | -2.4293424419 | 0.1584552846 |
| C | -0.7666889133 | -1.5419334245 | -0.2383971415 |
| C | -2.9976529557 | -0.2778584372 | -0.2463057247 |
| C | -0.8347875116 | 0.9680568996 | -0.2906353903 |
| C | -2.2823179102 | 1.0146459693 | 0.1801578521 |
| C | -0.1058646475 | -0.2600113462 | 0.2503871708 |
| C | -2.2436062215 | -1.5421207653 | 0.1940012253 |
| H | -3.0946628462 | -0.2818086265 | -1.3367006324 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8341175819 | 0.8698365577 | -1.3817662814 |
| H | -2.3140602309 | 1.1170976653 | 1.2702233083 |
| H | -0.1806892022 | -0.2443846316 | 1.3574480432 |
| H | -2.2919979339 | -1.6245954879 | 1.2846425987 |
| H | -0.6864532677 | -1.5888483203 | -1.3283324708 |
| H | -4.0139672738 | -0.2970803525 | 0.1532718412 |
| H | -2.8004184768 | 1.8844048735 | -0.2314382790 |
| H | -2.7451943993 | -2.4275452144 | -0.2018448565 |
| N | 1.2699924728 | -0.0097499360 | -0.1724741244 |
| C | 1.5161363610 | 1.4246122841 | 0.0801322688 |
| H | 2.1743983185 | 1.8376528872 | -0.6848790050 |
| H | 2.0161457819 | 1.5711444158 | 1.0496123173 |
| C | 0.1225549750 | 2.1031048703 | 0.0858138450 |
| H | 0.0675177984 | 2.9457943505 | -0.6025574301 |
| H | -0.1118478226 | 2.4822610872 | 1.0822854497 |
| C | 2.2752342868 | -0.8940786363 | 0.3921118877 |
| H | 1.9273099642 | -1.9209993005 | 0.2729249365 |
| H | 2.3899071179 | -0.7217177014 | 1.4789148521 |
| C | 3.6337010722 | -0.7544460707 | -0.2874061587 |
| H | 4.0572651153 | 0.2400331537 | -0.1438531493 |
| H | 3.5425077632 | -0.9316529171 | -1.3595873207 |
| H | 4.3405733303 | -1.4763004041 | 0.1243260836 |

**perhydro-N-ethylindazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.2932168895 | -2.4541139294 | 0.1388959565 |
| C | -0.7847038070 | -1.5574776035 | -0.2445549079 |
| C | -2.9916202614 | -0.2332793381 | -0.1480136398 |
| C | -0.8106065244 | 0.9454757269 | -0.3147513807 |
| C | -2.2255197002 | 1.0458693419 | 0.2380458312 |
| C | -0.0950270932 | -0.2890489541 | 0.2291352009 |
| C | -2.2473481691 | -1.5221760723 | 0.2416804744 |
| H | -3.1506746424 | -0.2272698467 | -1.2308995352 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8860910145 | 0.8050362748 | -1.3971580710 |
| H | -2.1974186066 | 1.1554175223 | 1.3272120792 |
| H | -0.1413671707 | -0.2654320737 | 1.3378556395 |
| H | -2.2543307500 | -1.6214245457 | 1.3317060751 |
| H | -0.7429344237 | -1.6066496059 | -1.3360511566 |
| H | -3.9836096555 | -0.2331645034 | 0.3085845624 |
| H | -2.7446199025 | 1.9234876529 | -0.1544495580 |
| H | -2.7869685099 | -2.3879616578 | -0.1471072267 |
| N | 1.2777080090 | -0.0182505206 | -0.1976978421 |
| N | 1.5056839578 | 1.3545553805 | 0.2306774808 |
| C | 0.2294900753 | 2.0567452066 | -0.0627824352 |
| H | 0.3498898222 | 2.6928250376 | -0.9397609003 |
| H | -0.0318393215 | 2.6954917252 | 0.7821388072 |
| H | 1.5954263811 | 1.3216723481 | 1.2526970966 |
| C | 2.3039102250 | -0.8864443536 | 0.3474796075 |
| H | 1.9966371547 | -1.9140159738 | 0.1487612103 |
| H | 2.3595823987 | -0.7788382913 | 1.4485136433 |
| C | 3.6734325222 | -0.6300380629 | -0.2689646400 |
| H | 3.9966439111 | 0.3928602123 | -0.0856002714 |
| H | 3.6367134091 | -0.7839534490 | -1.3474768130 |
| H | 4.4140785761 | -1.3102786473 | 0.1542617130 |

**octahydro-1Methylpurine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.2639090023 | -0.6540931032 | -0.3640054474 |
| C | -2.4666356388 | 0.0301516562 | -0.0261886824 |
| C | -0.2834284862 | 0.7179361498 | 0.3006410846 |
| N | -1.5741290312 | -1.1579816783 | -0.0211910669 |
| H | -3.1273521686 | 0.0367050074 | -0.9013203519 |
| H | -0.2526673610 | 0.5594926578 | 1.3853212417 |
| H | -0.1582366509 | -0.5007765221 | -1.4573303945 |
| H | -3.0928081665 | 0.0150724156 | 0.8688457423 |
| N | 0.8676930748 | -1.4752321765 | 0.0272257547 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 2.0921101007 | -0.7094424403 | -0.2656042633 |
| H | 2.1985673785 | -0.6849991870 | -1.3528347354 |
| H | 2.9465395177 | -1.2497447683 | 0.1380144247 |
| N | 2.1589959312 | 0.6743885433 | 0.2152111316 |
| C | 0.9700759126 | 1.4841813487 | -0.0974616623 |
| H | 0.9625382752 | 1.6915916351 | -1.1731899432 |
| H | 1.0492554097 | 2.4435338809 | 0.4141865833 |
| N | -1.6104287512 | 1.2378601965 | -0.0372147972 |
| H | 0.8013582237 | -1.6738517251 | 1.0216483993 |
| H | 2.3186416260 | 0.6838224649 | 1.2153530059 |
| H | -1.5862928573 | 1.6126053554 | -0.9788280580 |
| C | -2.0466240086 | -2.2832368254 | -0.8023574595 |
| H | -1.3109746789 | -3.0850836316 | -0.7591404343 |
| H | -2.2167681542 | -2.0273175761 | -1.8622570156 |
| H | -2.9835714943 | -2.6604226777 | -0.3905010562 |

**N-ethylperhydropurine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.1723337111 | -2.3807394498 | -0.3327856595 |
| C | -0.7161163535 | -1.4541369527 | -0.5238626209 |
| C | -2.7943996832 | -0.2932421979 | 0.1001585252 |
| C | -0.8474666091 | 0.9924251157 | -0.2166367296 |
| N | -2.0447241934 | 0.8612694443 | 0.6056447026 |
| C | 0.0188162075 | -0.2362207477 | 0.0129926653 |
| N | -1.9812757369 | -1.5012875289 | 0.2210150148 |
| H | -3.1113265043 | -0.1255316115 | -0.9515702992 |
| H | -1.1258024598 | 1.0121449877 | -1.2867921436 |
| H | 0.1121300585 | -0.3644679050 | 1.1006925688 |
| H | -0.8432952461 | -1.3541984091 | -1.6130805790 |
| H | -3.6915072069 | -0.4228721522 | 0.7051541582 |
| N | 1.2623227473 | 0.1990791130 | -0.6032111212 |
| C | 1.4279646465 | 1.5573566411 | -0.0643748332 |
| H | 2.0298631930 | 2.1684609856 | -0.7417102461 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.9239667148 | 1.5538445338 | 0.9165029800 |
| N | 0.0580523660 | 2.0945589347 | 0.0902848289 |
| H | -0.0868742434 | 2.8620014526 | -0.5492963211 |
| H | -2.5269432760 | -2.3092364539 | -0.0452015802 |
| H | -2.6200557000 | 1.6930911283 | 0.5408684246 |
| C | 2.4243052103 | -0.6773307860 | -0.5090346679 |
| H | 3.2466047398 | -0.1779005989 | -1.0281199364 |
| H | 2.2044773248 | -1.5749396887 | -1.0918753314 |
| C | 2.8917963096 | -1.0974777345 | 0.8927745363 |
| H | 3.7658574502 | -1.7452028917 | 0.8064534920 |
| H | 2.1214946778 | -1.6536448865 | 1.4276999824 |
| H | 3.1756952775 | -0.2434763414 | 1.5073271901 |

**perhydrofluorene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.3882967323 | 0.0877092503 | 2.5378638137 |
| C | -1.6902188525 | -0.2744143853 | 1.5519293923 |
| C | -3.5779495847 | -0.1762666149 | -0.1815902196 |
| C | -1.1918181852 | -0.2935312003 | -0.9190002437 |
| C | -2.5758019911 | 0.2374783523 | -1.2727048030 |
| C | -0.7359746746 | 0.2069810470 | 0.4656651398 |
| C | -3.1162081890 | 0.2096359371 | 1.2324859455 |
| H | -3.7136696977 | -1.2619327425 | -0.2274270642 |
| H | -1.2821244327 | -1.3833213420 | -0.8326425790 |
| H | -2.5405324562 | 1.3294092037 | -1.3541506095 |
| H | -0.7682912794 | 1.3058819601 | 0.4584642434 |
| H | -3.1440981525 | 1.2998691701 | 1.3316357132 |
| H | -1.6711640073 | -1.3690477942 | 1.5982847123 |
| H | -4.5576793979 | 0.2638099646 | -0.3809601369 |
| H | -2.9071281092 | -0.1383904339 | -2.2444539967 |
| H | -3.8212431933 | -0.1827042898 | 1.9689040448 |
| C | 0.7359746746 | -0.2069810470 | 0.4656651398 |
| C | 2.5758019911 | -0.2374783523 | -1.2727048030 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 3.1162081890 | -0.2096359371 | 1.2324859455 |
| C | 3.5779495847 | 0.1762666149 | -0.1815902196 |
| C | 1.6902188525 | 0.2744143853 | 1.5519293923 |
| C | 1.1918181852 | 0.2935312003 | -0.9190002437 |
| H | 2.5405324562 | -1.3294092037 | -1.3541506095 |
| H | 3.1440981525 | -1.2998691701 | 1.3316357132 |
| H | 3.7136696977 | 1.2619327425 | -0.2274270642 |
| H | 1.6711640073 | 1.3690477942 | 1.5982847123 |
| H | 1.2821244327 | 1.3833213420 | -0.8326425790 |
| H | 0.7682912794 | -1.3058819601 | 0.4584642434 |
| H | 2.9071281092 | 0.1383904339 | -2.2444539967 |
| H | 3.8212431933 | 0.1827042898 | 1.9689040448 |
| H | 4.5576793979 | -0.2638099646 | -0.3809601369 |
| H | 1.3882967323 | -0.0877092503 | 2.5378638137 |
| C | 0.0000000000 | 0.0000000000 | -1.8647573368 |
| H | -0.2026360626 | 0.8523361084 | -2.5165486841 |
| H | 0.2026360626 | -0.8523361084 | -2.5165486841 |

**perhydro-9-ethylfluorene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.8690857033 | -2.8098025308 | -0.1821944004 |
| C | -2.0260057333 | -1.7536301905 | -0.4151606839 |
| C | -3.6609535666 | 0.1956321905 | -0.1140968946 |
| C | -1.1909699057 | 0.6023643629 | -0.1014288245 |
| C | -2.5316217511 | 1.0736880342 | 0.4509571057 |
| C | -0.9449119792 | -0.8806608133 | 0.2111059745 |
| C | -3.4073235129 | -1.3060876323 | 0.0923810311 |
| H | -3.7561653267 | 0.3958156476 | -1.1864031519 |
| H | -1.2516633825 | 0.6761393360 | -1.1961963931 |
| H | -2.5198239604 | 1.0076632336 | 1.5444062036 |
| H | -0.9961591922 | -1.0156949200 | 1.3010198112 |
| H | -3.4782290681 | -1.5362486058 | 1.1606685339 |
| H | -1.9836826445 | -1.6619244968 | -1.5063597588 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -4.6168645572 | 0.4729466971 | 0.3360699265 |
| H | -2.7173313439 | 2.1223417831 | 0.2028752470 |
| H | -4.1948324782 | -1.8828941329 | -0.3979949784 |
| C | 0.5155438234 | -1.0341446947 | -0.2042308765 |
| C | 2.6029614336 | 0.3785321081 | -0.0197454895 |
| C | 2.7433619507 | -2.1682503835 | -0.3029549441 |
| C | 3.4058891959 | -0.9043402807 | 0.2613738837 |
| C | 1.2786197469 | -2.3081101836 | 0.1385558843 |
| C | 1.1628430151 | 0.1999196917 | 0.4599485793 |
| H | 2.6224018539 | 0.5973575737 | -1.0917491114 |
| H | 2.7787871279 | -2.1342382046 | -1.3969654665 |
| H | 3.5145823061 | -1.0150729825 | 1.3454935566 |
| H | 1.2321469884 | -2.4824526352 | 1.2194859579 |
| H | 1.2253430661 | -0.0364879354 | 1.5289625666 |
| H | 0.5647991502 | -0.9015176875 | -1.2945240208 |
| H | 3.0896523037 | 1.2172198481 | 0.4809363964 |
| H | 3.3156452608 | -3.0497165344 | -0.0046837227 |
| H | 4.4173818242 | -0.8060372156 | -0.1395521961 |
| H | 0.8258849990 | -3.1803304010 | -0.3398812462 |
| C | 0.0994815459 | 1.3497779864 | 0.3283260667 |
| C | 0.4213176003 | 2.5124936200 | -0.6248576078 |
| H | 0.8478994819 | 2.1221681597 | -1.5534024778 |
| H | -0.5245445914 | 2.9815979950 | -0.9124441737 |
| C | 1.3309376712 | 3.5980803252 | -0.0478174607 |
| H | 1.4850607244 | 4.4034397260 | -0.7681970456 |
| H | 2.3117434091 | 3.2126529706 | 0.2274702573 |
| H | 0.8875653729 | 4.0379611953 | 0.8482751134 |
| H | -0.0596251545 | 1.7815709762 | 1.3215208293 |

**perhydro-9H-carbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.4467566739 | -2.5482999030 | 0.0348839776 |
| C | -1.7194701128 | -1.5481532903 | -0.3107508923 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -3.5488160056 | 0.2465824161 | -0.1686197350 |
| C | -1.1498982738 | 0.9000642107 | -0.2847983177 |
| C | -2.5108346783 | 1.2934723482 | 0.2726249932 |
| C | -0.7383657759 | -0.5006937295 | 0.1996133493 |
| C | -3.1363181515 | -1.1932056590 | 0.1781627201 |
| H | -3.6876229276 | 0.3247551452 | -1.2520575224 |
| H | -1.2551736769 | 0.8398653085 | -1.3792757640 |
| H | -2.4512971636 | 1.3465072521 | 1.3633486705 |
| H | -0.7882058881 | -0.5018654439 | 1.2966486822 |
| H | -3.1701129339 | -1.3216348320 | 1.2648903500 |
| H | -1.6969537315 | -1.5753213836 | -1.4056290000 |
| H | -4.5197188239 | 0.4679077867 | 0.2795442482 |
| H | -2.8051052063 | 2.2862114205 | -0.0765525319 |
| H | -3.8641369834 | -1.8943297296 | -0.2363610486 |
| C | 0.7363595657 | -0.5069017076 | -0.1965093371 |
| C | 2.5010480291 | 1.2941244195 | -0.2458104011 |
| C | 3.1280373050 | -1.1989415044 | -0.2008365445 |
| C | 3.5444268199 | 0.2370799016 | 0.1613572603 |
| C | 1.7150117034 | -1.5652881200 | 0.2934719817 |
| C | 1.1522381726 | 0.8801922258 | 0.3171278281 |
| H | 2.4404761115 | 1.3664306486 | -1.3374793914 |
| H | 3.1540092502 | -1.3136391211 | -1.2894079186 |
| H | 3.6984746125 | 0.3011900529 | 1.2428580950 |
| H | 1.6997966094 | -1.6063025816 | 1.3879066799 |
| H | 1.2770135527 | 0.7949101889 | 1.4057566406 |
| H | 0.7844156871 | -0.4880961394 | -1.2943769745 |
| H | 2.7996837675 | 2.2775097794 | 0.1261723350 |
| H | 3.8619385275 | -1.9022922902 | 0.1986162842 |
| H | 4.5078355657 | 0.4657160184 | -0.2989594233 |
| H | 1.4430348092 | -2.5614892538 | -0.0634441588 |
| N | -0.0058217758 | 1.7673446019 | 0.0706782283 |
| H | 0.1933716939 | 2.4272479641 | -0.6689343636 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**perhydro-N-ethylcarbazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -1.7430180821 | -2.9029095523 | 0.0860098770 |
| C | -1.9279264785 | -1.8881329315 | -0.2744040110 |
| C | -3.6016275647 | 0.0502949458 | -0.1905138798 |
| C | -1.1509169770 | 0.5048958967 | -0.2497729829 |
| C | -2.4912546938 | 1.0086016875 | 0.2751040036 |
| C | -0.8762825653 | -0.9190691332 | 0.2489583024 |
| C | -3.3208709119 | -1.4164306229 | 0.1764124147 |
| H | -3.7050352895 | 0.1319239587 | -1.2774750296 |
| H | -1.2346201951 | 0.4554761736 | -1.3524375917 |
| H | -2.4516358414 | 1.0532342493 | 1.3671840843 |
| H | -0.9398270631 | -0.9054804243 | 1.3448794484 |
| H | -3.3933987771 | -1.5316872253 | 1.2626632713 |
| H | -1.8824584287 | -1.9283554148 | -1.3680391248 |
| H | -4.5610672094 | 0.3573686229 | 0.2308523851 |
| H | -2.7030144603 | 2.0208802926 | -0.0773884703 |
| H | -4.0941242149 | -2.0575883550 | -0.2526320356 |
| C | 0.5885214438 | -1.0644952370 | -0.1400741953 |
| C | 2.5150194855 | 0.5168763295 | -0.3456845961 |
| C | 2.8779242213 | -2.0298573844 | -0.1866519300 |
| C | 3.4526475027 | -0.6286737403 | 0.0837153753 |
| C | 1.4527376066 | -2.2109170630 | 0.3640274528 |
| C | 1.1593425032 | 0.2875401861 | 0.3220966814 |
| H | 2.4110621048 | 0.5259923840 | -1.4343755342 |
| H | 2.8563382831 | -2.2031832663 | -1.2673509050 |
| H | 3.6532194107 | -0.5268837205 | 1.1549802496 |
| H | 1.4689491970 | -2.2112161477 | 1.4588855920 |
| H | 1.3638062412 | 0.2105626875 | 1.3999561227 |
| H | 0.6287646484 | -1.0803582076 | -1.2380713915 |
| H | 2.9567784261 | 1.4727537234 | -0.0587049172 |
| H | 3.5467200958 | -2.7852485064 | 0.2317056769 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 4.4167542064 | -0.5255949867 | -0.4185902271 |
| H | 1.0525494403 | -3.1788026956 | 0.0528235750 |
| N | 0.0448887940 | 1.2545124678 | 0.1434832350 |
| C | 0.2838963064 | 2.5176369342 | -0.5347738652 |
| H | 0.9396083233 | 2.4033024631 | -1.4100719901 |
| H | -0.6742941334 | 2.8658683166 | -0.9246214858 |
| C | 0.8498755194 | 3.5970927636 | 0.3879795261 |
| H | 1.0043618471 | 4.5311615873 | -0.1568276853 |
| H | 1.8082373418 | 3.2977916790 | 0.8134326380 |
| H | 0.1648029375 | 3.7846912657 | 1.2151569370 |

**perhydro-1,8-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.5218801736 | -2.5635808704 | 0.0531227605 |
| C | -1.7536425518 | -1.5567350200 | -0.3012994634 |
| C | -3.4565318920 | 0.3482713883 | -0.1019648100 |
| C | -1.1447655917 | 0.8622945334 | -0.3056889608 |
| N | -2.3839118061 | 1.2392475326 | 0.3600754942 |
| C | -0.7303926922 | -0.5375856706 | 0.1796814585 |
| C | -3.1371128735 | -1.1190795947 | 0.2199372124 |
| H | -3.6213486320 | 0.4377534216 | -1.1900341958 |
| H | -1.3147501311 | 0.8003008483 | -1.3977202873 |
| H | -0.7773753589 | -0.5119201771 | 1.2737219371 |
| H | -3.1616790274 | -1.2504701778 | 1.3045399255 |
| H | -1.7577865513 | -1.5970744524 | -1.3955840711 |
| H | -4.3860809044 | 0.6386006633 | 0.3889657841 |
| H | -3.9215709472 | -1.7534109423 | -0.1981787155 |
| C | 0.7379702321 | -0.5452841414 | -0.2307144560 |
| N | 2.4101278879 | 1.2523232475 | -0.2565842690 |
| C | 3.1361449302 | -1.1304947463 | -0.2158795481 |
| C | 3.4553416275 | 0.3138362269 | 0.1910794870 |
| C | 1.7403268967 | -1.5809515786 | 0.2542399087 |
| C | 1.1310845576 | 0.8425847040 | 0.2920783627 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.1857641587 | -1.2086756753 | -1.3050327725 |
| H | 3.5808738297 | 0.3472462363 | 1.2855445275 |
| H | 1.7144470824 | -1.6457079399 | 1.3471208687 |
| H | 1.1856815130 | 0.7793220277 | 1.3932401421 |
| H | 0.7976391111 | -0.5003640279 | -1.3247677643 |
| H | 3.9095855847 | -1.7871178302 | 0.1877252246 |
| H | 4.4031143023 | 0.6221758671 | -0.2516578913 |
| H | 1.5164377944 | -2.5787880091 | -0.1288250653 |
| N | 0.0105437497 | 1.7392659451 | -0.0488987519 |
| H | 2.6412483730 | 2.1825789014 | 0.0762524427 |
| H | -2.6134354983 | 2.2051979010 | 0.1586409391 |
| H | 0.2567550007 | 2.2348644097 | -0.8972404528 |

**perhydro-N-methyl-1,8-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.5595591693 | -2.7656484751 | -0.1448494101 |
| C | -1.7745376215 | -1.7270714658 | -0.4057729593 |
| C | -3.4701187479 | 0.1599314707 | -0.0953865430 |
| C | -1.1436449585 | 0.6723020395 | -0.1283380864 |
| N | -2.4172321391 | 0.9874257251 | 0.5089124897 |
| C | -0.7581421918 | -0.7733259833 | 0.2072719870 |
| C | -3.1750891547 | -1.3328016342 | 0.1007533255 |
| H | -3.5767911812 | 0.3559231515 | -1.1762708758 |
| H | -1.2565111442 | 0.7397720999 | -1.2336066896 |
| H | -0.8150389737 | -0.8700275048 | 1.2966811312 |
| H | -3.2454980926 | -1.5646991867 | 1.1663834077 |
| H | -1.7380676799 | -1.6593156661 | -1.4980185131 |
| H | -4.4214234004 | 0.4137089006 | 0.3737219211 |
| H | -3.9439342120 | -1.9186516843 | -0.4074403405 |
| C | 0.7065502628 | -0.7534282916 | -0.2066114706 |
| N | 2.4151841406 | 0.9903319871 | -0.1127657478 |
| C | 3.0852524327 | -1.4011346936 | -0.3134952425 |
| C | 3.4449444744 | -0.0100672397 | 0.2212562775 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.6895750213 | -1.8583804978 | 0.1459312946 |
| C | 1.1413640545 | 0.5638673613 | 0.4499735487 |
| H | 3.1088049847 | -1.3751140289 | -1.4058861381 |
| H | 3.5916929217 | -0.0846087224 | 1.3115002764 |
| H | 1.6876880786 | -2.0332624645 | 1.2267073799 |
| H | 1.2583457605 | 0.3751737827 | 1.5334481566 |
| H | 0.7546311089 | -0.5962143378 | -1.2904960121 |
| H | 3.8505631495 | -2.1106423065 | 0.0076833480 |
| H | 4.3906602492 | 0.3203819048 | -0.2098579079 |
| H | 1.4252604100 | -2.8047785964 | -0.3305712067 |
| N | -0.0067151861 | 1.4872932663 | 0.2865934842 |
| C | 0.1899202740 | 2.6879019173 | -0.5052419640 |
| H | 0.4475986657 | 2.4938028844 | -1.5561473288 |
| H | -0.7265759348 | 3.2798397131 | -0.4838320939 |
| H | 0.9720631376 | 3.3128027852 | -0.0738658854 |
| H | 2.6936062127 | 1.8796987094 | 0.2859948770 |
| H | -2.6407435519 | 1.9691350807 | 0.3965935105 |

**perhydro-N-ethyl-1,8-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.7064971685 | -2.9045617345 | -0.3936100367 |
| C | -1.8679716941 | -1.8371636438 | -0.5590027037 |
| C | -3.4833759834 | 0.0898347722 | -0.1097164231 |
| C | -1.1359616988 | 0.4956296421 | -0.0322589934 |
| N | -2.4155019794 | 0.8081484971 | 0.6014239208 |
| C | -0.8303951743 | -0.9945098767 | 0.1686282337 |
| C | -3.2628442989 | -1.4269268249 | -0.0501935070 |
| H | -3.5459163999 | 0.3925854599 | -1.1690678498 |
| H | -1.2196718920 | 0.6794052748 | -1.1251681600 |
| H | -0.9259955379 | -1.1855679103 | 1.2426258417 |
| H | -3.3732282008 | -1.7542624565 | 0.9866184798 |
| H | -1.7978382694 | -1.6676809799 | -1.6384117775 |
| H | -4.4370859121 | 0.3439204595 | 0.3543665539 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -4.0434759162 | -1.9241050062 | -0.6298637663 |
| C | 0.6445175420 | -1.0083868202 | -0.2053827209 |
| N | 2.4255154520 | 0.6376132366 | 0.0084868733 |
| C | 2.9871627560 | -1.7603675605 | -0.3789568297 |
| C | 3.4130165515 | -0.4299066628 | 0.2546029360 |
| C | 1.5700962081 | -2.1882568965 | 0.0459976813 |
| C | 1.1414521553 | 0.2175998798 | 0.5728006790 |
| H | 3.0132409798 | -1.6558776844 | -1.4665566333 |
| H | 3.5643116764 | -0.5922727926 | 1.3345058534 |
| H | 1.5585120068 | -2.4587296466 | 1.1066308217 |
| H | 1.3009857745 | -0.0819722216 | 1.6278820608 |
| H | 0.7234170615 | -0.7469421577 | -1.2668719334 |
| H | 3.7185383419 | -2.5263098263 | -0.1128960255 |
| H | 4.3693469408 | -0.1106613994 | -0.1610533655 |
| H | 1.2606457698 | -3.0737042909 | -0.5132463453 |
| N | 0.0232117069 | 1.1651309292 | 0.5224748197 |
| C | 0.2249779967 | 2.5807772698 | 0.2920502696 |
| H | -0.6378587786 | 3.1180321764 | 0.6991042982 |
| H | 1.0684600434 | 2.9054416369 | 0.9071315239 |
| H | 2.7502305852 | 1.4806054137 | 0.4686746443 |
| H | -2.5979796611 | 1.8041604861 | 0.5626647138 |
| C | 0.4540028601 | 3.0268158751 | -1.1604889893 |
| H | 1.3279739931 | 2.5338497972 | -1.5829842555 |
| H | 0.6061644321 | 4.1078610237 | -1.2013521044 |
| H | -0.4057612684 | 2.7943275623 | -1.7905917845 |

**perhydrodibenzoborole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.3361796412 | 0.0601550030 | 2.4703716072 |
| C | -1.6656814442 | -0.2744047153 | 1.4832045929 |
| C | -3.6102457572 | -0.1686335300 | -0.1767322950 |
| C | -1.2396584615 | -0.1742418873 | -1.0202943329 |
| C | -2.6652660423 | 0.2992289317 | -1.2946649047 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.7312661723 | 0.2299872866 | 0.3872684912 |
| C | -3.1016838524 | 0.2090702712 | 1.2217743968 |
| H | -3.7117609167 | -1.2577627356 | -0.2362277976 |
| H | -1.2635611719 | -1.2883851080 | -1.0099176540 |
| H | -2.6799355837 | 1.3929691950 | -1.3479307032 |
| H | -0.7304830257 | 1.3289383809 | 0.4312830677 |
| H | -3.1316130514 | 1.2985687163 | 1.3308785957 |
| H | -1.6447076440 | -1.3702027169 | 1.4990620575 |
| H | -4.6108197772 | 0.2431747268 | -0.3290140145 |
| H | -3.0185081100 | -0.0613772267 | -2.2634167372 |
| H | -3.7765171600 | -0.1927295786 | 1.9810629270 |
| C | 0.7312661723 | -0.2299872866 | 0.3872684912 |
| C | 2.6652660423 | -0.2992289317 | -1.2946649047 |
| C | 3.1016838524 | -0.2090702712 | 1.2217743968 |
| C | 3.6102457572 | 0.1686335300 | -0.1767322950 |
| C | 1.6656814442 | 0.2744047153 | 1.4832045929 |
| C | 1.2396584615 | 0.1742418873 | -1.0202943329 |
| H | 2.6799355837 | -1.3929691950 | -1.3479307032 |
| H | 3.1316130514 | -1.2985687163 | 1.3308785957 |
| H | 3.7117609167 | 1.2577627356 | -0.2362277976 |
| H | 1.6447076440 | 1.3702027169 | 1.4990620575 |
| H | 1.2635611719 | 1.2883851080 | -1.0099176540 |
| H | 0.7304830257 | -1.3289383809 | 0.4312830677 |
| H | 3.0185081100 | 0.0613772267 | -2.2634167372 |
| H | 3.7765171600 | 0.1927295786 | 1.9810629270 |
| H | 4.6108197772 | -0.2431747268 | -0.3290140145 |
| H | 1.3361796412 | -0.0601550030 | 2.4703716072 |
| B | 0.0000000000 | 0.0000000000 | -1.9585902867 |
| H | 0.0000000000 | 0.0000000000 | -3.1521403069 |

**perhydro-5Me-dibenzoborole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.3303513766 | -2.7569108491 | 0.0803187104 |

Continued on Next Page...

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.6599703472 | -1.7745739060 | -0.2684269271 |
| C | -3.6068187743 | -0.1158037404 | -0.1887714873 |
| C | -1.2352654303 | 0.7290431158 | -0.2053196845 |
| C | -2.6616584464 | 1.0081082313 | 0.2653090247 |
| C | -0.7304170765 | -0.6697476736 | 0.2254216389 |
| C | -3.0981189838 | -1.5096266857 | 0.2061118291 |
| H | -3.7070020475 | -0.0695305689 | -1.2786295751 |
| H | -1.2634512291 | 0.6963555398 | -1.3167288405 |
| H | -2.6775712574 | 1.0752288767 | 1.3586288853 |
| H | -0.7371866876 | -0.6982703030 | 1.3251465773 |
| H | -3.1321917547 | -1.6066637042 | 1.2967013010 |
| H | -1.6342279565 | -1.8046885242 | -1.3638927836 |
| H | -4.6079688924 | 0.0411632471 | 0.2203333082 |
| H | -3.0199949211 | 1.9710413806 | -0.1071886257 |
| H | -3.7710883776 | -2.2738256666 | -0.1897074604 |
| C | 0.7341504064 | -0.6740723800 | -0.2243140579 |
| C | 2.6672597439 | 0.9990429666 | -0.2990111331 |
| C | 3.0995812709 | -1.5187177851 | -0.1999860636 |
| C | 3.6126263589 | -0.1192543618 | 0.1685183587 |
| C | 1.6629329736 | -1.7723767191 | 0.2849485254 |
| C | 1.2426796857 | 0.7310108799 | 0.1838125406 |
| H | 2.6781045264 | 1.0489297307 | -1.3933360467 |
| H | 3.1287478496 | -1.6347213614 | -1.2888498959 |
| H | 3.7187302764 | -0.0549337221 | 1.2569230373 |
| H | 1.6414617279 | -1.7838468000 | 1.3808530201 |
| H | 1.2766977446 | 0.7130066558 | 1.2945918780 |
| H | 0.7398612794 | -0.7197061087 | -1.3234552957 |
| H | 3.0297232097 | 1.9666724635 | 0.0567637397 |
| H | 3.7727578735 | -2.2772690906 | 0.2062188843 |
| H | 4.6119024757 | 0.0289540346 | -0.2483621698 |
| H | 1.3297740185 | -2.7597216848 | -0.0458587565 |
| B | 0.0036527667 | 1.6860756335 | -0.0213525074 |
| C | -0.0091627472 | 3.2516685535 | -0.0004728531 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.9195261413 | 3.7135410940 | -0.3403751857 |
| H | -0.1431918068 | 3.5654285223 | 1.0438332860 |
| H | -0.8445302159 | 3.6900167098 | -0.5503961955 |

**perhydro[b,d]dibenzofuran**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.4918670784 | 0.0160089986 | 2.5645199496 |
| C | -1.7386453377 | -0.3228202697 | 1.5557820812 |
| C | -3.5177591159 | -0.1516417954 | -0.2947809879 |
| C | -1.1230274097 | -0.2916626246 | -0.8673348552 |
| C | -2.4486693720 | 0.2900337171 | -1.3138582651 |
| C | -0.7370372658 | 0.1962047683 | 0.5328323814 |
| C | -3.1435766151 | 0.1740142078 | 1.1624761464 |
| H | -3.6654643880 | -1.2319597767 | -0.3909123308 |
| H | -1.2360906970 | -1.3855591967 | -0.8281069858 |
| H | -2.3776549958 | 1.3804395965 | -1.3539162138 |
| H | -0.7921821445 | 1.2927034535 | 0.5343546830 |
| H | -3.1792963309 | 1.2587187444 | 1.3051178903 |
| H | -1.7185045931 | -1.4174689833 | 1.5753635615 |
| H | -4.4766557810 | 0.3098388386 | -0.5376705710 |
| H | -2.7117392613 | -0.0555063999 | -2.3153445024 |
| H | -3.8936841832 | -0.2483641048 | 1.8344704960 |
| C | 0.7370372658 | -0.1962047683 | 0.5328323814 |
| C | 2.4486693720 | -0.2900337171 | -1.3138582651 |
| C | 3.1435766151 | -0.1740142078 | 1.1624761464 |
| C | 3.5177591159 | 0.1516417954 | -0.2947809879 |
| C | 1.7386453377 | 0.3228202697 | 1.5557820812 |
| C | 1.1230274097 | 0.2916626246 | -0.8673348552 |
| H | 2.3776549958 | -1.3804395965 | -1.3539162138 |
| H | 3.1792963309 | -1.2587187444 | 1.3051178903 |
| H | 3.6654643880 | 1.2319597767 | -0.3909123308 |
| H | 1.7185045931 | 1.4174689833 | 1.5753635615 |
| H | 1.2360906970 | 1.3855591967 | -0.8281069858 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.7921821445 | -1.2927034535 | 0.5343546830 |
| H | 2.7117392613 | 0.0555063999 | -2.3153445024 |
| H | 3.8936841832 | 0.2483641048 | 1.8344704960 |
| H | 4.4766557810 | -0.3098388386 | -0.5376705710 |
| H | 1.4918670784 | -0.0160089986 | 2.5645199496 |
| O | 0.0000000000 | 0.0000000000 | -1.7149889547 |

**perhydrodibenzothiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2566224215 | 0.1433242108 | 2.6437577195 |
| C | -1.6297596653 | -0.2454073214 | 1.6935010173 |
| C | -3.6225809227 | -0.1773616670 | 0.0893377605 |
| C | -1.2978349384 | -0.3389631486 | -0.7829321711 |
| C | -2.6879490264 | 0.2112456924 | -1.0699549119 |
| C | -0.7361517552 | 0.2032682793 | 0.5372216814 |
| C | -3.0698762311 | 0.2403550873 | 1.4595784830 |
| H | -3.7675831900 | -1.2622444894 | 0.0767512856 |
| H | -1.3731206226 | -1.4264106013 | -0.7005937701 |
| H | -2.6364121598 | 1.2985510096 | -1.1718464412 |
| H | -0.7771677709 | 1.2992681257 | 0.4918837597 |
| H | -3.0861946413 | 1.3324738446 | 1.5334720455 |
| H | -1.6114100169 | -1.3377951160 | 1.7709047634 |
| H | -4.6084562688 | 0.2664509823 | -0.0639042208 |
| H | -3.0780693473 | -0.1783386619 | -2.0121197026 |
| H | -3.7245210580 | -0.1307705320 | 2.2509806169 |
| C | 0.7361517552 | -0.2032682793 | 0.5372216814 |
| C | 2.6879490264 | -0.2112456924 | -1.0699549119 |
| C | 3.0698762311 | -0.2403550873 | 1.4595784830 |
| C | 3.6225809227 | 0.1773616670 | 0.0893377605 |
| C | 1.6297596653 | 0.2454073214 | 1.6935010173 |
| C | 1.2978349384 | 0.3389631486 | -0.7829321711 |
| H | 2.6364121598 | -1.2985510096 | -1.1718464412 |
| H | 3.0861946413 | -1.3324738446 | 1.5334720455 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.7675831900 | 1.2622444894 | 0.0767512856 |
| H | 1.6114100169 | 1.3377951160 | 1.7709047634 |
| H | 1.3731206226 | 1.4264106013 | -0.7005937701 |
| H | 0.7771677709 | -1.2992681257 | 0.4918837597 |
| H | 3.0780693473 | 0.1783386619 | -2.0121197026 |
| H | 3.7245210580 | 0.1307705320 | 2.2509806169 |
| H | 4.6084562688 | -0.2664509823 | -0.0639042208 |
| H | 1.2566224215 | -0.1433242108 | 2.6437577195 |
| S | 0.0000000000 | 0.0000000000 | -2.0623008302 |

**perhydro-3,6-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.5022416312 | -2.5211367908 | 0.0875725522 |
| C | -1.7415448124 | -1.5202767815 | -0.2771100270 |
| C | -3.5099204530 | 0.1920861157 | -0.1456044494 |
| C | -1.1492930383 | 0.9040369579 | -0.2778733552 |
| C | -2.5129577746 | 1.2776639102 | 0.2841377335 |
| C | -0.7317866449 | -0.4933985733 | 0.2127076754 |
| N | -3.0504433020 | -1.1371279211 | 0.2647245867 |
| H | -3.6516496581 | 0.2656825642 | -1.2378896711 |
| H | -1.2628375908 | 0.8348398901 | -1.3706882834 |
| H | -0.7766585108 | -0.4986221169 | 1.3069327005 |
| H | -1.7242616268 | -1.5575747800 | -1.3800864026 |
| H | -4.4827611013 | 0.3694458102 | 0.3149765252 |
| C | 0.7300190933 | -0.5001931078 | -0.2186249769 |
| C | 2.5091906836 | 1.2766268796 | -0.2462848592 |
| N | 3.0442061519 | -1.1408514335 | -0.2805350366 |
| C | 3.5047175953 | 0.1787716366 | 0.1590064614 |
| C | 1.7347863112 | -1.5384901151 | 0.2541369581 |
| C | 1.1493332835 | 0.8839541852 | 0.3025315562 |
| H | 3.6451224758 | 0.2313725173 | 1.2517636560 |
| H | 1.7180734013 | -1.5941645960 | 1.3559322060 |
| H | 1.2652295883 | 0.7920866686 | 1.3913629950 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.7751257116 | -0.4854323611 | -1.3135118450 |
| H | 4.4771112862 | 0.3657712415 | -0.2985930434 |
| H | 1.4996542749 | -2.5336531374 | -0.1278792648 |
| N | -0.0031627643 | 1.7781224986 | 0.0563130433 |
| H | -2.8450632961 | 2.2493042324 | -0.0889169384 |
| H | -2.4619990804 | 1.3388516905 | 1.3729029349 |
| H | 2.8410363638 | 2.2376177436 | 0.1540773286 |
| H | 2.4711838600 | 1.3586229452 | -1.3362854236 |
| H | 3.7419971116 | -1.8401326846 | -0.0654428656 |
| H | -3.7467096976 | -1.8329196129 | 0.0338591356 |
| H | 0.1930347899 | 2.4173885246 | -0.7023296065 |

**perhydro-4,5-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 1.6277119589 | -1.5361686030 | 0.2324156159 |
| C | 3.5051662787 | 0.1826656231 | 0.1753758121 |
| C | 1.1425360318 | 0.9210024729 | 0.2903382972 |
| C | 2.5169790644 | 1.2841278578 | -0.2528540045 |
| C | 0.7337136392 | -0.4816008998 | -0.2082483175 |
| C | 3.0051578018 | -1.2306003899 | -0.1827457592 |
| H | 3.6568840242 | 0.2421431472 | 1.2582197238 |
| H | 1.2348313302 | 0.8464992453 | 1.3852957695 |
| H | 0.7801633445 | -0.4751971146 | -1.3053408855 |
| H | 4.4829638669 | 0.3476221783 | -0.2840626941 |
| C | -0.7320274075 | -0.4863728158 | 0.1987389925 |
| C | -2.5061245962 | 1.2825837897 | 0.2327236524 |
| C | -2.9966773906 | -1.2386250556 | 0.2019504654 |
| C | -3.5011871574 | 0.1734078811 | -0.1627059594 |
| N | -1.6227548559 | -1.5530747954 | -0.2185080801 |
| C | -1.1473630532 | 0.9008648886 | -0.3270415855 |
| H | -3.6716748508 | 0.2239267217 | -1.2423608975 |
| H | -1.2689350538 | 0.8007857494 | -1.4153821467 |
| H | -0.7755001126 | -0.4600779427 | 1.2966372214 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -4.4695702785 | 0.3438233001 | 0.3140686153 |
| N | 0.0068919574 | 1.7904236080 | -0.0801655918 |
| H | -2.8432193124 | 2.2495055382 | -0.1488915996 |
| H | -2.4473540802 | 1.3679543404 | 1.3236709478 |
| H | 3.6673659067 | -1.9838332684 | 0.2464222356 |
| H | 3.0493141150 | -1.3586557840 | -1.2692719215 |
| H | -1.5792622987 | -1.6753155831 | -1.2245968184 |
| H | 1.5782607647 | -1.6403349005 | 1.2402614521 |
| H | -3.6653079695 | -1.9921120735 | -0.2163243247 |
| H | -3.0345380034 | -1.3579395157 | 1.2898363786 |
| H | 2.8481122195 | 2.2585016598 | 0.1142627385 |
| H | 2.4648421216 | 1.3566509394 | -1.3429470034 |
| H | -0.1916340046 | 2.4704668012 | 0.6408306711 |

**pyrimidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -2.1454664073 | 0.0000000000 | -1.1148667707 |
| C | -1.1802887238 | 0.0000000000 | -0.6205300403 |
| N | 1.1922501213 | 0.0000000000 | 0.7126859807 |
| N | -1.1922501213 | 0.0000000000 | 0.7126859807 |
| C | 0.0000000000 | 0.0000000000 | -1.3492461795 |
| C | 1.1802887238 | 0.0000000000 | -0.6205300403 |
| C | 0.0000000000 | 0.0000000000 | 1.3069149793 |
| H | 0.0000000000 | 0.0000000000 | -2.4298204865 |
| H | 2.1454664073 | 0.0000000000 | -1.1148667707 |
| H | 0.0000000000 | 0.0000000000 | 2.3909583473 |

**pyridazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 0.6644048378 | 0.0000000000 | 1.2216081575 |
| C | -0.6888506265 | 0.0000000000 | -1.1782054603 |
| C | 1.3187268964 | 0.0000000000 | 0.0634272412 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | -0.6644048378 | 0.0000000000 | 1.2216081575 |
| C | -1.3187268964 | 0.0000000000 | 0.0634272412 |
| C | 0.6888506265 | 0.0000000000 | -1.1782054603 |
| H | 2.3984050729 | 0.0000000000 | 0.1469585800 |
| H | -2.3984050729 | 0.0000000000 | 0.1469585800 |
| H | 1.2655869501 | 0.0000000000 | -2.0929065183 |
| H | -1.2655869501 | 0.0000000000 | -2.0929065183 |

**1,3,5-triazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | -1.3685449311 | 0.0000001370 | 0.0000000000 |
| C | 1.2904826641 | -0.0000001292 | 0.0000000000 |
| C | -0.6452416940 | -1.1175908500 | 0.0000000000 |
| C | -0.6452414702 | 1.1175909792 | 0.0000000000 |
| N | 0.6842723342 | 1.1851944637 | 0.0000000000 |
| N | 0.6842720969 | -1.1851946007 | 0.0000000000 |
| H | -1.1872440190 | 2.0563671487 | 0.0000000000 |
| H | 2.3744879498 | -0.0000002377 | 0.0000000000 |
| H | -1.1872444308 | -2.0563669110 | 0.0000000000 |

**1H-pyrrole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0132883425 | -0.9915809482 | -0.7104772925 |
| C | 0.0681608957 | 0.3175787023 | -1.1216279882 |
| N | 0.1011499627 | 1.1049863059 | 0.0000000000 |
| C | 0.0681608957 | 0.3175787023 | 1.1216279882 |
| C | 0.0132883425 | -0.9915809482 | 0.7104772925 |
| H | -0.0227713694 | -1.8524247157 | -1.3558469069 |
| H | 0.0861149436 | 0.7485018162 | -2.1069480507 |
| H | 0.0861149436 | 0.7485018162 | 2.1069480507 |
| H | -0.0227713694 | -1.8524247157 | 1.3558469069 |
| H | 0.1434484118 | 2.1072869851 | 0.0000000000 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**1H-imidazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| C | 1.1319211674 | -0.2999923147 | -0.0033713092 |
| C | 0.6344726584 | 0.9714943427 | 0.0545130224 |
| N | -0.7330505023 | 0.8212319463 | 0.0819688363 |
| C | -0.9928292443 | -0.5157939962 | 0.0402985349 |
| N | 0.1104080202 | -1.2196917943 | -0.0117054069 |
| H | 2.1633405243 | -0.6059321023 | -0.0392453587 |
| H | 1.1063622485 | 1.9367270773 | 0.0779893331 |
| H | -1.9954460669 | -0.9094300361 | 0.0504001026 |
| H | -1.4114178053 | 1.5609938773 | 0.1245162456 |

**1H-pyrazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | 0.9720421886 | -0.4423875768 | -0.0915163176 |
| N | 0.7804929765 | 0.8884959646 | -0.0745307601 |
| C | -0.5383190225 | 1.0288593543 | -0.0219190884 |
| C | -1.1979732517 | -0.2167042701 | -0.0051607622 |
| C | -0.1839176765 | -1.1457720806 | -0.0517021535 |
| H | -0.9687627174 | 2.0162242877 | 0.0020808145 |
| H | -2.2549767242 | -0.4089187334 | 0.0349371649 |
| H | -0.1962549872 | -2.2216073327 | -0.0591956138 |
| H | 1.9094362145 | -0.8002136130 | -0.1308272837 |

**1H-1,2,3-triazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | -0.4661458256 | -0.9483510151 | -0.1065185320 |
| N | -1.1411470969 | 0.2148995632 | -0.0720027228 |
| N | -0.2593201369 | 1.1637087203 | -0.0053834337 |
| C | 0.9879382682 | 0.6174671912 | 0.0044817961 |
| C | 0.8695686305 | -0.7458984118 | -0.0610706270 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 1.8724168604 | 1.2261303804 | 0.0564384182 |
| H | 1.5861532741 | -1.5460799879 | -0.0778309294 |
| H | -0.9754379737 | -1.8141974403 | -0.1601199694 |

**1H-1,2,4-triazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | 0.8261624896 | 0.6775149833 | -0.0732536584 |
| N | -0.4628462888 | 1.0865255047 | -0.0623883989 |
| C | -1.1132641224 | -0.0596570680 | -0.0029016971 |
| N | -0.3255433551 | -1.1692209397 | 0.0239405919 |
| C | 0.8895846363 | -0.6661045734 | -0.0216427401 |
| H | -2.1890167491 | -0.0988334622 | 0.0214004457 |
| H | 1.8145411911 | -1.2178645847 | -0.0195547808 |
| H | 1.5691451983 | 1.3532561400 | -0.1152787623 |

**naphthalene**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 3.3645215766 | -1.2402275820 | 0.0000000000 |
| C | 2.4238428070 | -0.7058025573 | 0.0000000000 |
| H | 1.2392614266 | -2.4798275384 | 0.0000000000 |
| C | 1.2406174149 | -1.3969645822 | 0.0000000000 |
| C | 1.2406174149 | 1.3969645822 | 0.0000000000 |
| C | 0.0000000000 | -0.7139541915 | 0.0000000000 |
| C | 2.4238428070 | 0.7058025573 | 0.0000000000 |
| C | 0.0000000000 | 0.7139541915 | 0.0000000000 |
| C | -1.2406174149 | -1.3969645822 | 0.0000000000 |
| H | 3.3645215766 | 1.2402275820 | 0.0000000000 |
| H | -1.2392614266 | 2.4798275384 | 0.0000000000 |
| H | 1.2392614266 | 2.4798275384 | 0.0000000000 |
| C | -2.4238428070 | -0.7058025573 | 0.0000000000 |
| H | -1.2392614266 | -2.4798275384 | 0.0000000000 |
| H | -3.3645215766 | -1.2402275820 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.4238428070 | 0.7058025573 | 0.0000000000 |
| H | -3.3645215766 | 1.2402275820 | 0.0000000000 |
| C | -1.2406174149 | 1.3969645822 | 0.0000000000 |

**isoquinoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.3876425423 | -1.0801058078 | 0.0000000000 |
| C | 2.4121289659 | -0.6093096780 | 0.0000000000 |
| H | 1.3315996086 | -2.4473962005 | 0.0000000000 |
| C | 1.2716538431 | -1.3667605000 | 0.0000000000 |
| C | 1.2572813257 | 1.3586618004 | 0.0000000000 |
| C | 0.0110103063 | -0.7267898023 | 0.0000000000 |
| N | 2.4172155366 | 0.7488879542 | 0.0000000000 |
| C | 0.0043139980 | 0.6954655646 | 0.0000000000 |
| C | -1.2252796880 | -1.4154964161 | 0.0000000000 |
| H | -1.2232458667 | 2.4705572066 | 0.0000000000 |
| C | -2.4055964573 | -0.7182729520 | 0.0000000000 |
| H | -1.2255805462 | -2.4979384934 | 0.0000000000 |
| H | -3.3470671454 | -1.2514424459 | 0.0000000000 |
| C | -2.4101528771 | 0.6943355266 | 0.0000000000 |
| H | -3.3529339432 | 1.2244455172 | 0.0000000000 |
| C | -1.2281926598 | 1.3878279578 | 0.0000000000 |
| H | 1.2745100570 | 2.4452887685 | 0.0000000000 |

**4H-quinolizine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.0176704482 | -0.7447053420 | 0.0000000000 |
| C | -2.4683030064 | -0.7111287829 | 0.0000000000 |
| N | -0.0703971522 | 0.6765097068 | 0.0000000000 |
| C | -1.3100597806 | -1.4009003457 | 0.0000000000 |
| H | -1.3043318954 | -2.4819104318 | 0.0000000000 |
| H | -3.4133321360 | -1.2373577677 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.1641710358 | -1.3940674291 | 0.0000000000 |
| H | 1.1341814620 | -2.4750917125 | 0.0000000000 |
| C | 2.5076576638 | -0.7177027927 | 0.0000000000 |
| H | 3.1073316309 | -1.0259677999 | -0.8687911667 |
| H | 3.1073316309 | -1.0259677999 | 0.8687911667 |
| C | 2.3326961249 | 0.7757343058 | 0.0000000000 |
| H | 3.2133134493 | 1.4040683607 | 0.0000000000 |
| C | 1.1435737845 | 1.3729066966 | 0.0000000000 |
| H | 1.0399672559 | 2.4485773967 | 0.0000000000 |
| C | -1.2649661700 | 1.3563015281 | 0.0000000000 |
| H | -1.1724167127 | 2.4327319433 | 0.0000000000 |
| C | -2.4573585347 | 0.7265462035 | 0.0000000000 |
| H | -3.3708802017 | 1.2993180628 | 0.0000000000 |

**cinnoline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 2.3307466872 | 0.8087174542 | 0.0000000000 |
| N | 1.1801993017 | 1.4067709809 | 0.0000000000 |
| C | 1.2864309387 | -1.3579570700 | 0.0000000000 |
| C | 0.0285854778 | 0.6769603455 | 0.0000000000 |
| C | 2.3907135884 | -0.5485966618 | 0.0000000000 |
| C | 0.0234383490 | -0.7442089592 | 0.0000000000 |
| C | -1.1996087951 | 1.3810506721 | 0.0000000000 |
| H | -1.2184227099 | -2.5134636510 | 0.0000000000 |
| H | 1.3822086163 | -2.4362738090 | 0.0000000000 |
| C | -2.3807965541 | 0.6909332319 | 0.0000000000 |
| H | -1.1631515296 | 2.4612992978 | 0.0000000000 |
| H | -3.3214896106 | 1.2247051349 | 0.0000000000 |
| C | -2.3873791499 | -0.7249024598 | 0.0000000000 |
| H | -3.3333495489 | -1.2496958046 | 0.0000000000 |
| C | -1.2145427820 | -1.4309579092 | 0.0000000000 |
| H | 3.3943627212 | -0.9516887927 | 0.0000000000 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**phtalazine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| N | 0.6817551513 | 0.0000000000 | 2.4235653419 |
| C | 1.3246894847 | 0.0000000000 | 1.2860513522 |
| C | -1.3246894847 | 0.0000000000 | 1.2860513522 |
| C | 0.7055726916 | 0.0000000000 | 0.0092410962 |
| N | -0.6817551513 | 0.0000000000 | 2.4235653419 |
| C | -0.7055726916 | 0.0000000000 | 0.0092410962 |
| C | 1.4051103650 | 0.0000000000 | -1.2149314263 |
| H | -2.4874012170 | 0.0000000000 | -1.2112953380 |
| H | -2.4075068439 | 0.0000000000 | 1.3610116213 |
| C | 0.7054859403 | 0.0000000000 | -2.3965485988 |
| H | 2.4874012170 | 0.0000000000 | -1.2112953380 |
| H | 1.2354931426 | 0.0000000000 | -3.3394410485 |
| C | -0.7054859403 | 0.0000000000 | -2.3965485988 |
| H | -1.2354931426 | 0.0000000000 | -3.3394410485 |
| C | -1.4051103650 | 0.0000000000 | -1.2149314263 |
| H | 2.4075068439 | 0.0000000000 | 1.3610116213 |

**quinazoline**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 3.2633700662 | -1.1843531666 | 0.0000000000 |
| C | 2.3173348222 | -0.6550314139 | 0.0000000000 |
| N | 1.2285588925 | -1.3809452058 | 0.0000000000 |
| C | 1.2702322663 | 1.3544820095 | 0.0000000000 |
| C | 0.0444754765 | -0.7095853528 | 0.0000000000 |
| N | 2.4066481217 | 0.7011073970 | 0.0000000000 |
| C | 0.0126792500 | 0.7101104314 | 0.0000000000 |
| C | -1.1752002545 | -1.4232576611 | 0.0000000000 |
| H | -1.2383026126 | 2.4710477416 | 0.0000000000 |
| H | 1.3199527725 | 2.4403299338 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.3646097248 | -0.7408736063 | 0.0000000000 |
| H | -1.1352785699 | -2.5033119355 | 0.0000000000 |
| H | -3.2980255312 | -1.2879802326 | 0.0000000000 |
| C | -2.3948129583 | 0.6721869536 | 0.0000000000 |
| H | -3.3474197470 | 1.1841153427 | 0.0000000000 |
| C | -1.2264992696 | 1.3883007651 | 0.0000000000 |

**quinoxaline**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2498780597 | 0.0000000000 | 3.2496342653 |
| C | -0.7080837417 | 0.0000000000 | 2.3096023603 |
| N | -1.4118479372 | 0.0000000000 | 1.2053159093 |
| N | 1.4118479372 | 0.0000000000 | 1.2053159093 |
| C | -0.7125313270 | 0.0000000000 | 0.0387859696 |
| C | 0.7080837417 | 0.0000000000 | 2.3096023603 |
| C | 0.7125313270 | 0.0000000000 | 0.0387859696 |
| C | -1.4055890716 | 0.0000000000 | -1.1930331485 |
| H | 1.2498780597 | 0.0000000000 | 3.2496342653 |
| H | 2.4863800865 | 0.0000000000 | -1.1673412333 |
| C | -0.7068126939 | 0.0000000000 | -2.3716404121 |
| H | -2.4863800865 | 0.0000000000 | -1.1673412333 |
| H | -1.2371734702 | 0.0000000000 | -3.3144217107 |
| C | 0.7068126939 | 0.0000000000 | -2.3716404121 |
| H | 1.2371734702 | 0.0000000000 | -3.3144217107 |
| C | 1.4055890716 | 0.0000000000 | -1.1930331485 |

**1,8-naphthyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.1910518200 | 0.0000000000 | 1.3601492408 |
| C | 2.2867909084 | 0.0000000000 | 0.7593983376 |
| N | 1.1530680933 | 0.0000000000 | 1.4181250504 |
| C | 1.2450311429 | 0.0000000000 | -1.3913347422 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.0000000000 | 0.0000000000 | 0.7019829947 |
| C | 2.3935563252 | 0.0000000000 | -0.6499524461 |
| C | 0.0000000000 | 0.0000000000 | -0.7251986279 |
| N | -1.1530680933 | 0.0000000000 | 1.4181250504 |
| H | 3.3688858196 | 0.0000000000 | -1.1161799355 |
| H | -1.2723558940 | 0.0000000000 | -2.4741411884 |
| H | 1.2723558940 | 0.0000000000 | -2.4741411884 |
| C | -2.2867909084 | 0.0000000000 | 0.7593983376 |
| H | -3.1910518200 | 0.0000000000 | 1.3601492408 |
| C | -2.3935563252 | 0.0000000000 | -0.6499524461 |
| H | -3.3688858196 | 0.0000000000 | -1.1161799355 |
| C | -1.2450311429 | 0.0000000000 | -1.3913347422 |

**1,5-naphthyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 3.3372529386 | -1.1700260431 | 0.0000000000 |
| C | 2.3697110102 | -0.6871559397 | 0.0000000000 |
| C | 1.2111812533 | -1.4147266106 | 0.0000000000 |
| N | 1.1700868987 | 1.4014288820 | 0.0000000000 |
| C | -0.0247107895 | -0.7302983520 | 0.0000000000 |
| C | 2.2940313979 | 0.7243762317 | 0.0000000000 |
| C | 0.0095177028 | 0.6926671475 | 0.0000000000 |
| N | -1.1853042637 | -1.4390563286 | 0.0000000000 |
| H | 3.2087960222 | 1.3081633781 | 0.0000000000 |
| H | -1.2174065255 | 2.4584215301 | 0.0000000000 |
| C | -2.3092228412 | -0.7620168626 | 0.0000000000 |
| H | -3.2240211771 | -1.3457562653 | 0.0000000000 |
| C | -2.3849087789 | 0.6495468124 | 0.0000000000 |
| H | -3.3524593910 | 1.1324068140 | 0.0000000000 |
| C | -1.2263989927 | 1.3771102563 | 0.0000000000 |
| H | 1.2022165358 | -2.4960386504 | 0.0000000000 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**pteridine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 3.2385741234 | -1.1797714310 | 0.0000000000 |
| C | 2.2863891417 | -0.6612056534 | 0.0000000000 |
| N | 1.1969761676 | -1.3864078004 | 0.0000000000 |
| N | 1.1383722764 | 1.4487546698 | 0.0000000000 |
| C | 0.0315948860 | -0.6924465120 | 0.0000000000 |
| C | 2.2508068853 | 0.7590827936 | 0.0000000000 |
| C | -0.0090305695 | 0.7223875644 | 0.0000000000 |
| C | -1.2131710130 | -1.3635183805 | 0.0000000000 |
| H | 3.1816918858 | 1.3168590030 | 0.0000000000 |
| N | -2.3505138297 | -0.7141961626 | 0.0000000000 |
| H | -1.2296498965 | -2.4485896654 | 0.0000000000 |
| C | -2.2704914531 | 0.6439424459 | 0.0000000000 |
| H | -3.2211190626 | 1.1641146354 | 0.0000000000 |
| N | -1.1895575417 | 1.3839684931 | 0.0000000000 |

**pyrazino[2,3-b]pyrazine**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | 3.2012844298 | -1.2497311225 | 0.0000000000 |
| C | 2.2606246492 | -0.7093131736 | 0.0000000000 |
| N | 1.1585760849 | -1.4147377019 | 0.0000000000 |
| N | 1.1585760849 | 1.4147377019 | 0.0000000000 |
| C | 0.0000000000 | -0.7118184453 | 0.0000000000 |
| C | 2.2606246492 | 0.7093131736 | 0.0000000000 |
| C | 0.0000000000 | 0.7118184453 | 0.0000000000 |
| N | -1.1585760849 | -1.4147377019 | 0.0000000000 |
| H | 3.2012844298 | 1.2497311225 | 0.0000000000 |
| C | -2.2606246492 | -0.7093131736 | 0.0000000000 |
| H | -3.2012844298 | -1.2497311225 | 0.0000000000 |
| C | -2.2606246492 | 0.7093131736 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -3.2012844298 | 1.2497311225 | 0.0000000000 |
| N | -1.1585760849 | 1.4147377019 | 0.0000000000 |

**pyrimido[4,5-d]pyrimidine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 2.3796244254 | 0.0000000000 | -0.6651881256 |
| H | 1.3184987749 | 0.0000000000 | -2.4237383816 |
| C | 1.2559943011 | 0.0000000000 | -1.3388759730 |
| N | 1.1653170155 | 0.0000000000 | 1.4071173355 |
| C | 0.0000000000 | 0.0000000000 | -0.6973918763 |
| C | 2.2628304129 | 0.0000000000 | 0.6910432253 |
| C | 0.0000000000 | 0.0000000000 | 0.7169297334 |
| C | -1.2559943011 | 0.0000000000 | -1.3388759730 |
| H | 3.2008905369 | 0.0000000000 | 1.2340569909 |
| N | -2.3796244254 | 0.0000000000 | -0.6651881256 |
| H | -1.3184987749 | 0.0000000000 | -2.4237383816 |
| C | -2.2628304129 | 0.0000000000 | 0.6910432253 |
| N | -1.1653170155 | 0.0000000000 | 1.4071173355 |
| H | -3.2008905369 | 0.0000000000 | 1.2340569909 |

**benzo[b]thiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.5438440000 | -2.4455990000 | 0.0000000000 |
| C | -1.4000230000 | -1.3728900000 | 0.0000000000 |
| C | -1.0357600000 | 1.4218570000 | 0.0000000000 |
| C | -0.1014710000 | -0.8430330000 | 0.0000000000 |
| C | -2.4861450000 | -0.5190080000 | 0.0000000000 |
| C | -2.3055940000 | 0.8714770000 | 0.0000000000 |
| C | 0.0595710000 | 0.5602660000 | 0.0000000000 |
| H | -3.4889200000 | -0.9246940000 | 0.0000000000 |
| H | -3.1690780000 | 1.5229840000 | 0.0000000000 |
| H | -0.8986890000 | 2.4945680000 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.1608140000 | -1.5268440000 | 0.0000000000 |
| H | 1.2579360000 | -2.6027980000 | 0.0000000000 |
| C | 2.2178340000 | -0.6832230000 | 0.0000000000 |
| H | 3.2644960000 | -0.9384930000 | 0.0000000000 |
| S | 1.7536390000 | 0.9961850000 | 0.0000000000 |

**1H-indole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.9024286322 | -2.4903481074 | 0.0746878951 |
| C | -0.9247166399 | -1.4084980280 | 0.0502771237 |
| C | -0.9915634242 | 1.4270185347 | -0.0139005601 |
| C | 0.2491484546 | -0.6571751919 | 0.0544577883 |
| C | -2.1249408594 | -0.7201587312 | 0.0136045958 |
| C | -2.1578667300 | 0.6843260175 | -0.0181593173 |
| C | 0.2403813531 | 0.7607655673 | 0.0227658836 |
| H | -3.0546415673 | -1.2730935693 | 0.0093152862 |
| H | -3.1144474547 | 1.1886868775 | -0.0463496643 |
| H | -1.0286405368 | 2.5083973482 | -0.0385222928 |
| N | 1.5666622226 | -1.0546325592 | 0.0869699011 |
| H | 1.8881271543 | -2.0043986749 | 0.1118295222 |
| C | 2.3789723751 | 0.0595822975 | 0.0765083630 |
| H | 3.4501618770 | -0.0454653244 | 0.0979756389 |
| C | 1.6092321512 | 1.1856421195 | 0.0377907478 |
| H | 1.9745222567 | 2.1981044242 | 0.0219690887 |

**2H-isoindole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.9914748910 | -0.0135805163 | 1.4257552931 |
| C | -2.1575094484 | 0.0128473986 | -0.7127782809 |
| C | 0.2393129339 | -0.0414850109 | -0.7232451851 |
| C | -0.9914748910 | -0.0135805163 | -1.4257552931 |
| C | 0.2393129339 | -0.0414850109 | 0.7232451851 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.1575094484 | 0.0128473986 | 0.7127782809 |
| H | -1.0045528692 | -0.0132661157 | -2.5081295101 |
| H | -3.1055715248 | 0.0343167868 | 1.2338852951 |
| H | -1.0045528692 | -0.0132661157 | 2.5081295101 |
| H | -3.1055715248 | 0.0343167868 | -1.2338852951 |
| C | 1.5676518063 | -0.0717943954 | 1.1311461261 |
| H | 2.0128405251 | -0.0817688414 | 2.1096504881 |
| C | 1.5676518063 | -0.0717943954 | -1.1311461261 |
| H | 2.0128405251 | -0.0817688414 | -2.1096504881 |
| N | 2.3314253554 | -0.0891999610 | 0.0000000000 |
| H | 3.3359865808 | -0.1122866540 | 0.0000000000 |

**indolizine(delta-coniceine)**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.0267672828 | -2.4659343540 | -0.2051772982 |
| C | -0.9998338090 | -1.4042575283 | -0.0031918401 |
| C | -2.0793579855 | 0.7078783073 | 0.4455413142 |
| N | 0.2812702692 | 0.6198642062 | 0.3310036087 |
| C | -0.8772613188 | 1.3330619545 | 0.5153879936 |
| C | 0.2584691036 | -0.7669531355 | 0.0666473181 |
| C | -2.1481576208 | -0.6892109218 | 0.1811237595 |
| H | -0.7593717189 | 2.3879246444 | 0.7123054524 |
| H | -3.1113351864 | -1.1762031053 | 0.1278250247 |
| H | -2.9795569210 | 1.2854633915 | 0.5932910772 |
| C | 1.5841319705 | 1.0463364791 | 0.3586661295 |
| H | 1.8240171862 | 2.0778038415 | 0.5460589384 |
| C | 1.5790734937 | -1.1777044854 | -0.0665864621 |
| H | 1.9013701983 | -2.1836676140 | -0.2723675797 |
| C | 2.3932464638 | -0.0454028584 | 0.1163277415 |
| H | 3.4693451571 | -0.0188108182 | 0.0768778031 |

**1H-benzo[d]imidazole**

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
| H | -0.9025316802 | -2.5151119053 | -0.0600900391 |
| C | -0.9119446537 | -1.4335860789 | -0.0397744206 |
| C | -0.9534036488 | 1.4169468367 | 0.0140095443 |
| C | 0.2605009258 | -0.6846183162 | -0.0446433339 |
| C | -2.1039893379 | -0.7264125374 | -0.0074183861 |
| C | -2.1243408853 | 0.6776814833 | 0.0190701611 |
| C | 0.2582302893 | 0.7258744859 | -0.0183183051 |
| H | -3.0400676491 | -1.2682627558 | -0.0024481490 |
| H | -3.0777264473 | 1.1878577997 | 0.0439004438 |
| H | -0.9635980955 | 2.4977201224 | 0.0342662322 |
| N | 1.5977406929 | -1.0282183241 | -0.0726980885 |
| H | 1.9819922140 | -1.9557187738 | -0.0947133607 |
| N | 1.5586725914 | 1.2081776974 | -0.0302393140 |
| C | 2.3098498829 | 0.1452358241 | -0.0622566367 |
| H | 3.3884358017 | 0.1460044420 | -0.0796483477 |

**1H-indazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.9111178462 | -2.5020392698 | 0.0000000000 |
| C | -0.9231542159 | -1.4205911744 | 0.0000000000 |
| C | -0.9706825583 | 1.4277666172 | 0.0000000000 |
| C | 0.2582215774 | -0.6716347451 | 0.0000000000 |
| C | -2.1108999623 | -0.7173548036 | 0.0000000000 |
| C | -2.1377326372 | 0.6923406626 | 0.0000000000 |
| C | 0.2522226609 | 0.7418530145 | 0.0000000000 |
| H | -3.0466783322 | -1.2601195194 | 0.0000000000 |
| H | -3.0930600682 | 1.1990537551 | 0.0000000000 |
| H | -0.9979964558 | 2.5092636656 | 0.0000000000 |
| N | 1.5727051124 | -1.0339175756 | 0.0000000000 |
| H | 1.9667022179 | -1.9566807979 | 0.0000000000 |
| N | 2.4054160736 | 0.0351392536 | 0.0000000000 |
| C | 1.6321209302 | 1.0993587274 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 2.0734935036 | 2.0825591897 | 0.0000000000 |

**1H-pyrrolo[2,3-b]pyridine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | -0.8583051272 | -1.4313290106 | 0.0000000000 |
| C | -1.0130511981 | 1.4107814947 | 0.0000000000 |
| C | 0.2103721389 | -0.6464909373 | 0.0000000000 |
| C | -2.0225010822 | -0.7843114724 | 0.0000000000 |
| C | -2.1456550210 | 0.6121193122 | 0.0000000000 |
| C | 0.2285155431 | 0.7740685273 | 0.0000000000 |
| H | -2.9115119949 | -1.4040691564 | 0.0000000000 |
| H | -3.1322497797 | 1.0539192736 | 0.0000000000 |
| H | -1.0926345851 | 2.4902053883 | 0.0000000000 |
| N | 1.5142424503 | -1.0736174016 | 0.0000000000 |
| H | 1.7948279914 | -2.0377904821 | 0.0000000000 |
| C | 2.3469830786 | 0.0250284359 | 0.0000000000 |
| H | 3.4160383394 | -0.1001956126 | 0.0000000000 |
| C | 1.6036292238 | 1.1713103073 | 0.0000000000 |
| H | 1.9941070229 | 2.1743783336 | 0.0000000000 |

**imidazo[1,2-a]pyrazine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.8370601997 | -2.4523862407 | 0.0000000000 |
| C | -0.8883920952 | -1.3746696910 | 0.0000000000 |
| N | -2.1036628392 | 0.6996248981 | 0.0000000000 |
| C | 0.2864808516 | 0.7208975255 | 0.0000000000 |
| C | -0.9724488222 | 1.3578781583 | 0.0000000000 |
| N | 0.2930191576 | -0.6795338255 | 0.0000000000 |
| C | -2.0471284010 | -0.6640973717 | 0.0000000000 |
| H | -1.0012776729 | 2.4410324656 | 0.0000000000 |
| H | -2.9936504169 | -1.1863263049 | 0.0000000000 |
| C | 1.6061858762 | -1.0619634985 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.9053500623 | -2.0941429731 | 0.0000000000 |
| C | 2.3278397500 | 0.1153328233 | 0.0000000000 |
| H | 3.4013879225 | 0.2114898396 | 0.0000000000 |
| N | 1.5219268269 | 1.2045651950 | 0.0000000000 |

**7H-purine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.9629672313 | -1.3777152392 | 0.0495530332 |
| C | -2.0232306194 | 0.6527452556 | -0.0218647796 |
| C | 0.2075749356 | 0.7221933077 | 0.0233223042 |
| N | -0.9316697034 | 1.4094901984 | -0.0172994089 |
| C | 0.2372934568 | -0.6887672490 | 0.0582706944 |
| N | -2.0995890221 | -0.6890188698 | 0.0089208405 |
| H | -2.9715048845 | 1.1751115469 | -0.0546094117 |
| H | -1.0297636568 | -2.4602115892 | 0.0743171778 |
| N | 1.5754368361 | -1.0150408992 | 0.0942892549 |
| C | 2.2581991875 | 0.1745189268 | 0.0797652040 |
| H | 3.3364580951 | 0.1970605829 | 0.1018902801 |
| N | 1.4909448417 | 1.2286006024 | 0.0379511943 |
| H | 1.9811237783 | -1.9338735900 | 0.1243209741 |

**1,4-dihydropentalene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.3413203522 | 1.1981084792 | 0.0000000000 |
| C | -0.0144542616 | 0.6778925260 | 0.0000000000 |
| C | 0.0144542616 | -0.6778925260 | 0.0000000000 |
| C | 1.4349455295 | -1.1496864188 | 0.0000000000 |
| C | 2.1996011074 | 0.1563879165 | 0.0000000000 |
| H | 1.6196262955 | 2.2419402954 | 0.0000000000 |
| H | 1.6794587667 | -1.7597232287 | -0.8759428567 |
| H | 1.6794587667 | -1.7597232287 | 0.8759428567 |
| H | 3.2770833178 | 0.2155079701 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -1.4349455295 | 1.1496864188 | 0.0000000000 |
| H | -1.6794587667 | 1.7597232287 | -0.8759428567 |
| H | -1.6794587667 | 1.7597232287 | 0.8759428567 |
| C | -2.1996011074 | -0.1563879165 | 0.0000000000 |
| H | -3.2770833178 | -0.2155079701 | 0.0000000000 |
| C | -1.3413203522 | -1.1981084792 | 0.0000000000 |
| H | -1.6196262955 | -2.2419402954 | 0.0000000000 |

**1H-pyrrolizine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.3346637841 | 1.1758317122 | 0.0000000000 |
| C | 0.0392819489 | 0.7250451906 | 0.0000000000 |
| N | 0.0746765506 | -0.6539144556 | 0.0000000000 |
| C | 1.3715417484 | -1.0995381325 | 0.0000000000 |
| C | 2.1727063139 | 0.0195988051 | 0.0000000000 |
| H | 1.6610073014 | 2.2015878165 | 0.0000000000 |
| H | 1.6149890193 | -2.1467383430 | 0.0000000000 |
| H | 3.2495441456 | 0.0141471366 | 0.0000000000 |
| C | -1.4017700992 | 1.1495904515 | 0.0000000000 |
| H | -1.6658278125 | 1.7475247150 | -0.8771496022 |
| H | -1.6658278125 | 1.7475247150 | 0.8771496022 |
| C | -2.1175255808 | -0.1890371121 | 0.0000000000 |
| H | -3.1877146107 | -0.3085475082 | 0.0000000000 |
| C | -1.2249082787 | -1.1824417767 | 0.0000000000 |
| H | -1.3804396177 | -2.2485132142 | 0.0000000000 |

**1,4-dihydropyrrolo[3,2-b]pyrrole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.3265372456 | -1.1774090454 | 0.0000000000 |
| C | 2.1187425754 | -0.0495657617 | 0.0000000000 |
| N | 1.3286179922 | 1.0841305460 | 0.0000000000 |
| C | 0.0089046330 | 0.6960191860 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.0089046330 | -0.6960191860 | 0.0000000000 |
| H | 3.1915930085 | 0.0308911366 | 0.0000000000 |
| N | -1.3286179922 | -1.0841305460 | 0.0000000000 |
| C | -2.1187425754 | 0.0495657617 | 0.0000000000 |
| H | -3.1915930085 | -0.0308911366 | 0.0000000000 |
| C | -1.3265372456 | 1.1774090454 | 0.0000000000 |
| H | -1.6746523311 | -2.0244708162 | 0.0000000000 |
| H | 1.6746523311 | 2.0244708162 | 0.0000000000 |
| H | 1.6832035007 | -2.1925755403 | 0.0000000000 |
| H | -1.6832035007 | 2.1925755403 | 0.0000000000 |

**1,4-dihydroimidazo[4,5-d]imidazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 1.2767527909 | -1.1954378525 | -0.0632665450 |
| C | 2.0270698628 | -0.1117693450 | 0.0358058686 |
| N | 1.3057735600 | 1.0616207589 | 0.1101007772 |
| C | -0.0164284943 | 0.6837798128 | 0.0517785684 |
| C | 0.0164284943 | -0.6837798128 | -0.0517785684 |
| H | 3.1035565448 | -0.1113469775 | 0.0594536343 |
| N | -1.3057735600 | -1.0616207589 | -0.1101007772 |
| C | -2.0270698628 | 0.1117693450 | -0.0358058686 |
| H | -3.1035565448 | 0.1113469775 | -0.0594536343 |
| N | -1.2767527909 | 1.1954378525 | 0.0632665450 |
| H | -1.6844137819 | -1.9885487074 | -0.1855782455 |
| H | 1.6844137819 | 1.9885487074 | 0.1855782455 |

**N-ethylindole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.5735549293 | -1.4188884306 | 0.0738327103 |
| C | -2.6979824894 | -0.3389398097 | -0.4050164390 |
| C | -0.7689216745 | 1.0328746960 | -0.0076841183 |
| C | -2.1334703130 | 0.9192205116 | -0.3017507787 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.0046553948 | -0.1490624395 | 0.1798155749 |
| C | -1.9248274254 | -1.4967875912 | -0.2183946677 |
| H | -2.3932861629 | -2.4679422040 | -0.3058988770 |
| H | 0.0128207423 | -2.3171888424 | 0.2126545718 |
| H | -3.7507255739 | -0.4378464005 | -0.6335300667 |
| H | -2.7373527671 | 1.8057656839 | -0.4467370493 |
| N | 1.2903641463 | 0.2284724805 | 0.4701503482 |
| C | 1.3518298977 | 1.6072071314 | 0.4562421170 |
| H | 2.2852852244 | 2.1045973827 | 0.6613769008 |
| C | 0.1253612258 | 2.1351761331 | 0.1739084930 |
| H | -0.1128810143 | 3.1832092726 | 0.1128792486 |
| C | 2.4190627136 | -0.6629847518 | 0.6716903394 |
| H | 2.0788949312 | -1.5158586531 | 1.2613812076 |
| H | 3.1506991303 | -0.1326644761 | 1.2819630409 |
| C | 3.0627937452 | -1.1404868353 | -0.6293839071 |
| H | 3.4416275932 | -0.2973569944 | -1.2072649858 |
| H | 2.3449232681 | -1.6786913661 | -1.2475314718 |
| H | 3.8971118863 | -1.8098092172 | -0.4137512813 |

**N-ethylindazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.4504549234 | -2.4513853371 | 0.0000000000 |
| C | -0.9520197157 | -1.4938253370 | 0.0000000000 |
| C | -2.2953833601 | 1.0181236644 | 0.0000000000 |
| C | -0.2406941771 | -0.2875986233 | 0.0000000000 |
| C | -2.3302317152 | -1.4108720744 | 0.0000000000 |
| C | -2.9980672055 | -0.1691723031 | 0.0000000000 |
| C | -0.8945121264 | 0.9661962584 | 0.0000000000 |
| H | -2.9148124724 | -2.3212045448 | 0.0000000000 |
| H | -4.0794483240 | -0.1545464908 | 0.0000000000 |
| H | -2.8138305329 | 1.9677700745 | 0.0000000000 |
| N | 1.0989117857 | -0.0264607874 | 0.0000000000 |
| N | 1.3413215895 | 1.3068834835 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 0.1700082935 | 1.9089775483 | 0.0000000000 |
| H | 0.1212716911 | 2.9855902762 | 0.0000000000 |
| C | 2.1754838372 | -1.0108158197 | 0.0000000000 |
| H | 2.0529607850 | -1.6492036988 | -0.8791688155 |
| H | 2.0529607850 | -1.6492036988 | 0.8791688155 |
| C | 3.5597346886 | -0.3843983443 | 0.0000000000 |
| H | 4.3046114736 | -1.1804987462 | 0.0000000000 |
| H | 3.7133858116 | 0.2377432503 | 0.8790478616 |
| H | 3.7133858116 | 0.2377432503 | -0.8790478616 |

**N-methylpurine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.7304145824 | -1.4568204739 | 0.0000000000 |
| C | -2.4671391934 | 0.0382389076 | 0.0000000000 |
| C | -0.4194529271 | 0.9283323766 | 0.0000000000 |
| N | -1.7327200943 | 1.1454794442 | 0.0000000000 |
| C | 0.1307548472 | -0.3730566438 | 0.0000000000 |
| N | -2.0426524418 | -1.2372038009 | 0.0000000000 |
| H | -3.5418629588 | 0.1736221794 | 0.0000000000 |
| H | -0.3935097936 | -2.4879257365 | 0.0000000000 |
| N | 1.4973368810 | -0.1958397244 | 0.0000000000 |
| C | 1.6857980687 | 1.1624658601 | 0.0000000000 |
| H | 2.6832843876 | 1.5756677298 | 0.0000000000 |
| N | 0.5866800575 | 1.8686347033 | 0.0000000000 |
| C | 2.5191349247 | -1.2235815867 | 0.0000000000 |
| H | 3.4967009793 | -0.7473810478 | 0.0000000000 |
| H | 2.4362489227 | -1.8512570935 | -0.8875876660 |
| H | 2.4362489227 | -1.8512570935 | 0.8875876660 |

**N-ethylpurine**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -0.6833361031 | -1.4606173815 | 0.1863080771 |

Continued on Next Page...

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -2.7128200232 | -0.4708386368 | -0.2022463888 |
| C | -0.9684927483 | 0.9150613157 | -0.0531512730 |
| N | -2.2800276596 | 0.7843321252 | -0.2399693874 |
| C | -0.1209955983 | -0.1951624642 | 0.1645594336 |
| N | -1.9941561017 | -1.5885295130 | 0.0001267454 |
| H | -3.7756377697 | -0.6184200807 | -0.3509780762 |
| H | -0.1098667211 | -2.3670466759 | 0.3487854836 |
| N | 1.1441790127 | 0.3315980234 | 0.3241074478 |
| C | 0.9876999240 | 1.6875412548 | 0.1915885083 |
| H | 1.8387174834 | 2.3467046357 | 0.2774079238 |
| N | -0.2381692168 | 2.0820585669 | -0.0300090803 |
| C | 2.3942892766 | -0.3874773575 | 0.5342635912 |
| H | 3.1088030542 | 0.3277653201 | 0.9414329666 |
| H | 2.2271919527 | -1.1420339540 | 1.3044631660 |
| C | 2.9456416423 | -1.0282134439 | -0.7364359771 |
| H | 3.8784065282 | -1.5479121724 | -0.5154688016 |
| H | 3.1459091602 | -0.2742785274 | -1.4975146849 |
| H | 2.2459059074 | -1.7525970344 | -1.1520606740 |

**9H-fluorene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.3119043545 | 0.0000000000 | 2.5289475456 |
| C | -1.6473136605 | 0.0000000000 | 1.4999514642 |
| C | -2.5358034799 | 0.0000000000 | -1.1664785171 |
| C | -0.7329294847 | 0.0000000000 | 0.4508786283 |
| C | -3.0067449394 | 0.0000000000 | 1.2073433752 |
| C | -3.4493241280 | 0.0000000000 | -0.1140519417 |
| C | -1.1806546438 | 0.0000000000 | -0.8808435344 |
| H | -3.7289922349 | 0.0000000000 | 2.0129430716 |
| H | -4.5106822126 | 0.0000000000 | -0.3236440980 |
| H | -2.8867213462 | 0.0000000000 | -2.1909737510 |
| C | 0.7329294847 | 0.0000000000 | 0.4508786283 |
| C | 3.4493241280 | 0.0000000000 | -0.1140519417 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.6473136605 | 0.0000000000 | 1.4999514642 |
| C | 1.1806546438 | 0.0000000000 | -0.8808435344 |
| C | 2.5358034799 | 0.0000000000 | -1.1664785171 |
| C | 3.0067449394 | 0.0000000000 | 1.2073433752 |
| H | 1.3119043545 | 0.0000000000 | 2.5289475456 |
| H | 2.8867213462 | 0.0000000000 | -2.1909737510 |
| H | 3.7289922349 | 0.0000000000 | 2.0129430716 |
| H | 4.5106822126 | 0.0000000000 | -0.3236440980 |
| C | 0.0000000000 | 0.0000000000 | -1.8238126941 |
| H | 0.0000000000 | 0.8767215555 | -2.4778838957 |
| H | 0.0000000000 | -0.8767215555 | -2.4778838957 |

**9-ethylfluorene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.6598050624 | -2.8744522927 | -1.3087103370 |
| C | 0.3276450839 | -1.9009703102 | -1.6453919621 |
| C | -0.5389383913 | 0.6187668669 | -2.5346674817 |
| C | -0.0059894195 | -0.9050731511 | -0.7328262079 |
| C | 0.2274696859 | -1.6280769039 | -3.0053623158 |
| C | -0.2023116885 | -0.3789148363 | -3.4482312453 |
| C | -0.4385382777 | 0.3542501307 | -1.1786911375 |
| H | 0.4845399598 | -2.3922141498 | -3.7269239903 |
| H | -0.2761209418 | -0.1828314205 | -4.5096544003 |
| H | -0.8745563331 | 1.5855064320 | -2.8890668872 |
| C | -0.0059894195 | -0.9050731511 | 0.7328262079 |
| C | -0.2023116885 | -0.3789148363 | 3.4482312453 |
| C | 0.3276450839 | -1.9009703102 | 1.6453919621 |
| C | -0.4385382777 | 0.3542501307 | 1.1786911375 |
| C | -0.5389383913 | 0.6187668669 | 2.5346674817 |
| C | 0.2274696859 | -1.6280769039 | 3.0053623158 |
| H | 0.6598050624 | -2.8744522927 | 1.3087103370 |
| H | -0.8745563331 | 1.5855064320 | 2.8890668872 |
| H | 0.4845399598 | -2.3922141498 | 3.7269239903 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.2761209418 | -0.1828314205 | 4.5096544003 |
| C | -0.7504784984 | 1.2578266969 | 0.0000000000 |
| C | -0.0093019080 | 2.6124176316 | 0.0000000000 |
| H | -0.3398310664 | 3.1819502128 | 0.8723024648 |
| H | -0.3398310664 | 3.1819502128 | -0.8723024648 |
| C | 1.5154385081 | 2.5143362154 | 0.0000000000 |
| H | 1.8805688274 | 1.9859318869 | 0.8809937604 |
| H | 1.9623085772 | 3.5093258276 | 0.0000000000 |
| H | 1.8805688274 | 1.9859318869 | -0.8809937604 |
| H | -1.8238716692 | 1.4809747094 | 0.0000000000 |

**N-ethylcarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.3066840104 | -3.0812115012 | -1.3970709307 |
| C | 0.1631292934 | -2.0489630262 | -1.6886859644 |
| C | -0.2079771966 | 0.6434829905 | -2.4728586817 |
| C | 0.0251256893 | -1.0541821644 | -0.7218849342 |
| C | 0.1156278709 | -1.7007093241 | -3.0300943797 |
| C | -0.0676828942 | -0.3671061829 | -3.4137369184 |
| C | -0.1642505067 | 0.2899750727 | -1.1256762182 |
| H | 0.2228067282 | -2.4635088361 | -3.7890632683 |
| H | -0.0984305666 | -0.1162929025 | -4.4657014049 |
| H | -0.3418389940 | 1.6694683350 | -2.7864335741 |
| C | 0.0251256893 | -1.0541821644 | 0.7218849342 |
| C | -0.0676828942 | -0.3671061829 | 3.4137369184 |
| C | 0.1631292934 | -2.0489630262 | 1.6886859644 |
| C | -0.1642505067 | 0.2899750727 | 1.1256762182 |
| C | -0.2079771966 | 0.6434829905 | 2.4728586817 |
| C | 0.1156278709 | -1.7007093241 | 3.0300943797 |
| H | 0.3066840104 | -3.0812115012 | 1.3970709307 |
| H | -0.3418389940 | 1.6694683350 | 2.7864335741 |
| H | 0.2228067282 | -2.4635088361 | 3.7890632683 |
| H | -0.0984305666 | -0.1162929025 | 4.4657014049 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | -0.2884112359 | 1.0896532163 | 0.0000000000 |
| C | -0.4690995985 | 2.5292212469 | 0.0000000000 |
| H | -1.0674625069 | 2.7916952809 | 0.8731281817 |
| H | -1.0674625069 | 2.7916952809 | -0.8731281817 |
| C | 0.8427162490 | 3.3138790667 | 0.0000000000 |
| H | 1.4381822231 | 3.0790655718 | 0.8820620055 |
| H | 0.6410962787 | 4.3862248406 | 0.0000000000 |
| H | 1.4381822231 | 3.0790655718 | -0.8820620055 |

**N-methyl-1,8-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 0.0157532838 | -2.8552735197 | -1.5017356694 |
| C | 0.0069101152 | -1.7968209961 | -1.7272670357 |
| N | -0.0152199578 | 0.9687530129 | -2.3645277625 |
| C | 0.0000636117 | -0.8423576405 | -0.7198666849 |
| C | 0.0019814616 | -1.3489403980 | -3.0435843777 |
| C | -0.0098707317 | 0.0221034005 | -3.3067000256 |
| C | -0.0114399174 | 0.5223284596 | -1.1182206226 |
| H | 0.0075919525 | -2.0490907816 | -3.8666761652 |
| H | -0.0143180080 | 0.3752341043 | -4.3312751351 |
| C | 0.0000636117 | -0.8423576405 | 0.7198666849 |
| C | -0.0098707317 | 0.0221034005 | 3.3067000256 |
| C | 0.0069101152 | -1.7968209961 | 1.7272670357 |
| C | -0.0114399174 | 0.5223284596 | 1.1182206226 |
| N | -0.0152199578 | 0.9687530129 | 2.3645277625 |
| C | 0.0019814616 | -1.3489403980 | 3.0435843777 |
| H | 0.0157532838 | -2.8552735197 | 1.5017356694 |
| H | 0.0075919525 | -2.0490907816 | 3.8666761652 |
| H | -0.0143180080 | 0.3752341043 | 4.3312751351 |
| N | -0.0243774976 | 1.3315532121 | 0.0000000000 |
| C | -0.0061253106 | 2.7804612789 | 0.0000000000 |
| H | -0.5129485436 | 3.1368486254 | 0.8927468848 |
| H | -0.5129485436 | 3.1368486254 | -0.8927468848 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.0163732630 | 3.1628839752 | 0.0000000000 |

**N-ethyl-1,8-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -0.3274169681 | -3.0999060970 | -1.5012123974 |
| C | -0.1747993187 | -2.0525236584 | -1.7270372538 |
| N | 0.2238943489 | 0.6840448419 | -2.3648356009 |
| C | -0.0388133711 | -1.1074156014 | -0.7198400085 |
| C | -0.1080129716 | -1.6099186003 | -3.0434379119 |
| C | 0.0902492816 | -0.2532570390 | -3.3067167591 |
| C | 0.1587887885 | 0.2431281238 | -1.1178245095 |
| H | -0.2082600532 | -2.3029064805 | -3.8664937113 |
| H | 0.1428948859 | 0.0957101837 | -4.3313823423 |
| C | -0.0388133711 | -1.1074156014 | 0.7198400085 |
| C | 0.0902492816 | -0.2532570390 | 3.3067167591 |
| C | -0.1747993187 | -2.0525236584 | 1.7270372538 |
| C | 0.1587887885 | 0.2431281238 | 1.1178245095 |
| N | 0.2238943489 | 0.6840448419 | 2.3648356009 |
| C | -0.1080129716 | -1.6099186003 | 3.0434379119 |
| H | -0.3274169681 | -3.0999060970 | 1.5012123974 |
| H | -0.2082600532 | -2.3029064805 | 3.8664937113 |
| H | 0.1428948859 | 0.0957101837 | 4.3313823423 |
| N | 0.2809678554 | 1.0444040706 | 0.0000000000 |
| C | 0.4799577722 | 2.4875175481 | 0.0000000000 |
| H | 1.0668511777 | 2.7275531491 | 0.8848347016 |
| H | 1.0668511777 | 2.7275531491 | -0.8848347016 |
| C | -0.8303574603 | 3.2701612627 | 0.0000000000 |
| H | -1.4203169542 | 3.0380854489 | -0.8862385309 |
| H | -0.6229718587 | 4.3412255753 | 0.0000000000 |
| H | -1.4203169542 | 3.0380854489 | 0.8862385309 |

**5H-dibenzoborole**

Continued on Next Page. . .

**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
| H | -1.2528245953 | 0.0000000000 | 2.4415044785 |
| C | -1.6148371411 | 0.0000000000 | 1.4213125443 |
| C | -2.6005108970 | 0.0000000000 | -1.2065078972 |
| C | -0.7433186452 | 0.0000000000 | 0.3484413226 |
| C | -2.9926038769 | 0.0000000000 | 1.1731741860 |
| C | -3.4853743564 | 0.0000000000 | -0.1245374249 |
| C | -1.2299050651 | 0.0000000000 | -0.9833631301 |
| H | -3.6826415817 | 0.0000000000 | 2.0070828858 |
| H | -4.5537337566 | 0.0000000000 | -0.2943948635 |
| H | -2.9876955764 | 0.0000000000 | -2.2180020788 |
| C | 0.7433186452 | 0.0000000000 | 0.3484413226 |
| C | 3.4853743564 | 0.0000000000 | -0.1245374249 |
| C | 1.6148371411 | 0.0000000000 | 1.4213125443 |
| C | 1.2299050651 | 0.0000000000 | -0.9833631301 |
| C | 2.6005108970 | 0.0000000000 | -1.2065078972 |
| C | 2.9926038769 | 0.0000000000 | 1.1731741860 |
| H | 1.2528245953 | 0.0000000000 | 2.4415044785 |
| H | 2.9876955764 | 0.0000000000 | -2.2180020788 |
| H | 3.6826415817 | 0.0000000000 | 2.0070828858 |
| H | 4.5537337566 | 0.0000000000 | -0.2943948635 |
| B | 0.0000000000 | 0.0000000000 | -1.9384213280 |
| H | 0.0000000000 | 0.0000000000 | -3.1275767173 |

**dibenzo-5Me-borole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2450673200 | -2.7690330196 | 0.0000000000 |
| C | -1.6100371570 | -1.7498959274 | 0.0000000000 |
| C | -2.5941601735 | 0.8752458787 | 0.0000000000 |
| C | -0.7388398623 | -0.6747549416 | 0.0000000000 |
| C | -2.9866800298 | -1.5049292720 | 0.0000000000 |
| C | -3.4788848326 | -0.2064736146 | 0.0000000000 |
| C | -1.2232370822 | 0.6554314304 | 0.0000000000 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -3.6764457657 | -2.3390461687 | 0.0000000000 |
| H | -4.5473251210 | -0.0361524343 | 0.0000000000 |
| H | -2.9865202120 | 1.8852982896 | 0.0000000000 |
| C | 0.7465028652 | -0.6796239823 | 0.0000000000 |
| C | 3.4903094216 | -0.2236624526 | 0.0000000000 |
| C | 1.6128276499 | -1.7583694048 | 0.0000000000 |
| C | 1.2389257255 | 0.6476813620 | 0.0000000000 |
| C | 2.6105810127 | 0.8619649832 | 0.0000000000 |
| C | 2.9909221420 | -1.5193771608 | 0.0000000000 |
| H | 1.2442686900 | -2.7762574526 | 0.0000000000 |
| H | 3.0062879061 | 1.8706555465 | 0.0000000000 |
| H | 3.6764216235 | -2.3570438568 | 0.0000000000 |
| H | 4.5595688647 | -0.0588676377 | 0.0000000000 |
| B | 0.0133158045 | 1.6241498046 | 0.0000000000 |
| C | 0.0012794081 | 3.1861042561 | 0.0000000000 |
| H | 0.9888539892 | 3.6480233080 | 0.0000000000 |
| H | -0.5464332735 | 3.5639932334 | 0.8700601184 |
| H | -0.5464332735 | 3.5639932334 | -0.8700601184 |

**dibenzo[b,d]furan**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.4654793533 | 0.0000000000 | 2.5592977280 |
| C | -1.7199672914 | 0.0000000000 | 1.5079276099 |
| C | -2.4133576566 | 0.0000000000 | -1.2435397730 |
| C | -0.7243127255 | 0.0000000000 | 0.5318341814 |
| C | -3.0479247250 | 0.0000000000 | 1.1040286278 |
| C | -3.3890953599 | 0.0000000000 | -0.2528541787 |
| C | -1.0975807341 | 0.0000000000 | -0.8199047933 |
| H | -3.8332470464 | 0.0000000000 | 1.8474310879 |
| H | -4.4322091639 | 0.0000000000 | -0.5385207803 |
| H | -2.6638473781 | 0.0000000000 | -2.2944972619 |
| C | 0.7243127255 | 0.0000000000 | 0.5318341814 |
| C | 3.3890953599 | 0.0000000000 | -0.2528541787 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | 1.7199672914 | 0.0000000000 | 1.5079276099 |
| C | 1.0975807341 | 0.0000000000 | -0.8199047933 |
| C | 2.4133576566 | 0.0000000000 | -1.2435397730 |
| C | 3.0479247250 | 0.0000000000 | 1.1040286278 |
| H | 1.4654793533 | 0.0000000000 | 2.5592977280 |
| H | 2.6638473781 | 0.0000000000 | -2.2944972619 |
| H | 3.8332470464 | 0.0000000000 | 1.8474310879 |
| H | 4.4322091639 | 0.0000000000 | -0.5385207803 |
| O | 0.0000000000 | 0.0000000000 | -1.6467788956 |

**dibenzo[b,d]thiophene**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.2232811117 | 0.0000000000 | 2.6610785609 |
| C | -1.6073944566 | 0.0000000000 | 1.6496089655 |
| C | -2.6286478462 | 0.0000000000 | -0.9677089589 |
| C | -0.7250928805 | 0.0000000000 | 0.5649036063 |
| C | -2.9737729295 | 0.0000000000 | 1.4270595651 |
| C | -3.4822623862 | 0.0000000000 | 0.1244362948 |
| C | -1.2560692636 | 0.0000000000 | -0.7389065161 |
| H | -3.6548264806 | 0.0000000000 | 2.2671302721 |
| H | -4.5520899030 | 0.0000000000 | -0.0347091328 |
| H | -3.0221586679 | 0.0000000000 | -1.9749056836 |
| C | 0.7250928805 | 0.0000000000 | 0.5649036063 |
| C | 3.4822623862 | 0.0000000000 | 0.1244362948 |
| C | 1.6073944566 | 0.0000000000 | 1.6496089655 |
| C | 1.2560692636 | 0.0000000000 | -0.7389065161 |
| C | 2.6286478462 | 0.0000000000 | -0.9677089589 |
| C | 2.9737729295 | 0.0000000000 | 1.4270595651 |
| H | 1.2232811117 | 0.0000000000 | 2.6610785609 |
| H | 3.0221586679 | 0.0000000000 | -1.9749056836 |
| H | 3.6548264806 | 0.0000000000 | 2.2671302721 |
| H | 4.5520899030 | 0.0000000000 | -0.0347091328 |
| S | 0.0000000000 | 0.0000000000 | -1.9715079466 |

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**Table S9** – Continued

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|

**9H-carbazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -1.4061314923 | 0.0000000000 | 2.5492435215 |
| C | -1.6938772423 | 0.0000000000 | 1.5060536445 |
| C | -2.4730852356 | 0.0000000000 | -1.2147670047 |
| C | -0.7232565693 | 0.0000000000 | 0.5041667303 |
| C | -3.0338216209 | 0.0000000000 | 1.1498833597 |
| C | -3.4162402075 | 0.0000000000 | -0.1974707336 |
| C | -1.1297745141 | 0.0000000000 | -0.8517098930 |
| H | -3.7946388546 | 0.0000000000 | 1.9183288391 |
| H | -4.4678386606 | 0.0000000000 | -0.4513240184 |
| H | -2.7758026739 | 0.0000000000 | -2.2536887426 |
| C | 0.7232565693 | 0.0000000000 | 0.5041667303 |
| C | 3.4162402075 | 0.0000000000 | -0.1974707336 |
| C | 1.6938772423 | 0.0000000000 | 1.5060536445 |
| C | 1.1297745141 | 0.0000000000 | -0.8517098930 |
| C | 2.4730852356 | 0.0000000000 | -1.2147670047 |
| C | 3.0338216209 | 0.0000000000 | 1.1498833597 |
| H | 1.4061314923 | 0.0000000000 | 2.5492435215 |
| H | 2.7758026739 | 0.0000000000 | -2.2536887426 |
| H | 3.7946388546 | 0.0000000000 | 1.9183288391 |
| H | 4.4678386606 | 0.0000000000 | -0.4513240184 |
| N | 0.0000000000 | 0.0000000000 | -1.6486825309 |
| H | 0.0000000000 | 0.0000000000 | -2.6518148745 |

**1,8-diazacarbazole**

| Atom | *x* (Å) | *y* (Å) | *z* (Å) |
|---|---|---|---|
| H | -1.5035184768 | 0.0000000000 | 2.5720371984 |
| C | -1.7288427574 | 0.0000000000 | 1.5136152156 |
| N | -2.3677840238 | 0.0000000000 | -1.2534217702 |
| C | -0.7211455610 | 0.0000000000 | 0.5581367909 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| C | -3.0444739040 | 0.0000000000 | 1.0654484320 |
| C | -3.3091369107 | 0.0000000000 | -0.3057317588 |
| C | -1.1235266813 | 0.0000000000 | -0.8043813493 |
| H | -3.8674215836 | 0.0000000000 | 1.7657191677 |
| H | -4.3338628078 | 0.0000000000 | -0.6579823186 |
| C | 0.7211455610 | 0.0000000000 | 0.5581367909 |
| C | 3.3091369107 | 0.0000000000 | -0.3057317588 |
| C | 1.7288427574 | 0.0000000000 | 1.5136152156 |
| C | 1.1235266813 | 0.0000000000 | -0.8043813493 |
| N | 2.3677840238 | 0.0000000000 | -1.2534217702 |
| C | 3.0444739040 | 0.0000000000 | 1.0654484320 |
| H | 1.5035184768 | 0.0000000000 | 2.5720371984 |
| H | 3.8674215836 | 0.0000000000 | 1.7657191677 |
| H | 4.3338628078 | 0.0000000000 | -0.6579823186 |
| N | 0.0000000000 | 0.0000000000 | -1.6019833281 |
| H | 0.0000000000 | 0.0000000000 | -2.6072818873 |

**3,6-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | -1.4673749250 | 0.0000000000 | 2.5299545116 |
| C | -1.7193177481 | 0.0000000000 | 1.4751869057 |
| C | -2.4753429270 | 0.0000000000 | -1.1833918164 |
| C | -0.7237671925 | 0.0000000000 | 0.5013347598 |
| N | -3.0147986894 | 0.0000000000 | 1.1747592587 |
| C | -3.3665008406 | 0.0000000000 | -0.1200260570 |
| C | -1.1265280144 | 0.0000000000 | -0.8524953534 |
| H | -4.4321296677 | 0.0000000000 | -0.3174326644 |
| C | 0.7237671925 | 0.0000000000 | 0.5013347598 |
| C | 3.3665008406 | 0.0000000000 | -0.1200260570 |
| C | 1.7193177481 | 0.0000000000 | 1.4751869057 |
| C | 1.1265280144 | 0.0000000000 | -0.8524953534 |
| C | 2.4753429270 | 0.0000000000 | -1.1833918164 |
| N | 3.0147986894 | 0.0000000000 | 1.1747592587 |

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**Table S9** – Continued

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| H | 1.4673749250 | 0.0000000000 | 2.5299545116 |
| H | 4.4321296677 | 0.0000000000 | -0.3174326644 |
| N | 0.0000000000 | 0.0000000000 | -1.6498483325 |
| H | 2.8269916622 | 0.0000000000 | -2.2058728774 |
| H | -2.8269916622 | 0.0000000000 | -2.2058728774 |
| H | 0.0000000000 | 0.0000000000 | -2.6538050023 |

**4,5-diazacarbazole**

| Atom | $x$ (Å) | $y$ (Å) | $z$ (Å) |
|---|---|---|---|
| N | 1.5844915471 | 0.0000000000 | 1.5110683072 |
| C | 2.4748732380 | 0.0000000000 | -1.1904560334 |
| C | 0.7250698918 | 0.0000000000 | 0.4923090659 |
| C | 2.8742229381 | 0.0000000000 | 1.1924977772 |
| C | 3.3588033849 | 0.0000000000 | -0.1226639464 |
| C | 1.1250864089 | 0.0000000000 | -0.8678166354 |
| H | 4.4259082881 | 0.0000000000 | -0.2962698864 |
| C | -0.7250698918 | 0.0000000000 | 0.4923090659 |
| C | -3.3588033849 | 0.0000000000 | -0.1226639464 |
| N | -1.5844915471 | 0.0000000000 | 1.5110683072 |
| C | -1.1250864089 | 0.0000000000 | -0.8678166354 |
| C | -2.4748732380 | 0.0000000000 | -1.1904560334 |
| C | -2.8742229381 | 0.0000000000 | 1.1924977772 |
| H | -4.4259082881 | 0.0000000000 | -0.2962698864 |
| N | 0.0000000000 | 0.0000000000 | -1.6690759059 |
| H | 2.8234437666 | 0.0000000000 | -2.2149715632 |
| H | -3.5730451164 | 0.0000000000 | 2.0210086577 |
| H | 3.5730451164 | 0.0000000000 | 2.0210086577 |
| H | -2.8234437666 | 0.0000000000 | -2.2149715632 |
| H | 0.0000000000 | 0.0000000000 | -2.6728725803 |