## Supporting Materials for the Article

# Theoretical Explanation of Reactivity and Stability of Phosphorus(V) Porphyrins

Ivan N. Meshkov,[a@] Alexander G. Martynov,[a] Aslan Yu. Tsivadze,[a,b] and Yulia G. Gorbunova[a,b]

[a]*A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of Russian Academy of Sciences, 119071 Moscow, Russia*
[b]*N.S. Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences, 119991 Moscow, Russia*
[@]*Corresponding author E-mail: ivan.n.meshkov@gmail.com*

# Теоретическое объяснение особенностей реакционной способности и устойчивости порфиринатов фосфора(V)

И. Н. Мешков,[a@] А. Г. Мартынов,[a] А. Ю. Цивадзе,[a,b] Ю. Г. Горбунова[a,b]

[a]*Институт физической химии и электрохимии им. А.Н. Фрумкина Российской Академии Наук, 119071 Москва, Россия*
[b]*Институт общей и неорганической химии им. Н.С. Курнакова Российской Академии Наук, 119071 Москва, Россия*
[@]*E-mail: ivan.n.meshkov@gmail.com*

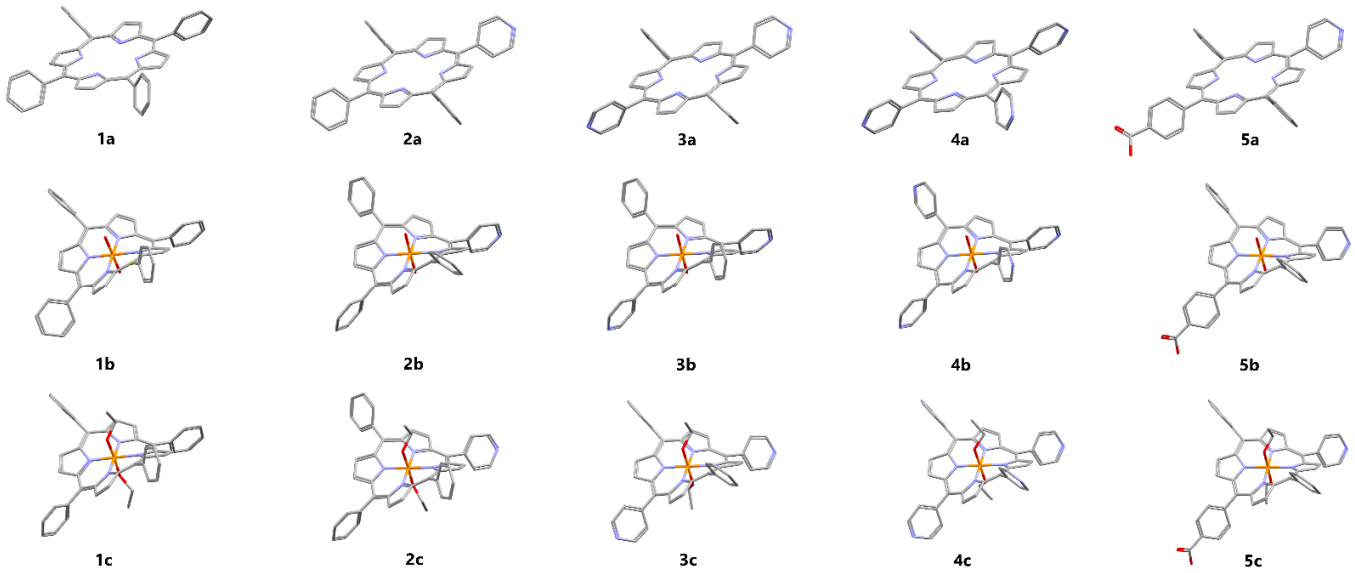


**Figure S1.** Optimized geometry of the studied P(V) porphyrins **1a-5c**.

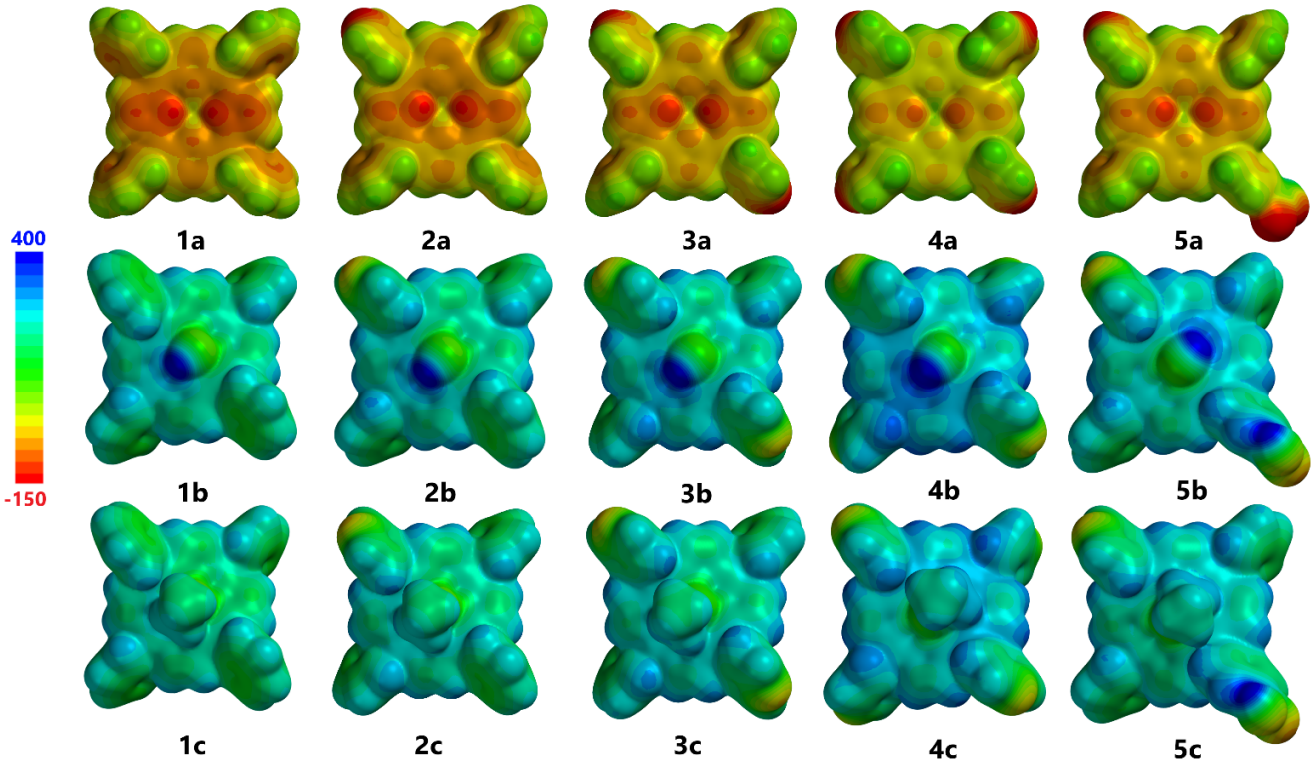


**Figure S2.** The comparative calculated electrostatic potential maps of the studied porphyrins **1a-5c**; the range of the potential is -150 – 400 kJ/mol.

Calculated atom coordinates and total energies.

Compound **1a**.
Total energy: -1913.8043027 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 0.688349 | -4.24487 | -0.16438 |
| C1 | -0.68108 | -4.24581 | -0.16324 |
| C2 | -1.12985 | -2.88967 | -0.03772 |
| N3 | 0.001819 | -2.10926 | 0.023511 |
| C4 | 1.134752 | -2.88782 | -0.03934 |
| C5 | 4.257671 | 0.680512 | 0.200711 |
| C6 | 4.258605 | -0.67336 | 0.19957 |
| C7 | 2.865588 | -1.0849 | 0.053196 |
| N8 | 2.039643 | 0.001876 | -0.01339 |
| C9 | 2.863785 | 1.089609 | 0.054751 |
| C10 | 2.465415 | -2.43768 | 0.004237 |
| C11 | -0.68835 | 4.24487 | -0.16438 |
| C12 | 0.681076 | 4.245811 | -0.16324 |
| C13 | 1.129849 | 2.88967 | -0.03772 |
| N14 | -0.00182 | 2.109261 | 0.023511 |
| C15 | -1.13475 | 2.887819 | -0.03934 |
| C16 | 2.461013 | 2.441998 | 0.007115 |
| C17 | -4.25767 | -0.68051 | 0.200711 |
| C18 | -4.2586 | 0.673364 | 0.19957 |
| C19 | -2.86559 | 1.084904 | 0.053196 |
| N20 | -2.03964 | -0.00188 | -0.01339 |
| C21 | -2.86378 | -1.08961 | 0.054751 |
| C22 | -2.46101 | -2.442 | 0.007115 |
| C23 | -2.46542 | 2.437676 | 0.004237 |
| C24 | 3.522192 | 3.498615 | 0.00077 |
| C25 | 3.528592 | -3.49226 | -0.00489 |
| C26 | -3.52219 | -3.49862 | 0.00077 |
| C27 | -3.52859 | 3.492264 | -0.00489 |
| C28 | 3.656029 | 4.390819 | 1.07675 |
| C29 | 4.644832 | 5.37527 | 1.070105 |
| C30 | 5.517304 | 5.486354 | -0.01398 |
| C31 | 5.394862 | 4.605977 | -1.09054 |
| C32 | 4.406613 | 3.621167 | -1.083 |
| C33 | 3.665477 | -4.38583 | 1.069594 |
| C34 | 4.655743 | -5.36879 | 1.059977 |
| C35 | 5.526701 | -5.47694 | -0.02559 |
| C36 | 5.401308 | -4.59509 | -1.10064 |
| C37 | 4.411606 | -3.61178 | -1.09012 |
| C38 | -3.66548 | 4.385828 | 1.069594 |

| | | | |
|---|---|---|---|
| C39 | -4.65574 | 5.368793 | 1.059977 |
| C40 | -5.5267 | 5.476941 | -0.02559 |
| C41 | -5.40131 | 4.595094 | -1.10064 |
| C42 | -4.41161 | 3.611778 | -1.09012 |
| C43 | -3.65603 | -4.39082 | 1.07675 |
| C44 | -4.64483 | -5.37527 | 1.070105 |
| C45 | -5.5173 | -5.48635 | -0.01398 |
| C46 | -5.39486 | -4.60598 | -1.09054 |
| C47 | -4.40661 | -3.62117 | -1.083 |
| H48 | 1.3447 | -5.09714 | -0.25618 |
| H49 | -1.33607 | -5.09925 | -0.25397 |
| H50 | 0.001268 | -1.09496 | 0.059123 |
| H51 | 5.102702 | 1.345076 | 0.308593 |
| H52 | 5.10479 | -1.33665 | 0.306375 |
| H53 | -1.3447 | 5.097137 | -0.25618 |
| H54 | 1.33607 | 5.099255 | -0.25397 |
| H55 | -0.00127 | 1.094964 | 0.059123 |
| H56 | -5.1027 | -1.34508 | 0.308593 |
| H57 | -5.10479 | 1.336654 | 0.306375 |
| H58 | 2.98571 | 4.300749 | 1.927197 |
| H59 | 4.736509 | 6.051686 | 1.915985 |
| H60 | 6.287571 | 6.253064 | -0.01956 |
| H61 | 6.066467 | 4.687668 | -1.94123 |
| H62 | 4.309194 | 2.942245 | -1.92561 |
| H63 | 2.996319 | -4.29806 | 1.921199 |
| H64 | 4.749717 | -6.04634 | 1.904696 |
| H65 | 6.298089 | -6.2425 | -0.03351 |
| H66 | 6.071753 | -4.67449 | -1.95246 |
| H67 | 4.311869 | -2.93171 | -1.93153 |
| H68 | -2.99632 | 4.298062 | 1.921199 |
| H69 | -4.74972 | 6.046338 | 1.904696 |
| H70 | -6.29809 | 6.242502 | -0.03351 |
| H71 | -6.07175 | 4.674486 | -1.95246 |
| H72 | -4.31187 | 2.931714 | -1.93153 |
| H73 | -2.98571 | -4.30075 | 1.927197 |
| H74 | -4.73651 | -6.05169 | 1.915985 |
| H75 | -6.28757 | -6.25306 | -0.01956 |
| H76 | -6.06647 | -4.68767 | -1.94123 |
| H77 | -4.30919 | -2.94225 | -1.92561 |

Compound **2a**.
Total energy: -1929.838105 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 0.133562 | -4.30539 | 0.065316 |
| C1 | -1.22352 | -4.12729 | 0.075878 |
| C2 | -1.49114 | -2.72141 | -0.01163 |
| N3 | -0.26772 | -2.09415 | -0.07585 |
| C4 | 0.752667 | -3.01507 | -0.02971 |
| C5 | 4.320365 | 0.123508 | -0.01918 |
| C6 | 4.14817 | -1.21886 | -0.03151 |
| C7 | 2.706157 | -1.44757 | -0.01877 |
| N8 | 2.023503 | -0.26478 | -0.0162 |
| C9 | 2.983231 | 0.709198 | -0.01751 |
| C10 | 2.129429 | -2.73618 | -0.02132 |
| C11 | -0.1328 | 4.30044 | -0.07438 |
| C12 | 1.22478 | 4.123629 | -0.07796 |
| C13 | 1.492599 | 2.718139 | 0.013937 |
| N14 | 0.270449 | 2.09012 | 0.075156 |
| C15 | -0.75091 | 3.010444 | 0.021718 |
| C16 | 2.755077 | 2.101107 | -0.00583 |
| C17 | -4.31711 | -0.12486 | 0.025719 |
| C18 | -4.14391 | 1.217502 | 0.035184 |
| C19 | -2.70228 | 1.445447 | 0.018672 |
| N20 | -2.01995 | 0.26108 | 0.015817 |
| C21 | -2.98006 | -0.71104 | 0.021742 |
| C22 | -2.75222 | -2.10418 | 0.012394 |
| C23 | -2.12854 | 2.734829 | 0.014467 |
| C24 | 3.941546 | 3.016607 | -0.02466 |
| C25 | 3.04423 | -3.91969 | 0.012829 |
| C26 | -3.93937 | -3.01865 | 0.037878 |
| C27 | -3.04419 | 3.920215 | -0.02535 |
| C28 | 4.250811 | 3.804714 | 1.09451 |
| C29 | 5.35313 | 4.659662 | 1.082594 |
| C30 | 6.163294 | 4.74321 | -0.05093 |
| C31 | 5.864209 | 3.966914 | -1.1718 |
| C32 | 4.762429 | 3.111307 | -1.15937 |
| C33 | -3.13921 | 4.794303 | 1.068768 |
| C34 | -3.99081 | 5.898719 | 1.026465 |
| C35 | -4.76039 | 6.148492 | -0.11069 |
| C36 | -4.67381 | 5.287148 | -1.20579 |
| C37 | -3.82284 | 4.182884 | -1.16328 |
| C38 | -4.25478 | -3.8085 | -1.0783 |
| C39 | -5.35753 | -4.66283 | -1.05925 |

| | | | |
|---|---|---|---|
| C40 | -6.16198 | -4.7439 | 0.07848 |
| C41 | -5.8569 | -3.96553 | 1.196334 |
| C42 | -4.7548 | -3.11053 | 1.17674 |
| C43 | 3.126627 | -4.81751 | -1.06048 |
| C44 | 3.993195 | -5.90695 | -0.97319 |
| N45 | 4.769438 | -6.16242 | 0.087596 |
| C46 | 4.688438 | -5.30237 | 1.111202 |
| C47 | 3.85538 | -4.1844 | 1.125059 |
| H48 | 0.669006 | -5.23901 | 0.140693 |
| H49 | -1.98179 | -4.89033 | 0.158181 |
| H50 | 0.138426 | 1.085651 | 0.12273 |
| H51 | 5.250478 | 0.671421 | -0.01026 |
| H52 | 4.912104 | -1.98165 | -0.05011 |
| H53 | -0.67171 | 5.231712 | -0.15309 |
| H54 | 1.983306 | 4.886592 | -0.15878 |
| H55 | -0.13533 | -1.0896 | -0.12207 |
| H56 | -5.24727 | -0.67279 | 0.020213 |
| H57 | -4.9048 | 1.983267 | 0.05305 |
| H58 | 3.624877 | 3.735799 | 1.979199 |
| H59 | 5.580507 | 5.257049 | 1.960863 |
| H60 | 7.021786 | 5.408318 | -0.06094 |
| H61 | 6.486346 | 4.02964 | -2.05999 |
| H62 | 4.527412 | 2.512733 | -2.0344 |
| H63 | -2.5479 | 4.59706 | 1.958136 |
| H64 | -4.05608 | 6.560996 | 1.885007 |
| H65 | -5.42278 | 7.008575 | -0.14321 |
| H66 | -5.26575 | 5.476423 | -2.09668 |
| H67 | -3.75183 | 3.516575 | -2.01763 |
| H68 | -3.63333 | -3.74154 | -1.9663 |
| H69 | -5.58951 | -5.26184 | -1.9352 |
| H70 | -7.0206 | -5.40873 | 0.094123 |
| H71 | -6.47454 | -4.02626 | 2.087805 |
| H72 | -4.51519 | -2.51024 | 2.049343 |
| H73 | 2.530629 | -4.66172 | -1.95417 |
| H74 | 4.069287 | -6.60835 | -1.80245 |
| H75 | 5.320419 | -5.51967 | 1.970631 |
| H76 | 3.830869 | -3.52865 | 1.989264 |

Compound **3a**.
Total energy: -1945.872570 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | -0.51188 | -4.27468 | 0.08233 |
| C1 | -1.82766 | -3.89711 | 0.089226 |
| C2 | -1.88294 | -2.46687 | -0.0003 |
| N3 | -0.58 | -2.02822 | -0.0551 |
| C4 | 0.291735 | -3.09035 | -0.00873 |
| C5 | 4.290866 | -0.5235 | -0.01049 |
| C6 | 3.91946 | -1.82468 | -0.02342 |
| C7 | 2.458775 | -1.83443 | -0.01018 |
| N8 | 1.961569 | -0.5623 | -0.00867 |
| C9 | 3.056441 | 0.25545 | -0.00682 |
| C10 | 1.695023 | -3.02086 | -0.00624 |
| C11 | 0.517248 | 4.276279 | 0.034755 |
| C12 | 1.832722 | 3.897769 | 0.037864 |
| C13 | 1.885489 | 2.464733 | 0.040991 |
| N14 | 0.581948 | 2.025424 | 0.034191 |
| C15 | -0.28831 | 3.089684 | 0.019123 |
| C16 | 3.040413 | 1.666146 | 0.020709 |
| C17 | -4.28285 | 0.522666 | -0.13297 |
| C18 | -3.91062 | 1.823831 | -0.13066 |
| C19 | -2.45435 | 1.833181 | -0.02122 |
| N20 | -1.95937 | 0.561182 | 0.029776 |
| C21 | -3.05287 | -0.25633 | -0.0256 |
| C22 | -3.03849 | -1.66788 | -0.00951 |
| C23 | -1.69091 | 3.019934 | -0.00854 |
| C24 | 4.352457 | 2.391951 | 0.018466 |
| C25 | 2.421956 | -4.3294 | 0.015561 |
| C26 | -4.35127 | -2.38951 | 0.008166 |
| C27 | -2.42113 | 4.326493 | -0.03875 |
| C28 | -4.75832 | -3.17237 | -1.08339 |
| C29 | -5.98292 | -3.84074 | -1.06331 |
| C30 | -6.81909 | -3.74051 | 0.049853 |
| C31 | -6.42435 | -2.96666 | 1.142526 |
| C32 | -5.20122 | -2.29634 | 1.121167 |
| C33 | 2.383027 | -5.20541 | -1.07726 |
| C34 | 3.073812 | -6.41505 | -1.00651 |
| N35 | 3.786602 | -6.80756 | 0.056856 |
| C36 | 3.820776 | -5.96807 | 1.099875 |
| C37 | 3.166658 | -4.73661 | 1.130935 |
| C38 | 4.793788 | 3.080763 | 1.158561 |
| C39 | 6.014652 | 3.756408 | 1.153824 |

| | | | |
|---|---|---|---|
| C40 | 6.813365 | 3.755537 | 0.009203 |
| C41 | 6.384186 | 3.07466 | -1.13121 |
| C42 | 5.163633 | 2.398973 | -1.12635 |
| C43 | -3.19689 | 4.755759 | 1.04637 |
| C44 | -3.85534 | 5.982967 | 0.969079 |
| N45 | -3.79798 | 6.797397 | -0.09247 |
| C46 | -3.05717 | 6.382764 | -1.12796 |
| C47 | -2.3594 | 5.175278 | -1.152 |
| H48 | -0.1195 | -5.27762 | 0.150716 |
| H49 | -2.69225 | -4.53817 | 0.163814 |
| H50 | -0.29891 | -1.0545 | -0.08883 |
| H51 | 5.291949 | -0.11915 | -0.00226 |
| H52 | 4.559306 | -2.69428 | -0.03992 |
| H53 | 0.126507 | 5.282099 | 0.039127 |
| H54 | 2.69965 | 4.540047 | 0.03638 |
| H55 | 0.300069 | 1.051187 | 0.042749 |
| H56 | -5.28043 | 0.118503 | -0.21814 |
| H57 | -4.54559 | 2.693395 | -0.21301 |
| H58 | -4.11317 | -3.24437 | -1.9536 |
| H59 | -6.28478 | -4.43615 | -1.91994 |
| H60 | -7.77187 | -4.26149 | 0.065164 |
| H61 | -7.06672 | -2.88641 | 2.014531 |
| H62 | -4.89306 | -1.69806 | 1.972887 |
| H63 | 1.827978 | -4.94178 | -1.97166 |
| H64 | 3.054969 | -7.10172 | -1.85093 |
| H65 | 4.399452 | -6.29732 | 1.961162 |
| H66 | 3.228051 | -4.10357 | 2.009961 |
| H67 | 4.177165 | 3.07698 | 2.052515 |
| H68 | 6.343012 | 4.280028 | 2.047084 |
| H69 | 7.763391 | 4.28169 | 0.006486 |
| H70 | 6.997214 | 3.071067 | -2.02778 |
| H71 | 4.828446 | 1.872917 | -2.01522 |
| H72 | -3.27865 | 4.142782 | 1.93803 |
| H73 | -4.45784 | 6.329602 | 1.806775 |
| H74 | -3.02042 | 7.048646 | -1.98832 |
| H75 | -1.78199 | 4.892514 | -2.02619 |

Compound **4a**.
Total energy: -1977.195099 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 4.281722 | -0.80831 | 0.024029 |
| C1 | 4.321442 | 0.555286 | 0.036675 |
| C2 | 2.925498 | 1.010587 | 0.010358 |
| N3 | 2.053746 | -0.06117 | 0.005475 |
| C4 | 2.86096 | -1.1821 | 0.012383 |
| C5 | -0.81163 | -4.26841 | -0.04747 |
| C6 | 0.567388 | -4.30825 | -0.04631 |
| C7 | 1.058584 | -2.9511 | -0.04816 |
| N8 | -0.05984 | -2.12817 | -0.04115 |
| C9 | -1.22349 | -2.88542 | -0.02911 |
| C10 | 2.41098 | -2.53096 | -0.02006 |
| C11 | -4.26797 | 0.804317 | 0.167544 |
| C12 | -4.30768 | -0.55939 | 0.163942 |
| C13 | -2.91747 | -1.01351 | 0.027906 |
| N14 | -2.04854 | 0.058395 | -0.03405 |
| C15 | -2.85364 | 1.178451 | 0.034051 |
| C16 | -2.54817 | -2.38696 | 0.003191 |
| C17 | 0.817423 | 4.259347 | -0.12487 |
| C18 | -0.56165 | 4.299796 | -0.12671 |
| C19 | -1.05317 | 2.947863 | -0.01099 |
| N20 | 0.064706 | 2.126654 | 0.051107 |
| C21 | 1.228407 | 2.880846 | -0.00984 |
| C22 | 2.554099 | 2.383627 | -0.00251 |
| C23 | -2.40585 | 2.528318 | 0.010109 |
| C24 | -3.64931 | -3.41291 | 0.024161 |
| C25 | 3.64854 | 3.416763 | -0.01721 |
| C26 | 3.446157 | -3.62419 | -0.01368 |
| C27 | -3.44232 | 3.618269 | -0.00193 |
| C28 | -3.83047 | -4.28507 | 1.120907 |
| C29 | -4.87677 | -5.22176 | 1.088658 |
| N30 | -5.74537 | -5.35295 | 0.060684 |
| C31 | -5.56685 | -4.51474 | -0.9855 |
| C32 | -4.55285 | -3.54525 | -1.05408 |
| C33 | -4.34162 | 3.768515 | -1.08169 |
| C34 | -5.28741 | 4.80629 | -1.04973 |
| N35 | -5.40382 | 5.695282 | -0.03725 |
| C36 | -4.54145 | 5.545298 | 0.993487 |
| C37 | -3.55992 | 4.542661 | 1.060184 |
| C38 | 4.525018 | 3.555934 | -1.11643 |
| C39 | 5.529007 | 4.537399 | -1.0739 |

| | | | |
|---|---|---|---|
| N40 | 5.721914 | 5.381538 | -0.03514 |
| C41 | 4.877702 | 5.244983 | 1.012076 |
| C42 | 3.843157 | 4.296676 | 1.071 |
| C43 | 4.276373 | -3.84735 | 1.107605 |
| C44 | 5.222353 | -4.88475 | 1.066694 |
| N45 | 5.399359 | -5.70786 | 0.008446 |
| C46 | 4.601275 | -5.48896 | -1.06084 |
| C47 | 3.6272 | -4.47864 | -1.12383 |
| H48 | 5.123225 | -1.49509 | 0.018427 |
| H49 | 5.199833 | 1.193797 | 0.06193 |
| H50 | -1.49165 | -5.11418 | -0.05443 |
| H51 | 1.198443 | -5.19119 | -0.03995 |
| H52 | -0.03155 | -1.106 | -0.0531 |
| H53 | -5.10204 | 1.492017 | 0.273252 |
| H54 | -5.17957 | -1.19949 | 0.264722 |
| H55 | 1.498899 | 5.099433 | -0.21357 |
| H56 | -1.19297 | 5.177787 | -0.21861 |
| H57 | 0.036455 | 1.105749 | 0.097922 |
| H58 | -3.17244 | -4.22383 | 1.990873 |
| H59 | -5.03013 | -5.89969 | 1.936137 |
| H60 | -6.27186 | -4.62823 | -1.817 |
| H61 | -4.46031 | -2.90452 | -1.93406 |
| H62 | -4.29543 | 3.09066 | -1.93695 |
| H63 | -5.98629 | 4.935031 | -1.88417 |
| H64 | -4.64463 | 6.264709 | 1.813943 |
| H65 | -2.90328 | 4.47228 | 1.930549 |
| H66 | 4.418367 | 2.913209 | -1.99329 |
| H67 | 6.212748 | 4.656918 | -1.92235 |
| H68 | 5.041335 | 5.9288 | 1.852934 |
| H69 | 3.20274 | 4.233122 | 1.954057 |
| H70 | 4.177868 | -3.22418 | 1.999375 |
| H71 | 5.869444 | -5.06902 | 1.931576 |
| H72 | 4.753349 | -6.156 | -1.91741 |
| H73 | 3.023214 | -4.3499 | -2.02523 |

Compound **5a**.
Total energy: -2118.404248 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 4.086694 | 2.563129 | -0.02345 |
| C1 | 3.108197 | 3.520112 | -0.04304 |
| C2 | 1.836526 | 2.860127 | 0.016581 |
| N3 | 2.097771 | 1.510591 | 0.074618 |
| C4 | 3.452742 | 1.278427 | 0.046879 |
| C5 | 3.203444 | -3.46628 | 0.003768 |
| C6 | 4.149655 | -2.49884 | 0.023249 |
| C7 | 3.434298 | -1.22583 | 0.015175 |
| N8 | 2.083052 | -1.42383 | 0.004467 |
| C9 | 1.914792 | -2.77998 | 0.000109 |
| C10 | 4.086976 | 0.025063 | 0.033623 |
| C11 | -2.83408 | -2.55791 | 0.014514 |
| C12 | -1.85505 | -3.51454 | 0.020294 |
| C13 | -0.58437 | -2.85378 | -0.04857 |
| N14 | -0.84672 | -1.50419 | -0.1007 |
| C15 | -2.20157 | -1.27258 | -0.05957 |
| C16 | 0.680698 | -3.46409 | -0.01933 |
| C17 | -1.95061 | 3.47276 | -0.0438 |
| C18 | -2.89704 | 2.504999 | -0.05139 |
| C19 | -2.18244 | 1.231843 | -0.03387 |
| N20 | -0.83134 | 1.430127 | -0.02853 |
| C21 | -0.66244 | 2.786297 | -0.0364 |
| C22 | 0.571808 | 3.470372 | -0.02171 |
| C23 | -2.8363 | -0.01915 | -0.04147 |
| C24 | 0.697202 | -4.96256 | 0.011819 |
| C25 | 5.58401 | 0.041767 | 0.019529 |
| C26 | 0.555163 | 4.968513 | -0.06781 |
| C27 | -4.33323 | -0.03516 | -0.00752 |
| C28 | 0.288908 | -5.70803 | -1.10469 |
| C29 | 0.301018 | -7.103 | -1.07324 |
| C30 | 0.719676 | -7.775 | 0.076123 |
| C31 | 1.127202 | -7.04416 | 1.193433 |
| C32 | 1.116114 | -5.64959 | 1.161725 |
| C33 | -5.07666 | -0.49694 | -1.1068 |
| C34 | -6.46663 | -0.52357 | -1.06845 |
| C35 | -7.15382 | -0.07398 | 0.066489 |
| C36 | -6.41864 | 0.376937 | 1.171605 |
| C37 | -5.02646 | 0.394943 | 1.134332 |
| C38 | 0.956834 | 5.726315 | 1.042773 |
| C39 | 0.945479 | 7.120902 | 0.995788 |

| | | | |
|---|---|---|---|
| C40 | 0.533852 | 7.78024 | -0.1634 |
| C41 | 0.132386 | 7.03711 | -1.27478 |
| C42 | 0.14294 | 5.642974 | -1.22758 |
| C43 | 6.321613 | 0.482001 | 1.126501 |
| C44 | 7.714924 | 0.484011 | 1.059876 |
| N45 | 8.412521 | 0.088438 | -0.01234 |
| C46 | 7.703917 | -0.33061 | -1.06866 |
| C47 | 6.310374 | -0.37359 | -1.1045 |
| H48 | 5.153392 | 2.717305 | -0.07398 |
| H49 | 3.238169 | 4.588971 | -0.11129 |
| H50 | -0.13812 | -0.77932 | -0.13138 |
| H51 | 3.348977 | -4.53593 | -0.00994 |
| H52 | 5.222042 | -2.62327 | 0.04387 |
| H53 | -3.89996 | -2.71381 | 0.076089 |
| H54 | -1.984 | -4.58368 | 0.086255 |
| H55 | 1.388783 | 0.785987 | 0.102479 |
| H56 | -2.09581 | 4.542594 | -0.04117 |
| H57 | -3.96936 | 2.629818 | -0.07347 |
| H58 | -0.03015 | -5.18632 | -2.00214 |
| H59 | -0.01261 | -7.66373 | -1.94899 |
| H60 | 0.728671 | -8.86067 | 0.101154 |
| H61 | 1.45049 | -7.55917 | 2.093429 |
| H62 | 1.427321 | -5.08219 | 2.033673 |
| H63 | -4.55261 | -0.83104 | -1.99678 |
| H64 | -7.04384 | -0.88469 | -1.91271 |
| H66 | -6.91945 | 0.674743 | 2.089956 |
| H67 | -4.46537 | 0.729885 | 2.000773 |
| H68 | 1.270758 | 5.214473 | 1.947708 |
| H69 | 1.254353 | 7.691203 | 1.867061 |
| H70 | 0.525622 | 8.865577 | -0.20067 |
| H71 | -0.18542 | 7.542246 | -2.18232 |
| H72 | -0.16288 | 5.066064 | -2.09519 |
| H73 | 5.814602 | 0.809956 | 2.028266 |
| H74 | 8.299153 | 0.818738 | 1.915332 |
| H75 | 8.279351 | -0.64633 | -1.93715 |
| H76 | 5.794148 | -0.71825 | -1.99458 |
| C3 | -8.65149 | -0.1342 | 0.046532 |
| O1 | -9.27706 | -0.83785 | -0.71083 |
| O2 | -9.3085 | 0.654702 | 0.939846 |
| H2 | -8.69092 | 1.273367 | 1.353789 |

Compound **1b**.
Total energy: -2405.450199 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | -0.18653 | -4.09063 | -0.3777 |
| C1 | -1.34846 | -3.8735 | 0.301277 |
| C2 | -1.46329 | -2.46263 | 0.519749 |
| N3 | -0.32996 | -1.83739 | 0.029902 |
| C4 | 0.484477 | -2.83059 | -0.4955 |
| C5 | 4.09113 | -0.1795 | 0.416262 |
| C6 | 3.879665 | -1.35316 | -0.24732 |
| C7 | 2.473064 | -1.46655 | -0.48529 |
| N8 | 1.844446 | -0.31783 | -0.03273 |
| C9 | 2.834072 | 0.499487 | 0.504546 |
| C10 | 1.823707 | -2.65234 | -0.84596 |
| C11 | 0.181833 | 4.098093 | -0.46612 |
| C12 | 1.352755 | 3.893628 | 0.207697 |
| C13 | 1.467409 | 2.490655 | 0.460661 |
| N14 | 0.323552 | 1.855454 | -0.00233 |
| C15 | -0.49508 | 2.840522 | -0.5477 |
| C16 | 2.651317 | 1.843617 | 0.836652 |
| C17 | -4.09694 | 0.188034 | 0.433715 |
| C18 | -3.88621 | 1.347184 | -0.25511 |
| C19 | -2.47864 | 1.463719 | -0.48725 |
| N20 | -1.84676 | 0.335814 | 0.013879 |
| C21 | -2.83628 | -0.48044 | 0.546205 |
| C22 | -2.64519 | -1.81889 | 0.898683 |
| C23 | -1.83809 | 2.643501 | -0.88307 |
| C24 | -3.74741 | -2.6266 | 1.49448 |
| C25 | 2.630081 | -3.76934 | -1.41623 |
| C26 | -2.65197 | 3.731684 | -1.49483 |
| C27 | 3.7592 | 2.655906 | 1.415761 |
| C28 | 2.884518 | -4.94004 | -0.68343 |
| C29 | 3.659064 | -5.96143 | -1.23231 |
| C30 | 4.188543 | -5.82845 | -2.51706 |
| C31 | 3.947152 | -4.66534 | -3.24979 |
| C32 | 3.177586 | -3.63922 | -2.70208 |
| C33 | 3.599474 | 3.235204 | 2.684535 |
| C34 | 4.615836 | 4.011449 | 3.240781 |
| C35 | 5.799466 | 4.228314 | 2.533683 |
| C36 | 5.962695 | 3.667128 | 1.265999 |
| C37 | 4.950894 | 2.885951 | 0.708981 |
| C38 | -2.87105 | 4.951883 | -0.83444 |
| C39 | -3.65401 | 5.94322 | -1.42463 |

| | | | |
|---|---|---|---|
| C40 | -4.22836 | 5.730422 | -2.67898 |
| C41 | -4.02352 | 4.517767 | -3.33918 |
| C42 | -3.24514 | 3.521757 | -2.75022 |
| C43 | -3.58068 | -3.18273 | 2.772681 |
| C44 | -4.5924 | -3.95396 | 3.344422 |
| C45 | -5.77684 | -4.18809 | 2.644163 |
| C46 | -5.94585 | -3.65034 | 1.367092 |
| C47 | -4.93917 | -2.87432 | 0.793891 |
| H48 | 0.206026 | -5.02825 | -0.73953 |
| H49 | -2.10171 | -4.59437 | 0.580171 |
| O50 | 0.042008 | -0.03427 | 1.674597 |
| H51 | 5.025807 | 0.213215 | 0.786013 |
| H52 | 4.602373 | -2.11374 | -0.50124 |
| H53 | -0.20758 | 5.029695 | -0.84662 |
| H54 | 2.109867 | 4.620909 | 0.459335 |
| H55 | -0.39807 | 0.744677 | 2.040645 |
| H56 | -5.03203 | -0.20227 | 0.804582 |
| H57 | -4.61174 | 2.096605 | -0.53249 |
| H58 | 2.495844 | -5.03878 | 0.325594 |
| H59 | 3.855134 | -6.85767 | -0.65177 |
| H60 | 4.78984 | -6.62542 | -2.94299 |
| H61 | 4.356358 | -4.55517 | -4.24918 |
| H62 | 2.98617 | -2.73826 | -3.27756 |
| H63 | 2.682424 | 3.06321 | 3.240359 |
| H64 | 4.481914 | 4.445226 | 4.22683 |
| H65 | 6.588794 | 4.83501 | 2.966085 |
| H66 | 6.875249 | 3.843493 | 0.704927 |
| H67 | 5.074769 | 2.472897 | -0.2875 |
| H68 | -2.45074 | 5.113412 | 0.153462 |
| H69 | -3.82272 | 6.878074 | -0.89911 |
| H70 | -4.83666 | 6.503821 | -3.13711 |
| H71 | -4.46908 | 4.345128 | -4.31387 |
| H72 | -3.08336 | 2.58029 | -3.26669 |
| H73 | -2.66132 | -2.99852 | 3.320639 |
| H74 | -4.45378 | -4.37124 | 4.33694 |
| H75 | -6.56215 | -4.79102 | 3.089002 |
| H76 | -6.85843 | -3.8418 | 0.811109 |
| H77 | -5.06538 | -2.48119 | -0.21033 |
| O78 | -0.07415 | -0.03005 | -1.66927 |
| P79 | -0.00858 | -0.00966 | 0.002421 |
| H80 | 0.696682 | 0.41461 | -2.0466 |

Compound **2b**.
Total energy: -2421.4799121 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 0.517455 | -4.08492 | -0.33459 |
| C1 | -0.65712 | -4.06233 | 0.360218 |
| C2 | -1.02184 | -2.68948 | 0.544723 |
| N3 | -0.0077 | -1.88495 | 0.047565 |
| C4 | 0.961094 | -2.73093 | -0.47944 |
| C5 | 4.079179 | 0.480821 | 0.445089 |
| C6 | 4.064986 | -0.70811 | -0.22979 |
| C7 | 2.697974 | -1.05107 | -0.47495 |
| N8 | 1.889091 | -0.02421 | -0.01047 |
| C9 | 2.729566 | 0.945469 | 0.531109 |
| C10 | 2.249726 | -2.32899 | -0.83852 |
| C11 | -0.47418 | 4.047529 | -0.49156 |
| C12 | 0.701316 | 4.042015 | 0.204548 |
| C13 | 1.045064 | 2.676608 | 0.463245 |
| N14 | 0.03659 | 1.862055 | -0.02634 |
| C15 | -0.92747 | 2.693492 | -0.58036 |
| C16 | 2.314244 | 2.239098 | 0.865138 |
| C17 | -4.04134 | -0.51527 | 0.394223 |
| C18 | -4.02515 | 0.649943 | -0.31475 |
| C19 | -2.65367 | 1.011785 | -0.52014 |
| N20 | -1.84561 | 0.022346 | 0.014839 |
| C21 | -2.68199 | -0.93717 | 0.557624 |
| C22 | -2.28329 | -2.22368 | 0.925251 |
| C23 | -2.214 | 2.27222 | -0.93554 |
| C24 | -3.28303 | -3.14512 | 1.541347 |
| C25 | 3.224354 | -3.28201 | -1.44243 |
| C26 | -3.181 | 3.192243 | -1.59714 |
| C27 | 3.241151 | 3.2177 | 1.497948 |
| C28 | 3.728851 | -3.0143 | -2.72526 |
| C29 | 4.65019 | -3.87717 | -3.31776 |
| C30 | 5.088824 | -5.01096 | -2.6316 |
| C31 | 4.603977 | -5.27821 | -1.34966 |
| C32 | 3.677174 | -4.42106 | -0.75673 |
| C33 | 2.889059 | 3.776717 | 2.738005 |
| C34 | 3.725899 | 4.702074 | 3.36045 |
| C35 | 4.918974 | 5.090043 | 2.748397 |
| C36 | 5.270496 | 4.551884 | 1.508655 |
| C37 | 4.438988 | 3.621881 | 0.885376 |
| C38 | -3.62506 | 4.375317 | -0.98397 |
| C39 | -4.54258 | 5.201947 | -1.63199 |

| | | | |
|---|---|---|---|
| C40 | -5.02693 | 4.860129 | -2.89641 |
| C41 | -4.59756 | 3.681863 | -3.50961 |
| C42 | -3.68473 | 2.849504 | -2.86277 |
| C43 | -3.87679 | -4.19203 | 0.824472 |
| C44 | -4.80867 | -5.0057 | 1.471444 |
| N45 | -5.17549 | -4.84664 | 2.748333 |
| C46 | -4.61011 | -3.84088 | 3.425288 |
| C47 | -3.67053 | -2.96665 | 2.875176 |
| H48 | 1.064885 | -4.9494 | -0.67926 |
| H49 | -1.25536 | -4.90426 | 0.675885 |
| O50 | -0.03427 | -0.07936 | -1.66695 |
| H51 | 4.938104 | 1.015161 | 0.822607 |
| H52 | 4.905064 | -1.33764 | -0.484 |
| H53 | -1.00896 | 4.900458 | -0.88192 |
| H54 | 1.322161 | 4.885991 | 0.466596 |
| H55 | -4.89969 | -1.07572 | 0.734918 |
| H56 | -4.86589 | 1.248048 | -0.63358 |
| H57 | 3.383909 | -2.13493 | -3.26206 |
| H58 | 5.022633 | -3.66436 | -4.31561 |
| H59 | 5.809234 | -5.68129 | -3.09118 |
| H60 | 4.953138 | -6.15133 | -0.80593 |
| H61 | 3.32276 | -4.62058 | 0.25066 |
| H62 | 1.962442 | 3.472582 | 3.216839 |
| H63 | 3.445428 | 5.118271 | 4.323699 |
| H64 | 5.569674 | 5.813058 | 3.231575 |
| H65 | 6.18969 | 4.862516 | 1.020435 |
| H66 | 4.704216 | 3.231735 | -0.09323 |
| H67 | -3.2751 | 4.631683 | 0.012114 |
| H68 | -4.88686 | 6.10914 | -1.14371 |
| H69 | -5.74069 | 5.506929 | -3.39821 |
| H70 | -4.97166 | 3.409089 | -4.49219 |
| H71 | -3.34755 | 1.934365 | -3.34182 |
| H72 | -3.63253 | -4.36129 | -0.21999 |
| H73 | -5.28595 | -5.82255 | 0.933371 |
| H74 | -4.92149 | -3.72533 | 4.461671 |
| H75 | -3.24236 | -2.16989 | 3.476069 |
| P76 | 7.48E-05 | -0.00745 | 0.006793 |
| H77 | 0.624515 | 0.522803 | -2.04741 |
| O78 | -0.01355 | 0.057851 | 1.681248 |
| H79 | 0.630563 | -0.5652 | 2.053312 |

Compound **3b**.
Total energy: -2437.509353 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 3.734499 | 1.697955 | 0.2985 |
| C1 | 3.090342 | 2.679822 | -0.39829 |
| C2 | 1.722448 | 2.280786 | -0.53922 |
| N3 | 1.57278 | 1.005729 | -0.01118 |
| C4 | 2.802417 | 0.630881 | 0.505404 |
| C5 | 1.777442 | -3.74767 | -0.36842 |
| C6 | 2.752449 | -3.10134 | 0.337909 |
| C7 | 2.339216 | -1.74092 | 0.502308 |
| N8 | 1.059148 | -1.59805 | -0.02113 |
| C9 | 0.689972 | -2.83298 | -0.54022 |
| C10 | 3.157986 | -0.67055 | 0.879424 |
| C11 | -3.6744 | -1.80694 | 0.368986 |
| C12 | -3.02378 | -2.78032 | -0.3337 |
| C13 | -1.67841 | -2.33601 | -0.54261 |
| N14 | -1.54403 | -1.05852 | -0.0254 |
| C15 | -2.7762 | -0.70052 | 0.50622 |
| C16 | -0.61566 | -3.16626 | -0.91427 |
| C17 | -1.73277 | 3.662519 | -0.38091 |
| C18 | -2.71432 | 3.013566 | 0.31007 |
| C19 | -2.28516 | 1.660195 | 0.500801 |
| N20 | -1.01062 | 1.518598 | -0.01934 |
| C21 | -0.64703 | 2.743872 | -0.54937 |
| C22 | 0.653871 | 3.097203 | -0.91976 |
| C23 | -3.11937 | 0.602962 | 0.881506 |
| C24 | 0.886636 | 4.423043 | -1.56044 |
| C25 | 4.482946 | -0.89676 | 1.524655 |
| C26 | -4.42773 | 0.911523 | 1.523327 |
| C27 | -0.921 | -4.47754 | -1.55646 |
| C28 | 4.693592 | -0.40682 | 2.823431 |
| C29 | 5.919889 | -0.59724 | 3.45935 |
| C30 | 6.953128 | -1.26734 | 2.802641 |
| C31 | 6.757969 | -1.74338 | 1.504844 |
| C32 | 5.531093 | -1.56047 | 0.867216 |
| C33 | -1.43331 | -4.5029 | -2.86014 |
| C34 | -1.71943 | -5.73599 | -3.44803 |
| N35 | -1.54011 | -6.91063 | -2.83384 |
| C36 | -1.06148 | -6.88021 | -1.58475 |
| C37 | -0.73865 | -5.70441 | -0.90497 |
| C38 | -5.65142 | 0.652067 | 0.884445 |
| C39 | -6.85465 | 0.965945 | 1.515452 |

| | | | |
|---|---|---|---|
| C40 | -6.85225 | 1.540717 | 2.787676 |
| C41 | -5.6407 | 1.812057 | 3.425378 |
| C42 | -4.43484 | 1.505043 | 2.796159 |
| C43 | 1.544635 | 5.473458 | -0.90734 |
| C44 | 1.709483 | 6.684842 | -1.58086 |
| N45 | 1.272579 | 6.91018 | -2.82524 |
| C46 | 0.63844 | 5.906042 | -3.44098 |
| C47 | 0.417102 | 4.656751 | -2.8594 |
| H48 | 4.772002 | 1.664166 | 0.594573 |
| H49 | 3.49967 | 3.611753 | -0.75715 |
| O50 | 0.027361 | 0.012887 | 1.654498 |
| H51 | 1.774917 | -4.7747 | -0.7 |
| H52 | 3.695597 | -3.50176 | 0.676794 |
| H53 | -4.68925 | -1.82143 | 0.735053 |
| H54 | -3.40039 | -3.74851 | -0.62804 |
| H55 | -1.71867 | 4.69093 | -0.70892 |
| H56 | -3.67328 | 3.397626 | 0.622964 |
| H57 | 3.888634 | 0.110981 | 3.336316 |
| H58 | 6.066638 | -0.22203 | 4.46726 |
| H59 | 7.908442 | -1.41284 | 3.296922 |
| H60 | 7.563893 | -2.25009 | 0.983142 |
| H61 | 5.394332 | -1.90844 | -0.15215 |
| H62 | -1.59605 | -3.58051 | -3.40836 |
| H63 | -2.11176 | -5.77787 | -4.46182 |
| H64 | -0.93326 | -7.84355 | -1.09568 |
| H65 | -0.37662 | -5.74697 | 0.117149 |
| H66 | -5.65898 | 0.2332 | -0.11704 |
| H67 | -7.79406 | 0.770323 | 1.007882 |
| H68 | -7.79075 | 1.782024 | 3.276662 |
| H69 | -5.6324 | 2.262033 | 4.413133 |
| H70 | -3.49212 | 1.710626 | 3.294282 |
| H71 | 1.900033 | 5.361909 | 0.111859 |
| H72 | 2.212588 | 7.51541 | -1.09023 |
| H73 | 0.287399 | 6.106017 | -4.45101 |
| H74 | -0.10095 | 3.877807 | -3.40953 |
| P75 | 0.010322 | -0.01906 | -0.01863 |
| H76 | -0.14254 | -0.86597 | 2.018963 |
| O77 | -0.02704 | -0.02206 | -1.69226 |
| H78 | 0.849065 | -0.20686 | -2.05622 |

Compound **4b**.
Total energy: -2469.568096 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 3.836703 | -1.47525 | 0.196543 |
| C1 | 4.071375 | -0.32033 | -0.49122 |
| C2 | 2.824897 | 0.376721 | -0.59921 |
| N3 | 1.819515 | -0.41442 | -0.0599 |
| C4 | 2.426425 | -1.55944 | 0.431545 |
| C5 | -1.46142 | -3.87814 | -0.29967 |
| C6 | -0.28721 | -4.12789 | 0.351561 |
| C7 | 0.401642 | -2.88124 | 0.493725 |
| N8 | -0.41218 | -1.86158 | 0.013334 |
| C9 | -1.574 | -2.46034 | -0.45976 |
| C10 | 1.753422 | -2.72355 | 0.812724 |
| C11 | -3.85117 | 1.3976 | 0.4804 |
| C12 | -4.11688 | 0.242407 | -0.19603 |
| C13 | -2.86773 | -0.41707 | -0.43126 |
| N14 | -1.84056 | 0.382223 | 0.044601 |
| C15 | -2.42768 | 1.521944 | 0.576643 |
| C16 | -2.73755 | -1.76124 | -0.79299 |
| C17 | 1.413202 | 3.816744 | -0.39366 |
| C18 | 0.277333 | 4.067114 | 0.318249 |
| C19 | -0.39109 | 2.815351 | 0.515422 |
| N20 | 0.383814 | 1.801655 | -0.02103 |
| C21 | 1.506915 | 2.397838 | -0.56841 |
| C22 | 2.660485 | 1.715655 | -0.96176 |
| C23 | -1.72061 | 2.676455 | 0.922843 |
| C24 | 3.777604 | 2.480192 | -1.58865 |
| C25 | 2.539422 | -3.85405 | 1.387766 |
| C26 | -2.40549 | 3.834345 | 1.564929 |
| C27 | -3.91596 | -2.46845 | -1.37334 |
| C28 | 3.072071 | -3.75087 | 2.678812 |
| C29 | 3.810788 | -4.82015 | 3.189002 |
| C31 | 3.549098 | -6.03652 | 1.273942 |
| C32 | 2.794077 | -5.0301 | 0.669661 |
| C33 | -4.34443 | -2.15278 | -2.66884 |
| C34 | -5.44966 | -2.82447 | -3.1941 |
| N35 | -6.13772 | -3.75716 | -2.52638 |
| C36 | -5.7312 | -4.04646 | -1.285 |
| C37 | -4.63846 | -3.43801 | -0.66524 |
| C38 | -3.42799 | 4.551752 | 0.929784 |
| C39 | -4.01386 | 5.624233 | 1.604225 |
| C41 | -2.67028 | 5.334812 | 3.428796 |

| | | | |
|---|---|---|---|
| C42 | -2.01598 | 4.248752 | 2.845131 |
| C43 | 4.967469 | 2.755841 | -0.90174 |
| C44 | 5.963363 | 3.487229 | -1.55061 |
| N45 | 5.852085 | 3.946255 | -2.80233 |
| C46 | 4.711585 | 3.685073 | -3.45071 |
| C47 | 3.650393 | 2.967451 | -2.89529 |
| H48 | 4.547926 | -2.24002 | 0.47011 |
| H49 | 5.0151 | 0.047642 | -0.86371 |
| O50 | 0.083151 | 0.010098 | 1.6635 |
| H51 | -2.21055 | -4.59303 | -0.60393 |
| H52 | 0.102702 | -5.08441 | 0.664454 |
| H53 | -4.55887 | 2.122232 | 0.852856 |
| H54 | -5.0812 | -0.16553 | -0.4591 |
| H55 | 2.154795 | 4.524207 | -0.73271 |
| H56 | -0.10735 | 5.021905 | 0.643324 |
| H57 | 2.907277 | -2.86195 | 3.279475 |
| H58 | 4.227918 | -4.76376 | 4.192105 |
| H60 | 3.763504 | -6.95544 | 0.732519 |
| H61 | 2.432864 | -5.15474 | -0.34616 |
| H62 | -3.82133 | -1.40845 | -3.26051 |
| H63 | -5.79528 | -2.60017 | -4.20086 |
| H64 | -6.30911 | -4.79905 | -0.75287 |
| H65 | -4.37312 | -3.70049 | 0.353805 |
| H66 | -3.74694 | 4.299513 | -0.07624 |
| H67 | -4.80712 | 6.197574 | 1.129346 |
| H69 | -2.38881 | 5.669083 | 4.425016 |
| H70 | -1.22848 | 3.728676 | 3.381094 |
| H71 | 5.109206 | 2.428313 | 0.123099 |
| H72 | 6.892784 | 3.718006 | -1.03452 |
| H73 | 4.637478 | 4.066689 | -4.46672 |
| H74 | 2.7502 | 2.783473 | -3.47323 |
| P75 | -0.00796 | -0.0068 | -0.00594 |
| H76 | -0.64688 | -0.48622 | 2.057378 |
| O77 | -0.09214 | 0.015451 | -1.67557 |
| H78 | 0.374057 | -0.74055 | -2.05722 |
| N1 | 4.051246 | -5.94775 | 2.510759 |
| N2 | -3.65416 | 6.016664 | 2.83173 |

Compound **5b**.
Total energy: -2610.039626 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | -1.75039 | -3.36737 | -0.71478 |
| C1 | -2.68414 | -2.54441 | -0.15363 |
| C2 | -2.06635 | -1.26975 | 0.051706 |
| N3 | -0.72459 | -1.36196 | -0.29411 |
| C4 | -0.51426 | -2.64724 | -0.76779 |
| C5 | 3.840112 | -2.42523 | 0.652857 |
| C6 | 3.118642 | -3.27074 | -0.14141 |
| C7 | 1.881997 | -2.6223 | -0.45459 |
| N8 | 1.90705 | -1.33496 | 0.072244 |
| C9 | 3.116952 | -1.19334 | 0.740304 |
| C10 | 0.738251 | -3.2394 | -0.97222 |
| C11 | 3.021964 | 3.289811 | -0.16474 |
| C12 | 3.761108 | 2.468833 | 0.63688 |
| C13 | 3.06057 | 1.224293 | 0.742216 |
| N14 | 1.858443 | 1.326223 | 0.060668 |
| C15 | 1.80194 | 2.606908 | -0.47385 |
| C16 | 3.631244 | 0.028068 | 1.184974 |
| C17 | -2.76131 | 2.377155 | -0.23977 |
| C18 | -1.85194 | 3.22347 | -0.80373 |
| C19 | -0.58514 | 2.55585 | -0.80546 |
| N20 | -0.75194 | 1.277129 | -0.30104 |
| C21 | -2.08747 | 1.143988 | 0.036911 |
| C22 | -2.72237 | -0.06685 | 0.329101 |
| C23 | 0.647557 | 3.184418 | -1.0116 |
| C24 | -4.14955 | -0.04616 | 0.760097 |
| C25 | 0.798349 | -4.59663 | -1.58549 |
| C26 | 0.675826 | 4.533526 | -1.64376 |
| C27 | 4.889008 | 0.079042 | 1.987138 |
| C28 | 0.404597 | -4.75457 | -2.92412 |
| C29 | 0.438748 | -6.0117 | -3.52651 |
| C30 | 0.854796 | -7.12725 | -2.7982 |
| C31 | 1.233276 | -6.98265 | -1.46233 |
| C32 | 1.205976 | -5.72652 | -0.85739 |
| C33 | 4.841232 | 0.48528 | 3.326549 |
| C34 | 6.027949 | 0.52562 | 4.060326 |
| N35 | 7.224553 | 0.205271 | 3.555512 |
| C36 | 7.265507 | -0.17148 | 2.272313 |
| C37 | 6.139852 | -0.25178 | 1.450516 |
| C38 | 1.03874 | 5.683878 | -0.92429 |
| C39 | 1.042333 | 6.931727 | -1.54675 |

| | | | |
|---|---|---|---|
| C40 | 0.684254 | 7.046737 | -2.89105 |
| C41 | 0.311861 | 5.910199 | -3.61064 |
| C42 | 0.301569 | 4.660999 | -2.99112 |
| C43 | -5.18148 | -0.5334 | -0.06055 |
| C44 | -6.50399 | -0.48066 | 0.364818 |
| C46 | -5.80234 | 0.547118 | 2.435958 |
| C47 | -4.47738 | 0.50904 | 2.005847 |
| H48 | -1.86643 | -4.39876 | -1.01112 |
| H49 | -3.71446 | -2.77113 | 0.072644 |
| O50 | 0.748093 | -0.02964 | -1.78018 |
| H51 | 4.806764 | -2.60427 | 1.098673 |
| H52 | 3.381053 | -4.2698 | -0.45295 |
| H53 | 3.263533 | 4.288647 | -0.49348 |
| H54 | 4.731993 | 2.661595 | 1.068277 |
| H55 | -3.81298 | 2.549072 | -0.06815 |
| H56 | -2.00735 | 4.234435 | -1.14835 |
| H57 | 0.084531 | -3.8869 | -3.4932 |
| H58 | 0.140961 | -6.11814 | -4.56489 |
| H59 | 0.878098 | -8.10585 | -3.26711 |
| H60 | 1.54141 | -7.84941 | -0.886 |
| H61 | 1.472991 | -5.6265 | 0.190312 |
| H62 | 3.897863 | 0.753409 | 3.791368 |
| H63 | 6.01233 | 0.830962 | 5.104364 |
| H64 | 8.247701 | -0.41915 | 1.875358 |
| H65 | 6.241672 | -0.54881 | 0.411601 |
| H66 | 1.288774 | 5.604592 | 0.129278 |
| H67 | 1.315435 | 7.814904 | -0.97777 |
| H68 | 0.688998 | 8.018883 | -3.3738 |
| H69 | 0.029887 | 5.99434 | -4.65548 |
| H70 | 0.016253 | 3.776591 | -3.55286 |
| H71 | -4.94775 | -0.92459 | -1.04554 |
| H72 | -7.31082 | -0.82865 | -0.27083 |
| H73 | -6.0275 | 1.009009 | 3.39342 |
| H74 | -3.69043 | 0.907156 | 2.638519 |
| P75 | 0.559061 | -0.01139 | -0.11863 |
| H76 | 1.682932 | -0.0155 | -2.02448 |
| O77 | 0.339188 | 0.029469 | 1.540415 |
| H78 | 0.337531 | -0.86537 | 1.905817 |
| C3 | -6.82515 | 0.04262 | 1.623793 |
| C8 | -8.28076 | 0.084633 | 2.005688 |
| O1 | -9.16485 | 0.045883 | 1.185668 |
| O2 | -8.5691 | 0.1777 | 3.326779 |
| H1 | -7.7807 | 0.021939 | 3.86477 |

Compound **1c**.
Total energy: -2562.693308 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 4.143161 | -0.49389 | -0.01288 |
| C1 | 4.054537 | 0.706916 | 0.627247 |
| C2 | 2.670798 | 1.074419 | 0.661244 |
| N3 | 1.91593 | 0.037571 | 0.132885 |
| C4 | 2.807483 | -0.9445 | -0.26912 |
| C5 | -0.43279 | -4.11036 | 0.368424 |
| C6 | 0.79506 | -4.07289 | -0.22146 |
| C7 | 1.151145 | -2.69385 | -0.38208 |
| N8 | 0.101048 | -1.90235 | 0.045739 |
| C9 | -0.88574 | -2.75715 | 0.502744 |
| C10 | 2.444982 | -2.24045 | -0.64858 |
| C11 | -4.04036 | 0.426681 | -0.47382 |
| C12 | -4.03072 | -0.75668 | 0.205229 |
| C13 | -2.66179 | -1.13016 | 0.396196 |
| N14 | -1.84708 | -0.11507 | -0.08304 |
| C15 | -2.68059 | 0.849927 | -0.62085 |
| C16 | -2.20161 | -2.38852 | 0.794525 |
| C17 | 0.505474 | 4.065519 | 0.194342 |
| C18 | -0.66024 | 4.003897 | -0.51415 |
| C19 | -1.0436 | 2.628231 | -0.5931 |
| N20 | -0.04979 | 1.850317 | -0.00949 |
| C21 | 0.911642 | 2.722818 | 0.475521 |
| C22 | 2.184177 | 2.355859 | 0.928643 |
| C23 | -2.29212 | 2.14227 | -0.99101 |
| C24 | 3.056094 | 3.405134 | 1.533507 |
| C25 | 3.459185 | -3.2042 | -1.16589 |
| C26 | -3.28779 | 3.02249 | -1.66622 |
| C27 | -3.13033 | -3.40838 | 1.36023 |
| C28 | 3.332236 | -3.69709 | -2.47415 |
| C29 | 4.266655 | -4.59837 | -2.98406 |
| C30 | 5.332462 | -5.02603 | -2.19124 |
| C31 | 5.457654 | -4.55417 | -0.88337 |
| C32 | 4.527684 | -3.64988 | -0.37141 |
| C33 | -4.20725 | -3.9192 | 0.617869 |
| C34 | -5.05197 | -4.88135 | 1.170422 |
| C35 | -4.83263 | -5.34627 | 2.468334 |
| C36 | -3.75907 | -4.8514 | 3.21027 |
| C37 | -2.9092 | -3.89283 | 2.659377 |
| C38 | -3.73958 | 2.677708 | -2.95047 |
| C39 | -4.67962 | 3.471187 | -3.60657 |

| | | | |
|---|---|---|---|
| C40 | -5.18966 | 4.611872 | -2.98479 |
| C41 | -4.75772 | 4.955241 | -1.7024 |
| C42 | -3.81342 | 4.167013 | -1.04522 |
| C43 | 4.187391 | 3.904154 | 0.868627 |
| C44 | 4.968739 | 4.899273 | 1.455581 |
| C45 | 4.630397 | 5.408794 | 2.710502 |
| C46 | 3.502408 | 4.925183 | 3.375034 |
| C47 | 2.71604 | 3.934297 | 2.788486 |
| H48 | 5.035117 | -1.05157 | -0.25208 |
| H49 | 4.860385 | 1.319161 | 1.001054 |
| O50 | 0.081725 | -0.12971 | -1.65253 |
| H51 | -1.01245 | -4.97601 | 0.650071 |
| H52 | 1.436495 | -4.90034 | -0.48347 |
| H53 | -4.8949 | 1.001562 | -0.79645 |
| H54 | -4.87702 | -1.34464 | 0.524684 |
| C55 | 0.793539 | 0.743019 | -2.54495 |
| H56 | 1.079118 | 4.941741 | 0.455852 |
| H57 | -1.22923 | 4.823732 | -0.92433 |
| H58 | 2.503911 | -3.36378 | -3.09261 |
| H59 | 4.161191 | -4.96479 | -4.00043 |
| H60 | 6.058758 | -5.72861 | -2.58771 |
| H61 | 6.275089 | -4.89662 | -0.25639 |
| H62 | 4.615803 | -3.30509 | 0.654314 |
| H63 | -4.36655 | -3.57926 | -0.40079 |
| H64 | -5.8757 | -5.27388 | 0.582356 |
| H65 | -5.49133 | -6.09506 | 2.896863 |
| H66 | -3.58132 | -5.21094 | 4.219022 |
| H67 | -2.076 | -3.507 | 3.239088 |
| H68 | -3.34316 | 1.790379 | -3.43477 |
| H69 | -5.01303 | 3.197395 | -4.60276 |
| H70 | -5.92454 | 5.227197 | -3.49423 |
| H71 | -5.16296 | 5.832344 | -1.20743 |
| H72 | -3.50286 | 4.423307 | -0.03688 |
| H73 | 4.440087 | 3.5275 | -0.11785 |
| H74 | 5.836849 | 5.281809 | 0.927857 |
| H75 | 5.240057 | 6.18295 | 3.16568 |
| H76 | 3.23333 | 5.318895 | 4.350251 |
| H77 | 1.838549 | 3.558365 | 3.305958 |
| P78 | 0.030479 | -0.03452 | 0.02035 |
| H79 | 0.226672 | 1.67105 | -2.67841 |
| O80 | 0.013994 | -0.06235 | 1.696813 |
| C82 | -0.87123 | 0.654931 | 2.570774 |
| H83 | 1.774789 | 1.002864 | -2.13376 |
| H85 | -1.86843 | 0.20197 | 2.544744 |

| | | | |
|---|---|---|---|
| H86 | -0.96682 | 1.698456 | 2.252294 |
| C3 | -0.28724 | 0.573622 | 3.971929 |
| H2 | 0.702209 | 1.037982 | 4.010436 |
| H3 | -0.18756 | -0.46757 | 4.290205 |
| H4 | -0.94313 | 1.090192 | 4.679589 |
| C8 | 0.943694 | 0.022603 | -3.87489 |
| H1 | 1.435254 | 0.680155 | -4.59864 |
| H5 | -0.03385 | -0.26066 | -4.27416 |
| H6 | 1.54787 | -0.88228 | -3.76641 |

Compound **2c**.
Total energy: -2578.722521 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 4.055175 | -0.27151 | 0.257989 |
| C1 | 3.940145 | 0.919399 | -0.39985 |
| C2 | 2.544598 | 1.198697 | -0.5422 |
| N3 | 1.815293 | 0.140258 | -0.02081 |
| C4 | 2.73311 | -0.78003 | 0.463054 |
| C5 | -0.32023 | -4.14789 | -0.19561 |
| C6 | 0.878828 | -4.02506 | 0.441924 |
| C7 | 1.178059 | -2.62804 | 0.531705 |
| N8 | 0.104619 | -1.90328 | 0.031585 |
| C9 | -0.83668 | -2.82674 | -0.39478 |
| C10 | 2.429035 | -2.09064 | 0.845658 |
| C11 | -4.1618 | 0.194942 | 0.447732 |
| C12 | -4.06523 | -1.00836 | -0.18319 |
| C13 | -2.67269 | -1.26125 | -0.41179 |
| N14 | -1.93625 | -0.17457 | 0.018302 |
| C15 | -2.84067 | 0.747687 | 0.519683 |
| C16 | -2.15505 | -2.5173 | -0.73883 |
| C17 | 0.140279 | 4.071927 | -0.49878 |
| C18 | -1.0534 | 3.984947 | 0.154983 |
| C19 | -1.29854 | 2.599452 | 0.419759 |
| N20 | -0.21597 | 1.854939 | -0.01629 |
| C21 | 0.691487 | 2.752453 | -0.56312 |
| C22 | 2.004746 | 2.433777 | -0.91036 |
| C23 | -2.53521 | 2.077964 | 0.814149 |
| C24 | 2.902184 | 3.463669 | -1.5113 |
| C25 | 3.510361 | -2.93241 | 1.435373 |
| C26 | -3.56728 | 3.006454 | 1.35848 |
| C27 | -3.07541 | -3.56166 | -1.27608 |
| C28 | 4.064125 | -4.02219 | 0.744491 |
| C29 | 5.086583 | -4.77607 | 1.319894 |
| C30 | 5.569789 | -4.45194 | 2.588893 |
| C31 | 5.032246 | -3.3646 | 3.279247 |
| C32 | 4.013589 | -2.6056 | 2.704687 |
| C33 | -3.57813 | -3.42744 | -2.57952 |
| C34 | -4.44296 | -4.38713 | -3.10553 |
| C35 | -4.82357 | -5.48556 | -2.33346 |
| C36 | -4.34047 | -5.61923 | -1.03053 |
| C37 | -3.47186 | -4.66451 | -0.50259 |
| C38 | -4.72932 | 3.318012 | 0.633295 |
| C39 | -5.67098 | 4.203596 | 1.155818 |

| | | | |
|---|---|---|---|
| C40 | -5.4663 | 4.789542 | 2.406072 |
| C41 | -4.3103 | 4.493606 | 3.130035 |
| C42 | -3.3637 | 3.612379 | 2.608127 |
| C43 | 3.308735 | 4.599752 | -0.79913 |
| C44 | 4.158414 | 5.516021 | -1.42042 |
| N45 | 4.615478 | 5.377339 | -2.67027 |
| C46 | 4.228338 | 4.288468 | -3.34416 |
| C47 | 3.385487 | 3.308808 | -2.81639 |
| H48 | 4.957705 | -0.79019 | 0.543412 |
| H49 | 4.730835 | 1.578277 | -0.72584 |
| O50 | -0.1411 | 0.026327 | -1.66971 |
| H51 | -0.83751 | -5.05518 | -0.46587 |
| H52 | 1.531794 | -4.81341 | 0.782817 |
| H53 | -5.05192 | 0.687196 | 0.807263 |
| H54 | -4.85573 | -1.70356 | -0.42127 |
| C55 | 0.438115 | -0.12933 | -3.97495 |
| H56 | 0.624531 | 4.958466 | -0.87866 |
| H57 | -1.74324 | 4.780334 | 0.392257 |
| H58 | 3.708852 | -4.26324 | -0.25276 |
| H59 | 5.511332 | -5.61143 | 0.771969 |
| H60 | 6.365275 | -5.04057 | 3.034803 |
| H61 | 5.405057 | -3.10604 | 4.265426 |
| H62 | 3.59708 | -1.75919 | 3.24243 |
| H63 | -3.27976 | -2.5751 | -3.1828 |
| H64 | -4.81786 | -4.27556 | -4.11813 |
| H65 | -5.49814 | -6.23126 | -2.74227 |
| H66 | -4.64598 | -6.46332 | -0.42002 |
| H67 | -3.11795 | -4.76102 | 0.519369 |
| H68 | -4.8817 | 2.885691 | -0.35081 |
| H69 | -6.56064 | 4.442052 | 0.581169 |
| H70 | -6.20164 | 5.477418 | 2.811445 |
| H71 | -4.14428 | 4.947141 | 4.102184 |
| H72 | -2.46779 | 3.379558 | 3.176033 |
| H73 | 2.984 | 4.760597 | 0.223704 |
| H74 | 4.48948 | 6.402124 | -0.88298 |
| H75 | 4.608402 | 4.190513 | -4.35879 |
| H76 | 3.102511 | 2.448443 | -3.4146 |
| P77 | -0.06035 | -0.02235 | 0.002798 |
| C78 | 0.630582 | -0.74962 | -2.60074 |
| O79 | -0.09045 | -0.09169 | 1.676369 |
| H80 | 0.282239 | -1.78817 | -2.5977 |
| C81 | 0.537066 | 0.816243 | 2.594955 |
| H82 | 1.689276 | -0.74833 | -2.3205 |
| H83 | -0.04468 | 1.742833 | 2.653619 |

| | | | |
|---|---|---|---|
| H84 | 1.54636 | 1.074448 | 2.255944 |
| C85 | 0.584004 | 0.131302 | 3.951474 |
| H86 | 1.037052 | 0.799316 | 4.690674 |
| H87 | 1.174752 | -0.78764 | 3.904316 |
| H88 | -0.42264 | -0.12746 | 4.290249 |
| H89 | 0.992957 | -0.70327 | -4.72353 |
| H90 | 0.796919 | 0.90372 | -3.99175 |
| H91 | -0.6188 | -0.12717 | -4.25438 |

Compound **3c**.
Total energy: -2594.752709 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 2.911536 | 2.908084 | 0.315154 |
| C1 | 1.954132 | 3.61374 | -0.35292 |
| C2 | 0.810411 | 2.761725 | -0.48954 |
| N3 | 1.119208 | 1.509125 | 0.018339 |
| C4 | 2.410386 | 1.580073 | 0.509143 |
| C5 | 2.97055 | -2.90432 | -0.3192 |
| C6 | 3.666514 | -1.94017 | 0.35117 |
| C7 | 2.805063 | -0.80617 | 0.493432 |
| N8 | 1.550636 | -1.12941 | -0.0083 |
| C9 | 1.631764 | -2.42801 | -0.49198 |
| C10 | 3.204884 | 0.482786 | 0.861093 |
| C11 | -2.84419 | -2.97713 | 0.301115 |
| C12 | -1.87516 | -3.67061 | -0.36295 |
| C13 | -0.7634 | -2.7853 | -0.5456 |
| N14 | -1.09661 | -1.53503 | -0.05901 |
| C15 | -2.38724 | -1.62655 | 0.440572 |
| C16 | 0.531331 | -3.20182 | -0.87151 |
| C17 | -2.91146 | 2.84787 | -0.36052 |
| C18 | -3.61621 | 1.880822 | 0.292323 |
| C19 | -2.74283 | 0.758228 | 0.467753 |
| N20 | -1.49042 | 1.078757 | -0.02321 |
| C21 | -1.57129 | 2.366027 | -0.5215 |
| C22 | -0.47503 | 3.162163 | -0.86298 |
| C23 | -3.16752 | -0.52838 | 0.814538 |
| C24 | -0.71777 | 4.508068 | -1.45622 |
| C25 | 4.543077 | 0.732202 | 1.469837 |
| C26 | -4.51681 | -0.7037 | 1.42193 |
| C27 | 0.719049 | -4.55538 | -1.47044 |
| C28 | 4.614308 | 1.289354 | 2.756836 |
| C29 | 5.85064 | 1.540301 | 3.350977 |
| C30 | 7.030099 | 1.247965 | 2.664341 |
| C31 | 6.969513 | 0.709081 | 1.377886 |
| C32 | 5.735245 | 0.452447 | 0.782117 |
| C33 | 0.287224 | -4.80066 | -2.78014 |
| C34 | 0.463461 | -6.07495 | -3.32137 |
| N35 | 1.020397 | -7.09357 | -2.65678 |
| C36 | 1.421525 | -6.85719 | -1.40249 |
| C37 | 1.295303 | -5.62104 | -0.76671 |
| C38 | -5.56287 | -1.34541 | 0.739342 |
| C39 | -6.81642 | -1.47768 | 1.335988 |

| | | | |
|---|---|---|---|
| C40 | -7.04188 | -0.97235 | 2.617648 |
| C41 | -6.01122 | -0.32362 | 3.299326 |
| C42 | -4.75811 | -0.18395 | 2.703949 |
| C43 | -0.43866 | 5.694731 | -0.76446 |
| C44 | -0.70394 | 6.915198 | -1.38687 |
| N45 | -1.21531 | 7.027321 | -2.61805 |
| C46 | -1.48874 | 5.891934 | -3.27062 |
| C47 | -1.2667 | 4.620158 | -2.74035 |
| H48 | 3.900676 | 3.233632 | 0.599224 |
| H49 | 2.00627 | 4.63457 | -0.69872 |
| O50 | -0.02795 | 0.040996 | 1.656241 |
| H51 | 3.323662 | -3.87589 | -0.62912 |
| H52 | 4.692283 | -1.97676 | 0.683565 |
| H53 | -3.80119 | -3.34006 | 0.642842 |
| H54 | -1.88054 | -4.71211 | -0.64694 |
| H55 | -3.25044 | 3.825798 | -0.66698 |
| H56 | -4.65385 | 1.897318 | 0.588773 |
| H57 | 3.697155 | 1.514054 | 3.293163 |
| H58 | 5.89108 | 1.963118 | 4.349925 |
| H59 | 7.9922 | 1.445115 | 3.126507 |
| H60 | 7.883784 | 0.496461 | 0.832562 |
| H61 | 5.694156 | 0.058178 | -0.22863 |
| H62 | -0.16919 | -4.01168 | -3.36921 |
| H63 | 0.140272 | -6.28361 | -4.33894 |
| H64 | 1.862224 | -7.69881 | -0.87224 |
| H65 | 1.620188 | -5.49976 | 0.261568 |
| H66 | -5.40225 | -1.71383 | -0.26912 |
| H67 | -7.6197 | -1.96737 | 0.794324 |
| H68 | -8.01828 | -1.07825 | 3.079722 |
| H69 | -6.18129 | 0.07459 | 4.294691 |
| H70 | -3.9564 | 0.321154 | 3.234598 |
| H71 | -0.04507 | 5.671281 | 0.246397 |
| H72 | -0.49997 | 7.847521 | -0.86454 |
| H73 | -1.90641 | 5.999869 | -4.26934 |
| H74 | -1.50914 | 3.734536 | -3.3192 |
| P75 | 0.020227 | -0.01853 | -0.017 |
| O77 | -0.04053 | -0.00347 | -1.69049 |
| C3 | 0.230919 | -1.03659 | 2.571423 |
| H2 | 1.309224 | -1.22064 | 2.6291 |
| H3 | -0.25199 | -1.95829 | 2.23013 |
| C8 | -0.30935 | -0.62329 | 3.930625 |
| H1 | 0.150986 | 0.310904 | 4.263282 |
| H4 | -0.08791 | -1.40016 | 4.668919 |
| H5 | -1.39281 | -0.48096 | 3.895202 |

| | | | |
|---|---|---|---|
| C14 | 1.065683 | 0.085198 | -2.60373 |
| H6 | 1.764624 | 0.868478 | -2.29138 |
| H8 | 1.609915 | -0.86517 | -2.6221 |
| C20 | 0.498212 | 0.39745 | -3.97864 |
| H7 | 1.308599 | 0.445373 | -4.71252 |
| H9 | -0.02218 | 1.35889 | -3.97719 |
| H10 | -0.2082 | -0.37555 | -4.29299 |

Compound **4c**.
Total energy: -2626.811151 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | 3.40713 | -2.2922 | 0.463589 |
| C1 | 3.952432 | -1.22064 | -0.17977 |
| C2 | 2.911329 | -0.2537 | -0.35937 |
| N3 | 1.714386 | -0.7876 | 0.095499 |
| C4 | 2.002176 | -2.04543 | 0.5966 |
| C5 | -2.28993 | -3.41242 | -0.33984 |
| C6 | -1.22937 | -3.92354 | 0.350396 |
| C7 | -0.27348 | -2.86989 | 0.51358 |
| N8 | -0.80534 | -1.69552 | -0.00022 |
| C9 | -2.05582 | -2.01024 | -0.51123 |
| C10 | 1.057064 | -3.02554 | 0.913095 |
| C11 | -3.4148 | 2.31977 | 0.179199 |
| C12 | -3.90742 | 1.223952 | -0.46507 |
| C13 | -2.8369 | 0.280133 | -0.58849 |
| N14 | -1.67724 | 0.840292 | -0.07901 |
| C15 | -2.0108 | 2.10893 | 0.371608 |
| C16 | -3.00964 | -1.06878 | -0.90572 |
| C17 | 2.325815 | 3.422874 | -0.28299 |
| C18 | 1.226769 | 3.949404 | 0.326244 |
| C19 | 0.270849 | 2.890266 | 0.472855 |
| N20 | 0.82744 | 1.709784 | 0.017377 |
| C21 | 2.095094 | 2.016185 | -0.43848 |
| C22 | 3.086234 | 1.078795 | -0.73889 |
| C23 | -1.08343 | 3.07964 | 0.756617 |
| C24 | 4.377 | 1.554122 | -1.31493 |
| C25 | 1.527546 | -4.29674 | 1.536311 |
| C26 | -1.53303 | 4.396723 | 1.293294 |
| C27 | -4.3055 | -1.5084 | -1.50361 |
| C28 | 2.036167 | -4.27992 | 2.841727 |
| C29 | 2.478928 | -5.47575 | 3.409123 |
| C31 | 1.984063 | -6.66053 | 1.521106 |
| C32 | 1.512066 | -5.52442 | 0.861401 |
| C33 | -4.60356 | -1.20304 | -2.83726 |
| C34 | -5.82549 | -1.62228 | -3.36671 |
| N35 | -6.74463 | -2.2982 | -2.66857 |
| C36 | -6.45946 | -2.57726 | -1.39162 |
| C37 | -5.26736 | -2.21005 | -0.76527 |
| C38 | -2.27604 | 5.302112 | 0.524005 |
| C39 | -2.64891 | 6.520286 | 1.093703 |
| C41 | -1.62051 | 6.018949 | 3.070083 |

| | | | |
|---|---|---|---|
| C42 | -1.1929 | 4.776782 | 2.597837 |
| C43 | 5.579498 | 1.539039 | -0.59633 |
| C44 | 6.73669 | 2.016345 | -1.21452 |
| N45 | 6.770486 | 2.493574 | -2.46407 |
| C46 | 5.617943 | 2.51274 | -3.14245 |
| C47 | 4.404271 | 2.064305 | -2.6194 |
| H48 | 3.899549 | -3.20264 | 0.76996 |
| H49 | 4.979806 | -1.08194 | -0.47948 |
| O50 | 0.037442 | 0.039997 | 1.68067 |
| H51 | -3.17882 | -3.93137 | -0.66433 |
| H52 | -1.08874 | -4.94038 | 0.683155 |
| H53 | -3.94819 | 3.210412 | 0.473205 |
| H54 | -4.92395 | 1.039211 | -0.77809 |
| H55 | 3.237673 | 3.927603 | -0.564 |
| H56 | 1.050475 | 4.975843 | 0.610047 |
| H57 | 2.080135 | -3.3547 | 3.40733 |
| H58 | 2.870233 | -5.48485 | 4.424123 |
| H60 | 1.985935 | -7.6225 | 1.013083 |
| H61 | 1.16333 | -5.59536 | -0.16379 |
| H62 | -3.89647 | -0.65702 | -3.4538 |
| H63 | -6.07438 | -1.40204 | -4.40257 |
| H64 | -7.22221 | -3.11812 | -0.83558 |
| H65 | -5.10265 | -2.44957 | 0.28032 |
| H66 | -2.53962 | 5.076691 | -0.50419 |
| H67 | -3.22159 | 7.239953 | 0.512685 |
| H69 | -1.37347 | 6.330988 | 4.082579 |
| H70 | -0.6144 | 4.116447 | 3.236119 |
| H71 | 5.613777 | 1.186791 | 0.429509 |
| H72 | 7.68036 | 2.019262 | -0.67332 |
| H73 | 5.662127 | 2.906546 | -4.15558 |
| H74 | 3.500009 | 2.102223 | -3.21826 |
| P75 | 0.015178 | 0.016762 | 0.008545 |
| O77 | 0.026197 | 0.063805 | -1.66285 |
| N1 | 2.457376 | -6.65182 | 2.77259 |
| N2 | -2.33695 | 6.883451 | 2.343068 |
| C3 | -1.0754 | -0.18315 | 2.564296 |
| H3 | -1.74432 | -0.94858 | 2.157552 |
| H4 | -1.64856 | 0.744872 | 2.666559 |
| C8 | -0.52126 | -0.61557 | 3.911625 |
| H2 | 0.018832 | -1.56272 | 3.82861 |
| H1 | -1.34153 | -0.74877 | 4.623658 |
| H5 | 0.162328 | 0.138694 | 4.310214 |
| C14 | 0.532439 | -0.94 | -2.56066 |
| H6 | 1.626725 | -0.89755 | -2.57834 |

| | | | |
|---|---|---|---|
| H8 | 0.238001 | -1.94121 | -2.22715 |
| C20 | -0.0324 | -0.64878 | -3.94075 |
| H7 | 0.364486 | -1.36886 | -4.6628 |
| H9 | 0.242681 | 0.357029 | -4.26937 |
| H10 | -1.12308 | -0.72511 | -3.94256 |

Compound **5c**.
Total energy: -2767.282878 hartrees
Cartesian Coordinates (Angstroms)

| Atom | X | Y | Z |
|---|---|---|---|
| C0 | -1.72992 | -3.39385 | -0.81237 |
| C1 | -2.70613 | -2.59157 | -0.29809 |
| C2 | -2.1245 | -1.304 | -0.0642 |
| N3 | -0.76906 | -1.36302 | -0.35235 |
| C4 | -0.50922 | -2.64426 | -0.8042 |
| C5 | 3.811394 | -2.315 | 0.742473 |
| C6 | 3.115397 | -3.18902 | -0.04159 |
| C7 | 1.871009 | -2.56918 | -0.38017 |
| N8 | 1.860582 | -1.27483 | 0.125998 |
| C9 | 3.060772 | -1.098 | 0.800742 |
| C10 | 0.762963 | -3.21252 | -0.94013 |
| C11 | 2.855665 | 3.400678 | -0.02571 |
| C12 | 3.606269 | 2.584647 | 0.768491 |
| C13 | 2.936323 | 1.319993 | 0.837396 |
| N14 | 1.73967 | 1.403202 | 0.148777 |
| C15 | 1.660563 | 2.688256 | -0.36745 |
| C16 | 3.539041 | 0.132048 | 1.259942 |
| C17 | -2.90066 | 2.327745 | -0.32355 |
| C18 | -1.99276 | 3.208593 | -0.83152 |
| C19 | -0.70952 | 2.572498 | -0.79225 |
| N20 | -0.85947 | 1.281028 | -0.3203 |
| C21 | -2.20302 | 1.107971 | -0.04281 |
| C22 | -2.82028 | -0.12146 | 0.20265 |
| C23 | 0.510069 | 3.240887 | -0.93821 |
| C24 | -4.26253 | -0.14041 | 0.579852 |
| C25 | 0.879092 | -4.57301 | -1.53895 |
| C26 | 0.519668 | 4.599194 | -1.55026 |
| C27 | 4.799047 | 0.207369 | 2.057303 |
| C28 | 0.554388 | -4.74992 | -2.89351 |
| C29 | 0.640859 | -6.01056 | -3.48327 |
| C30 | 1.042052 | -7.11222 | -2.72611 |
| C31 | 1.351831 | -6.94938 | -1.37469 |
| C32 | 1.271449 | -5.68944 | -0.78245 |
| C33 | 4.754182 | 0.607719 | 3.398506 |
| C34 | 5.945774 | 0.673718 | 4.122445 |
| N35 | 7.145288 | 0.38317 | 3.606747 |
| C36 | 7.183697 | 0.01159 | 2.321905 |
| C37 | 6.053201 | -0.092 | 1.509677 |
| C38 | 0.843555 | 5.747842 | -0.80972 |
| C39 | 0.829212 | 7.004062 | -1.41499 |

| | | | |
|---|---|---|---|
| C40 | 0.490804 | 7.130494 | -2.76334 |
| C41 | 0.155346 | 5.996217 | -3.50426 |
| C42 | 0.163772 | 4.738862 | -2.90169 |
| C43 | -5.25099 | -0.65117 | -0.27902 |
| C44 | -6.58888 | -0.63691 | 0.098743 |
| C46 | -5.9915 | 0.399475 | 2.197907 |
| C47 | -4.65176 | 0.400878 | 1.814346 |
| H48 | -1.80802 | -4.42804 | -1.11124 |
| H49 | -3.74048 | -2.84094 | -0.11928 |
| O50 | 0.70422 | 0.047493 | -1.76105 |
| H51 | 4.775824 | -2.46639 | 1.202714 |
| H52 | 3.400932 | -4.18755 | -0.33362 |
| H53 | 3.07547 | 4.411192 | -0.33304 |
| H54 | 4.566107 | 2.793487 | 1.216527 |
| H55 | -3.96306 | 2.467323 | -0.19382 |
| H56 | -2.16008 | 4.222567 | -1.16108 |
| H57 | 0.244087 | -3.89341 | -3.48453 |
| H58 | 0.395029 | -6.13028 | -4.53374 |
| H59 | 1.106826 | -8.09397 | -3.18438 |
| H60 | 1.647703 | -7.80557 | -0.77647 |
| H61 | 1.485973 | -5.57612 | 0.275926 |
| H62 | 3.809304 | 0.85369 | 3.87242 |
| H63 | 5.931869 | 0.975387 | 5.167596 |
| H64 | 8.167844 | -0.21182 | 1.915461 |
| H65 | 6.152683 | -0.3832 | 0.468916 |
| H66 | 1.076294 | 5.660045 | 0.247007 |
| H67 | 1.072191 | 7.885068 | -0.82916 |
| H68 | 0.48121 | 8.109297 | -3.23236 |
| H69 | -0.11267 | 6.08869 | -4.55208 |
| H70 | -0.09669 | 3.856689 | -3.47907 |
| H71 | -4.97167 | -1.03031 | -1.25674 |
| H72 | -7.36249 | -1.00305 | -0.5673 |
| H73 | -6.26359 | 0.850627 | 3.148252 |
| H74 | -3.90006 | 0.822416 | 2.474295 |
| P75 | 0.491694 | 0.013249 | -0.10089 |
| O77 | 0.175886 | 0.068431 | 1.543753 |
| C3 | -6.96998 | -0.13018 | 1.347914 |
| C8 | -8.43826 | -0.13107 | 1.678382 |
| O1 | -9.29212 | -0.18309 | 0.827665 |
| O2 | -8.77477 | -0.06169 | 2.989859 |
| C14 | 1.946711 | 0.006229 | -2.48221 |
| H2 | 2.354746 | -1.01008 | -2.45875 |
| H3 | 2.681884 | 0.677069 | -2.0252 |
| C20 | 1.660075 | 0.427038 | -3.91435 |

| | | | |
|---|---|---|---|
| H4 | 0.908881 | -0.2255 | -4.36715 |
| H5 | 2.577184 | 0.363275 | -4.50797 |
| H6 | 1.293852 | 1.456351 | -3.95562 |
| C35 | 0.205645 | -1.02963 | 2.469478 |
| H7 | -0.20344 | -1.93696 | 2.012249 |
| H9 | 1.242219 | -1.23655 | 2.7575 |
| C45 | -0.6126 | -0.62864 | 3.685979 |
| H8 | -0.57214 | -1.42059 | 4.440301 |
| H10 | -1.65938 | -0.46358 | 3.416427 |
| H11 | -0.22102 | 0.290908 | 4.129155 |
| H16 | -8.00181 | -0.20384 | 3.553584 |