# Supplementary material.

For the FODFT calculations, the values of $V_{ab}$ where calculated from the following expression:

$$|V_{ab}| = \frac{1}{1 - S_{ab}^2}\left[H_{ab} - S_{ab}\frac{H_{aa} + H_{bb}}{2}\right]$$

***Table SI**. Values of $S_{ab}$, $H_{aa}$, $H_{bb}$ and $H_{ab}$ for a series of halogenated porphyrin dimers at different intermolecular distances, calculated with FODFT. The twist angle ($\alpha$) between two mono-halogenated porphyrin monomers was set to 180 degrees*

| Molecule | ΔZ (Å) | $H_{ab}$ (eV) | $H_{aa}$ (eV) | $H_{bb}$ (eV) | $S_{ab}$ (eV) |
|---|---|---|---|---|---|
| Porphyrin | 3 | 1.06100 | -4.30947 | -4.31130 | 0.10332 |
| | 3.5 | 0.55322 | -4.31391 | -4.31589 | 0.05997 |
| | 4 | 0.28537 | -4.37886 | -4.38131 | 0.03356 |
| | 4.5 | 0.14692 | -4.45211 | -4.45538 | 0.01838 |
| | 5 | 0.07559 | -4.51950 | -4.52290 | 0.00994 |
| | 5.2 | 0.05824 | -4.54345 | -4.54711 | -0.00779 |
| | 5.4 | 0.04468 | -4.56605 | -4.56984 | -0.00608 |
| | 5.6 | 0.03428 | -4.58738 | -4.59105 | -0.00474 |
| | 5.8 | 0.02631 | -4.60767 | -4.61122 | -0.00370 |
| | 6 | 0.02021 | -4.62659 | -4.63001 | -0.00288 |
| $H_2$PorphyrinF | 3 | -0.95865 | -4.40408 | -4.40193 | 0.09138 |
| | 3.5 | -0.49137 | -4.39804 | -4.39806 | 0.05237 |
| | 4 | -0.25001 | -4.45375 | -4.45406 | 0.02901 |
| | 4.5 | -0.12704 | -4.51862 | -4.51917 | 0.01576 |
| | 5 | -0.06473 | -4.57810 | -4.57944 | 0.00847 |
| | 5.2 | -0.04940 | -4.59974 | -4.60130 | 0.00660 |
| | 5.4 | -0.03772 | -4.62021 | -4.62176 | 0.00514 |
| | 5.6 | -0.02885 | -4.63922 | -4.64078 | 0.00400 |
| | 5.8 | -0.02207 | -4.65712 | -4.65869 | 0.00311 |
| | 6 | -0.01690 | -4.67394 | -4.67563 | 0.00242 |
| $H_2$PorphyrinCl | 3 | -0.90108 | -4.49140 | -4.49093 | 0.08471 |
| | 3.5 | -0.45026 | -4.48098 | -4.48097 | 0.04736 |
| | 4 | -0.22294 | -4.53328 | -4.53298 | 0.02560 |
| | 4.5 | -0.11029 | -4.59448 | -4.59407 | 0.01359 |
| | 5 | -0.05472 | -4.65162 | -4.65105 | 0.00716 |
| | 5.2 | -0.04139 | -4.67238 | -4.67180 | 0.00553 |
| | 5.4 | -0.03133 | -4.69163 | -4.69102 | 0.00428 |
| | 5.6 | -0.02372 | -4.70998 | -4.70925 | 0.00331 |
| | 5.8 | -0.01798 | -4.72711 | -4.72645 | 0.00256 |
| | 6 | -0.01364 | -4.74311 | -4.74256 | 0.00199 |
| $H_2$PorphyrinBr | 3 | -0.88693 | -4.49548 | -4.49466 | 0.08322 |
| | 3.5 | -0.43833 | -4.48580 | -4.48600 | 0.04582 |
| | 4 | -0.21330 | -4.53616 | -4.53667 | 0.02428 |
| | 4.5 | -0.10334 | -4.59745 | -4.59805 | 0.01258 |
| | 5 | -0.05009 | -4.65429 | -4.65486 | 0.00644 |
| | 5.2 | -0.03751 | -4.67474 | -4.67534 | 0.00492 |
| | 5.4 | -0.02808 | -4.69402 | -4.69460 | 0.00376 |
| | 5.6 | -0.02102 | -4.71241 | -4.71290 | 0.00287 |
| | 5.8 | -0.01575 | -4.72916 | -4.72981 | 0.00220 |
| | 6 | -0.01180 | -4.74558 | -4.74605 | 0.00168 |
| $H_2$PorphyrinI | 3 | -0.85395 | -4.49010 | -4.49071 | 0.08054 |
| | 3.5 | -0.41515 | -4.47960 | -4.47709 | 0.04361 |
| | 4 | -0.19728 | -4.52926 | -4.52550 | 0.02251 |
| | 4.5 | -0.09234 | -4.58842 | -4.58455 | 0.01124 |
| | 5 | -0.04275 | -4.64388 | -4.64037 | 0.00547 |

| | | | | | |
|---|---|---|---|---|---|
| | 5.2 | -0.03131 | -4.66385 | -4.66066 | 0.00408 |
| | 5.4 | -0.02286 | -4.68265 | -4.67964 | 0.00304 |
| | 5.6 | -0.01666 | -4.70036 | -4.69744 | 0.00226 |
| | 5.8 | -0.01212 | -4.71702 | -4.71412 | 0.00167 |
| | 6 | -0.00880 | -4.73268 | -4.72984 | 0.00124 |
| $H_2PorphyrinF_4$ | 3 | 0.84556 | -4.65371 | -4.65234 | 0.07428 |
| | 3.5 | 0.40505 | -4.62923 | -4.62836 | 0.03997 |
| | 4 | 0.19312 | -4.66109 | -4.66016 | 0.02093 |
| | 4.5 | 0.09227 | -4.70422 | -4.70319 | 0.01081 |
| | 5 | 0.04431 | -4.74596 | -4.74476 | 0.00555 |
| | 5.2 | 0.03307 | -4.76144 | -4.76019 | 0.00425 |
| | 5.4 | 0.02471 | -4.77585 | -4.77460 | 0.00325 |
| | 5.6 | 0.01846 | -4.78913 | -4.78785 | 0.00249 |
| | 5.8 | 0.01380 | -4.80196 | -4.80063 | 0.00191 |
| | 6 | 0.01031 | -4.81404 | -4.81263 | 0.00147 |
| $H_2PorphyrinCl_4$ | 3 | 1.03619 | -4.90072 | -4.90089 | 0.08913 |
| | 3.5 | 0.49400 | -4.86615 | -4.86620 | 0.04721 |
| | 4 | 0.23103 | -4.89624 | -4.89627 | 0.02383 |
| | 4.5 | 0.10660 | -4.93771 | -4.93737 | 0.01158 |
| | 5 | 0.04841 | -4.97685 | -4.97654 | 0.00544 |
| | 5.2 | 0.03509 | -4.99115 | -4.99068 | 0.00399 |
| | 5.4 | 0.02532 | -5.00471 | -5.00432 | 0.00291 |
| | 5.6 | 0.01816 | -5.01750 | -5.01712 | 0.00211 |
| | 5.8 | 0.01294 | -5.02971 | -5.02925 | 0.00152 |
| | 6 | 1.03619 | -4.90072 | -4.90089 | 0.08913 |
| $H_2PorphyrinBr_4$ | 3 | 1.18589 | -4.92430 | -4.92471 | 0.10281 |
| | 3.5 | 0.58971 | -4.85756 | -4.85769 | 0.05696 |
| | 4 | 0.28796 | -4.88062 | -4.88073 | 0.03011 |
| | 4.5 | 0.13927 | -4.92304 | -4.92313 | 0.01538 |
| | 5 | 0.06684 | -4.96426 | -4.96426 | 0.00762 |
| | 5.2 | 0.04967 | -4.97929 | -4.97925 | 0.00571 |
| | 5.4 | 0.03684 | -4.99350 | -4.99346 | 0.00425 |
| | 5.6 | 0.02724 | -5.00702 | -5.00699 | 0.00315 |
| | 5.8 | 0.02006 | -5.01954 | -5.01938 | 0.00232 |
| | 6 | 0.01472 | -5.03134 | -5.03133 | 0.00170 |
| $H_2PorphyrinI_4$ | 3 | 1.49716 | -5.08826 | -5.08826 | 0.13104 |
| | 3.5 | 0.81916 | -4.87049 | -4.87043 | 0.08060 |
| | 4 | 0.43937 | -4.84671 | -4.84667 | 0.04727 |
| | 4.5 | 0.23295 | -4.87475 | -4.87475 | 0.02690 |
| | 5 | 0.12323 | -4.91237 | -4.91233 | 0.01497 |
| | 5.2 | 0.09554 | -4.92698 | -4.92695 | 0.01178 |
| | 5.4 | 0.07389 | -4.94072 | -4.94070 | 0.00924 |
| | 5.6 | 0.05720 | -4.95386 | -4.95386 | 0.00723 |
| | 5.8 | 0.04414 | -4.96644 | -4.96641 | 0.00564 |
| | 6 | 1.49716 | -5.08826 | -5.08826 | 0.13104 |

***Table SII**. Values of $S_{ab}$, $V_{ab}$ and $\Delta E_{ex}$ for a series of halogenated porphyrin dimers at different intermolecular distances, calculated with FDE-ET. The twist angle ($\alpha$) between two mono-halogenated porphyrin monomers was set to 180 degrees*

| Molecule | R (Å) | $V_{ab}$ (eV) | $S_{ab}$ (eV) | $\Delta E_{ex}$ (eV) |
|---|---|---|---|---|
| Porphyrin | 3 | 0.6828 | 0.1092 | 1.3657 |
| | 3.5 | 0.3247 | 0.0638 | 0.6502 |
| | 4 | 0.1529 | 0.0354 | 0.3064 |
| | 4.5 | 0.0737 | 0.0193 | 0.1484 |
| | 5 | 0.0352 | 0.0103 | 0.0723 |
| | 5.2 | 0.0267 | 0.0081 | 0.0553 |
| | 5.4 | 0.0200 | 0.0064 | 0.0422 |
| | 5.6 | 0.0149 | 0.0049 | 0.0323 |
| | 5.8 | 0.0110 | 0.0038 | 0.0237 |
| | 6 | 0.0083 | 0.0030 | 0.0545 |
| $H_2$PorphyrinF | 3 | 0.6158 | 0.0967 | 1.2317 |
| | 3.5 | 0.2891 | 0.0558 | 0.5781 |
| | 4 | 0.1353 | 0.0307 | 0.2707 |
| | 4.5 | 0.0624 | 0.0165 | 0.1249 |
| | 5 | 0.0301 | 0.0089 | 0.0604 |
| | 5.2 | 0.0223 | 0.0069 | 0.0448 |
| | 5.4 | 0.0165 | 0.0053 | 0.0330 |
| | 5.6 | 0.0124 | 0.0042 | 0.0250 |
| | 5.8 | 0.0094 | 0.0033 | 0.0189 |
| | 6 | 0.0069 | 0.0025 | 0.0138 |
| $H_2$PorphyrinCl | 3 | 0.5844 | 0.0902 | 1.1687 |
| | 3.5 | 0.2651 | 0.0504 | 0.5303 |
| | 4 | 0.1196 | 0.0269 | 0.2393 |
| | 4.5 | 0.0546 | 0.0142 | 0.1096 |
| | 5 | 0.0250 | 0.0075 | 0.0501 |
| | 5.2 | 0.0183 | 0.0058 | 0.0366 |
| | 5.4 | 0.0133 | 0.0045 | 0.0266 |
| | 5.6 | 0.0096 | 0.0034 | 0.0203 |
| | 5.8 | 0.0071 | 0.0026 | 0.0147 |
| | 6 | 0.0053 | 0.0021 | 0.0116 |
| $H_2$PorphyrinBr | 3 | 0.5766 | 0.0889 | 1.1533 |
| | 3.5 | 0.2592 | 0.0488 | 0.5184 |
| | 4 | 0.1138 | 0.0255 | 0.2275 |
| | 4.5 | 0.0519 | 0.0128 | 0.1038 |
| | 5 | 0.0228 | 0.0067 | 0.0456 |
| | 5.2 | 0.0166 | 0.0051 | 0.0332 |
| | 5.4 | 0.0122 | 0.0039 | 0.0244 |
| | 5.6 | 0.0088 | 0.0029 | 0.0175 |
| | 5.8 | 0.0062 | 0.0022 | 0.0127 |
| | 6 | 0.0045 | 0.0017 | 0.0099 |
| $H_2$PorphyrinI | 3 | 0.5596 | 0.0864 | 1.1193 |
| | 3.5 | 0.2447 | 0.0464 | 0.4896 |
| | 4 | 0.1049 | 0.0235 | 0.2104 |
| | 4.5 | 0.0449 | 0.0115 | 0.0908 |
| | 5 | 0.0190 | 0.0055 | 0.0387 |
| | 5.2 | 0.0132 | 0.0040 | 0.0265 |
| | 5.4 | 0.0093 | 0.0030 | 0.0186 |
| | 5.6 | 0.0065 | 0.0022 | 0.0153 |
| | 5.8 | 0.0044 | 0.0017 | 0.0142 |
| | 6 | 0.0028 | 0.0012 | 0.0057 |
| $H_2$PorphyrinF$_4$ | 3 | 0.5436 | 0.0786 | 1.0873 |
| | 3.5 | 0.2419 | 0.0425 | 0.4841 |
| | 4 | 0.1072 | 0.0221 | 0.2145 |
| | 4.5 | 0.0468 | 0.0111 | 0.0935 |
| | 5 | 0.0212 | 0.0058 | 0.0437 |
| | 5.2 | 0.0153 | 0.0045 | 0.0306 |

| | | | | |
|---|---|---|---|---|
| | 5.4 | 0.0110 | 0.0034 | 0.0225 |
| | 5.6 | 0.0080 | 0.0026 | 0.0166 |
| | 5.8 | 0.0058 | 0.0020 | 0.0116 |
| | 6 | 0.0041 | 0.0016 | 0.0084 |
| $H_2PorphyrinCl_4$ | 3 | 0.6467 | 0.0922 | 1.2935 |
| | 3.5 | 0.2849 | 0.0489 | 0.5698 |
| | 4 | 0.1244 | 0.0245 | 0.2489 |
| | 4.5 | 0.0551 | 0.0118 | 0.1107 |
| | 5 | 0.0250 | 0.0056 | 0.0503 |
| | 5.2 | 0.0179 | 0.0040 | 0.0388 |
| | 5.4 | 0.0124 | 0.0030 | 0.0255 |
| | 5.6 | 0.0084 | 0.0022 | 0.0168 |
| | 5.8 | 0.0060 | 0.0015 | 0.0148 |
| | 6 | 0.0098 | 0.0011 | 0.0200 |
| $H_2PorphyrinBr_4$ | 3 | 0.7526 | 0.1077 | 1.5053 |
| | 3.5 | 0.3424 | 0.0596 | 0.6848 |
| | 4 | 0.1530 | 0.0315 | 0.3061 |
| | 4.5 | 0.0712 | 0.0160 | 0.1424 |
| | 5 | 0.0304 | 0.0080 | 0.0608 |
| | 5.2 | 0.0216 | 0.0061 | 0.0436 |
| | 5.4 | 0.0180 | 0.0045 | 0.0360 |
| | 5.6 | 0.0151 | 0.0033 | 0.0307 |
| | 5.8 | 0.0118 | 0.0024 | 0.0245 |
| | 6 | 0.0159 | 0.0018 | 0.0322 |
| $H_2PorphyrinI_4$ | 3 | 1.0029 | 0.1471 | 2.0059 |
| | 3.5 | 0.4916 | 0.0885 | 0.9831 |
| | 4 | 0.2389 | 0.0515 | 0.4779 |
| | 4.5 | 0.1168 | 0.0292 | 0.2336 |
| | 5 | 0.0599 | 0.0164 | 0.1198 |
| | 5.2 | 0.0452 | 0.0128 | 0.0903 |
| | 5.4 | 0.0388 | 0.0101 | 0.0776 |
| | 5.6 | 0.0204 | 0.0080 | 0.0408 |
| | 5.8 | 0.0195 | 0.0062 | 0.0390 |
| | 6 | 0.0155 | 0.0048 | 0.0311 |

**Table SIII.** *Values of $S_{ab}$, $H_{aa}$, $H_{bb}$ and $H_{ab}$ for a series of halogenated porphyrin dimers at different twist angles, at an intermolecular distance of 3.6 Angstroms, calculated with FODFT*

| Molecule | $\alpha$ | $H_{ab}$ (eV) | $H_{aa}$ (eV) | $H_{bb}$ (eV) | $S_{ab}$ (eV) |
|---|---|---|---|---|---|
| Porphyrin | 0 | 0.485 | -4.325 | -4.327 | -0.053 |
| | 15 | 0.336 | -4.319 | -4.321 | -0.037 |
| | 30 | 0.044 | -4.308 | -4.310 | -0.006 |
| | 45 | -0.103 | -4.302 | -4.304 | 0.010 |
| | 60 | 0.027 | -4.311 | -4.313 | -0.004 |
| | 75 | 0.295 | -4.325 | -4.327 | -0.033 |
| | 90 | 0.431 | -4.331 | -4.333 | -0.048 |
| | 105 | 0.296 | -4.325 | -4.327 | -0.033 |
| | 120 | 0.027 | -4.312 | -4.314 | -0.004 |
| | 135 | -0.103 | -4.303 | -4.305 | 0.010 |
| | 150 | 0.044 | -4.309 | -4.311 | -0.006 |
| | 165 | 0.338 | -4.320 | -4.322 | -0.038 |
| | 180 | 0.487 | -4.325 | -4.327 | -0.054 |
| $H_2PorphyrinF$ | 0 | 0.449 | -4.404 | -4.405 | -0.048 |
| | 15 | -0.310 | -4.397 | -4.401 | 0.034 |
| | 30 | -0.041 | -4.385 | -4.390 | 0.005 |

| | | | | | |
|---|---|---|---|---|---|
| | 45 | 0.091 | -4.378 | -4.384 | -0.009 |
| | 60 | -0.029 | -4.388 | -4.393 | 0.004 |
| | 75 | 0.268 | -4.404 | -4.407 | -0.029 |
| | 90 | -0.384 | -4.412 | -4.412 | 0.042 |
| | 105 | -0.262 | -4.406 | -4.404 | 0.029 |
| | 120 | -0.022 | -4.392 | -4.388 | 0.003 |
| | 135 | 0.093 | -4.383 | -4.377 | -0.009 |
| | 150 | 0.039 | -4.390 | -4.385 | -0.005 |
| | 165 | -0.299 | -4.402 | -4.399 | 0.033 |
| | 180 | -0.429 | -4.407 | -4.407 | 0.047 |
| $H_2$PorphyrinCl | 0 | 0.467 | -4.472 | -4.472 | -0.050 |
| | 15 | 0.320 | -4.466 | -4.472 | -0.034 |
| | 30 | 0.051 | -4.457 | -4.467 | -0.006 |
| | 45 | 0.079 | -4.453 | -4.465 | -0.007 |
| | 60 | -0.027 | -4.467 | -4.477 | 0.004 |
| | 75 | -0.244 | -4.485 | -4.492 | 0.026 |
| | 90 | -0.350 | -4.496 | -4.496 | 0.037 |
| | 105 | -0.241 | -4.492 | -4.487 | 0.026 |
| | 120 | -0.025 | -4.479 | -4.469 | 0.003 |
| | 135 | 0.078 | -4.469 | -4.457 | -0.007 |
| | 150 | 0.042 | -4.476 | -4.464 | -0.005 |
| | 165 | -0.275 | -4.486 | -4.480 | 0.030 |
| | 180 | -0.391 | -4.489 | -4.489 | 0.042 |
| $H_2$PorphyrinBr | 0 | 0.493 | -4.473 | -4.474 | -0.053 |
| | 15 | 0.335 | -4.467 | -4.472 | -0.036 |
| | 30 | -0.057 | -4.459 | -4.470 | 0.007 |
| | 45 | 0.074 | -4.455 | -4.468 | -0.007 |
| | 60 | -0.027 | -4.471 | -4.482 | 0.003 |
| | 75 | -0.236 | -4.490 | -4.497 | 0.025 |
| | 90 | -0.340 | -4.501 | -4.501 | 0.036 |
| | 105 | -0.235 | -4.497 | -4.491 | 0.025 |
| | 120 | -0.027 | -4.485 | -4.474 | 0.003 |
| | 135 | 0.073 | -4.475 | -4.461 | -0.007 |
| | 150 | -0.044 | -4.481 | -4.469 | 0.005 |
| | 165 | -0.268 | -4.491 | -4.485 | 0.029 |
| | 180 | -0.380 | -4.494 | -4.494 | 0.040 |
| $H_2$PorphyrinI | 0 | 0.565 | -4.477 | -4.473 | -0.060 |
| | 15 | 0.375 | -4.459 | -4.462 | -0.041 |
| | 30 | -0.067 | -4.446 | -4.455 | 0.008 |
| | 45 | 0.072 | -4.443 | -4.454 | -0.007 |
| | 60 | -0.022 | -4.461 | -4.469 | 0.003 |
| | 75 | -0.221 | -4.482 | -4.484 | 0.024 |
| | 90 | -0.321 | -4.494 | -4.490 | 0.034 |
| | 105 | -0.226 | -4.491 | -4.479 | 0.024 |
| | 120 | 0.034 | -4.479 | -4.461 | -0.004 |
| | 135 | 0.058 | -4.468 | -4.450 | -0.005 |
| | 150 | -0.049 | -4.476 | -4.458 | 0.006 |
| | 165 | 0.255 | -4.485 | -4.473 | -0.028 |
| | 180 | -0.358 | -4.487 | -4.484 | 0.038 |
| $H_2$PorphyrinF$_4$ | 0 | 0.301 | -4.639 | -4.638 | 0.031 |
| | 15 | 0.211 | -4.633 | -4.632 | 0.022 |
| | 30 | 0.041 | -4.621 | -4.620 | 0.005 |
| | 45 | -0.042 | -4.613 | -4.612 | 0.004 |
| | 60 | -0.033 | -4.621 | -4.620 | 0.004 |
| | 75 | -0.188 | -4.634 | -4.633 | 0.019 |
| | 90 | 0.270 | -4.640 | -4.639 | 0.028 |
| $H_2$PorphyrinCl$_4$ | 0 | 0.365 | -4.875 | -4.875 | 0.036 |
| | 15 | 0.246 | -4.876 | -4.876 | 0.025 |
| | 30 | 0.065 | -4.873 | -4.873 | 0.007 |
| | 45 | 0.011 | -4.869 | -4.869 | 0.001 |
| | 60 | -0.053 | -4.875 | -4.875 | 0.005 |
| | 75 | -0.221 | -4.878 | -4.879 | 0.022 |
| | 90 | -0.335 | -4.878 | -4.878 | 0.033 |

| | | | | | |
|---|---|---|---|---|---|
| | 0 | 0.443 | -4.862 | -4.862 | 0.044 |
| | 15 | -0.295 | -4.861 | -4.861 | 0.030 |
| | 30 | 0.089 | -4.862 | -4.862 | 0.010 |
| $H_2PorphyrinBr_4$ | 45 | 0.012 | -4.859 | -4.859 | 0.002 |
| | 60 | 0.079 | -4.864 | -4.864 | 0.008 |
| | 75 | -0.269 | -4.864 | -4.864 | 0.027 |
| | 90 | 0.408 | -4.865 | -4.865 | 0.041 |
| | 0 | 0.640 | -4.849 | -4.849 | 0.065 |
| | 15 | 0.416 | -4.826 | -4.826 | 0.044 |
| | 30 | 0.127 | -4.816 | -4.816 | 0.014 |
| $H_2PorphyrinI_4$ | 45 | -0.030 | -4.812 | -4.812 | 0.003 |
| | 60 | -0.117 | -4.818 | -4.818 | 0.013 |
| | 75 | -0.391 | -4.830 | -4.830 | 0.041 |
| | 90 | -0.607 | -4.853 | -4.853 | 0.062 |

**Table SIV.** *Values of $S_{ab}$, $H_{aa}$, $H_{bb}$ and $H_{ab}$ for a series of halogenated porphyrin dimers at different twist angles, at an intermolecular distance of 3.6 Angstroms, calculated with FDE-ET*

| Molecule | $\alpha$ | $V_{ab}$ (eV) | $S_{ab}$ (eV) | $\Delta E_{ex}$ (eV) |
|---|---|---|---|---|
| | 0 | 0.282 | 0.057 | 0.564 |
| | 15 | 0.192 | 0.039 | 0.385 |
| | 30 | 0.017 | 0.005 | 0.037 |
| | 45 | 0.073 | 0.012 | 0.147 |
| | 60 | 0.025 | 0.003 | 0.055 |
| | 75 | 0.168 | 0.034 | 0.337 |
| Porphyrin | 90 | 0.250 | 0.051 | 0.500 |
| | 105 | 0.168 | 0.034 | 0.337 |
| | 120 | 0.025 | 0.003 | 0.051 |
| | 135 | 0.073 | 0.012 | 0.147 |
| | 150 | 0.017 | 0.005 | 0.037 |
| | 165 | 0.192 | 0.039 | 0.385 |
| | 180 | 0.282 | 0.057 | 0.564 |
| | 0 | 0.258 | 0.052 | 0.516 |
| | 15 | 0.176 | 0.036 | 0.352 |
| | 30 | 0.017 | 0.005 | 0.035 |
| | 45 | 0.063 | 0.010 | 0.127 |
| | 60 | 0.027 | 0.003 | 0.054 |
| | 75 | 0.152 | 0.031 | 0.304 |
| $H_2PorphyrinF$ | 90 | 0.221 | 0.044 | 0.442 |
| | 105 | 0.149 | 0.030 | 0.297 |
| | 120 | 0.020 | 0.002 | 0.041 |
| | 135 | 0.066 | 0.011 | 0.131 |
| | 150 | 0.017 | 0.004 | 0.035 |
| | 165 | 0.169 | 0.034 | 0.338 |
| | 180 | 0.247 | 0.050 | 0.493 |
| | 0 | 0.267 | 0.052 | 0.535 |
| | 15 | 0.181 | 0.036 | 0.362 |
| | 30 | 0.025 | 0.006 | 0.051 |
| | 45 | 0.055 | 0.009 | 0.110 |
| | 60 | 0.024 | 0.003 | 0.049 |
| $H_2PorphyrinCl$ | 75 | 0.138 | 0.027 | 0.276 |
| | 90 | 0.201 | 0.040 | 0.402 |
| | 105 | 0.138 | 0.027 | 0.275 |
| | 120 | 0.023 | 0.002 | 0.047 |
| | 135 | 0.055 | 0.009 | 0.111 |
| | 150 | 0.021 | 0.004 | 0.041 |
| | 165 | 0.157 | 0.031 | 0.313 |

| | | | | |
|---|---|---|---|---|
| | 180 | 0.226 | 0.045 | 0.452 |
| $H_2$PorphyrinBr | 0 | 0.285 | 0.056 | 0.570 |
| | 15 | 0.190 | 0.038 | 0.379 |
| | 30 | 0.028 | 0.007 | 0.058 |
| | 45 | 0.052 | 0.008 | 0.105 |
| | 60 | 0.023 | 0.002 | 0.047 |
| | 75 | 0.134 | 0.026 | 0.268 |
| | 90 | 0.196 | 0.038 | 0.391 |
| | 105 | 0.134 | 0.026 | 0.268 |
| | 120 | 0.025 | 0.003 | 0.050 |
| | 135 | 0.052 | 0.008 | 0.106 |
| | 150 | 0.021 | 0.004 | 0.042 |
| | 165 | 0.153 | 0.030 | 0.305 |
| | 180 | 0.220 | 0.043 | 0.440 |
| $H_2$PorphyrinI | 0 | 0.333 | 0.065 | 0.666 |
| | 15 | 0.214 | 0.043 | 0.428 |
| | 30 | 0.034 | 0.008 | 0.068 |
| | 45 | 0.048 | 0.008 | 0.096 |
| | 60 | 0.018 | 0.002 | 0.036 |
| | 75 | 0.125 | 0.025 | 0.251 |
| | 90 | 0.184 | 0.036 | 0.369 |
| | 105 | 0.130 | 0.025 | 0.259 |
| | 120 | 0.031 | 0.003 | 0.065 |
| | 135 | 0.041 | 0.007 | 0.082 |
| | 150 | 0.026 | 0.005 | 0.054 |
| | 165 | 0.146 | 0.029 | 0.292 |
| | 180 | 0.207 | 0.041 | 0.414 |
| $H_2$PorphyrinF$_4$ | 0 | 0.204 | 0.037 | 0.409 |
| | 15 | 0.142 | 0.026 | 0.284 |
| | 30 | 0.030 | 0.005 | 0.060 |
| | 45 | 0.037 | 0.006 | 0.075 |
| | 60 | 0.033 | 0.004 | 0.067 |
| | 75 | 0.127 | 0.023 | 0.254 |
| | 90 | 0.183 | 0.033 | 0.367 |
| $H_2$PorphyrinCl$_4$ | 0 | 0.241 | 0.043 | 0.482 |
| | 15 | 0.160 | 0.029 | 0.320 |
| | 30 | 0.043 | 0.008 | 0.087 |
| | 45 | 0.023 | 0.001 | 0.046 |
| | 60 | 0.037 | 0.006 | 0.074 |
| | 75 | 0.146 | 0.026 | 0.291 |
| | 90 | 0.224 | 0.039 | 0.448 |
| $H_2$PorphyrinBr$_4$ | 0 | 0.292 | 0.053 | 0.585 |
| | 15 | 0.188 | 0.035 | 0.377 |
| | 30 | 0.053 | 0.011 | 0.109 |
| | 45 | 0.008 | 0.002 | 0.017 |
| | 60 | 0.048 | 0.010 | 0.100 |
| | 75 | 0.173 | 0.032 | 0.346 |
| | 90 | 0.272 | 0.049 | 0.545 |
| $H_2$PorphyrinI$_4$ | 0 | 0.424 | 0.080 | 0.848 |
| | 15 | 0.261 | 0.052 | 0.522 |
| | 30 | 0.074 | 0.016 | 0.148 |
| | 45 | 0.009 | 0.004 | 0.018 |
| | 60 | 0.069 | 0.015 | 0.138 |
| | 75 | 0.248 | 0.050 | 0.495 |
| | 90 | 0.407 | 0.076 | 0.813 |

***Table SV**. Values of $S_{ab}$, $H_{aa}$, $H_{bb}$ and $H_{ab}$ for a series of metallated porphyrin dimers at different intermolecular distances, at a twist angle of 0°, calculated with FODFT*

| Molecule | ΔZ (Å) | $H_{ab}$ (eV) | $H_{aa}$ (eV) | $H_{bb}$ (eV) | $S_{ab}$ (eV) |
|---|---|---|---|---|---|
| ZnPorphyrin | 3.5 | 0.611 | -4.427 | -4.427 | 0.066 |
| | 4 | 0.317 | -4.476 | -4.476 | 0.037 |
| | 4.5 | 0.163 | -4.544 | -4.544 | 0.020 |
| | 5 | 0.083 | -4.604 | -4.605 | 0.011 |
| NiPorphyrin | 3.5 | -0.390 | -3.853 | -3.853 | 0.048 |
| | 4 | -0.223 | -3.923 | -3.923 | 0.030 |
| | 4.5 | -0.128 | -4.014 | -4.014 | 0.018 |
| | 5 | -0.074 | -4.102 | -4.102 | 0.011 |
| FePorphyrin | 3.5 | -0.171 | -3.927 | -3.927 | 0.020 |
| | 4 | 0.092 | -4.036 | -4.031 | -0.012 |
| | 4.5 | 0.051 | -3.257 | -4.115 | -0.007 |
| | 5 | 0.031 | -4.235 | -4.235 | -0.005 |
| TiPorphyrin | 3.5 | 0.616 | 4.517 | -4.517 | 0.066 |
| | 4 | 0.322 | 4.557 | -4.557 | 0.037 |
| | 4.5 | 0.167 | 4.614 | -4.614 | 0.021 |
| | 5 | 0.086 | 4.664 | -4.664 | 0.011 |
| CdPorphyrin | 3.5 | 0.615 | -4.436 | -4.436 | -0.066 |
| | 4 | 0.322 | -4.480 | -4.480 | -0.037 |
| | 4.5 | 0.167 | -4.541 | -4.541 | -0.020 |
| | 5 | 0.086 | -4.600 | -4.600 | -0.011 |
| PdPorphyrin | 3.5 | 0.581 | -4.460 | -4.460 | -0.062 |
| | 4 | 0.299 | -4.516 | -4.516 | -0.035 |
| | 4.5 | 0.153 | -4.591 | -4.591 | -0.019 |
| | 5 | 0.078 | -4.660 | -4.660 | -0.010 |
| PtPorphyrin | 3.5 | 0.312 | -4.243 | -4.243 | -0.032 |
| | 4 | 0.150 | -4.347 | -4.347 | -0.017 |
| | 4.5 | 0.074 | -4.448 | -4.448 | -0.009 |
| | 5 | 0.038 | -4.535 | -4.535 | -0.005 |

***Table SVI**. Values of $S_{ab}$, $H_{aa}$, $H_{bb}$ and $H_{ab}$ for a series of metallated porphyrin dimers at different intermolecular distances, at a twist angle of 45°, calculated with FODFT*

| Molecule | ΔZ (Å) | $H_{ab}$ (eV) | $H_{aa}$ (eV) | $H_{bb}$ (eV) | $S_{ab}$ (eV) |
|---|---|---|---|---|---|
| Porphyrin | 3 | -0.26261 | -4.28380 | -4.28699 | 0.02234 |
| | 3.5 | -0.12090 | -4.29017 | -4.29259 | 0.01122 |
| | 4 | -0.05165 | -4.36048 | -4.36275 | 0.00511 |
| | 4.5 | -0.02013 | -4.43874 | -4.44187 | 0.00207 |
| | 5 | -0.00667 | -4.51017 | -4.51364 | 0.00068 |
| TPP | 3 | -0.17052 | -4.170 | -4.172 | 0.01547 |
| | 3.5 | -0.08222 | -4.180 | -4.182 | 0.00823 |
| | 4 | -0.03772 | -4.241 | -4.243 | 0.00406 |
| | 4.5 | -0.01603 | -4.312 | -4.313 | 0.00183 |
| | 5 | -0.00614 | -4.376 | -4.378 | 0.00073 |
| TPP-OMet | 3 | -0.16371 | -3.96796 | -3.95667 | 0.01522 |
| | 3.5 | -0.07874 | -3.99121 | -3.96925 | 0.00809 |
| | 4 | -0.03609 | -4.06324 | -4.03235 | 0.00399 |
| | 4.5 | -0.01532 | -4.14271 | -4.10580 | 0.00180 |
| | 5 | -0.00584 | -4.21470 | -4.17336 | 0.00072 |

| | | | | | |
|---|---|---|---|---|---|
| TPP-OEt | 3 | -0.13563 | -3.89973 | -3.91638 | 0.01248 |
| | 3.5 | -0.06478 | -3.90250 | -3.92394 | 0.00656 |
| | 4 | -0.02940 | -3.97022 | -3.99253 | 0.00320 |
| | 4.5 | -0.01229 | -4.04943 | -4.06973 | 0.00142 |
| | 5 | -0.00456 | -4.12096 | -4.13925 | 0.00055 |
| *meso*-Tetra-Pyridineporphyrin | 3 | -0.19121 | -5.04853 | -5.04710 | 0.01581 |
| | 3.5 | -0.09411 | -5.02942 | -5.02896 | 0.00850 |
| | 4 | -0.04389 | -5.06156 | -5.06137 | 0.00423 |
| | 4.5 | -0.01896 | -5.10470 | -5.10460 | 0.00193 |
| | 5 | -0.00740 | -5.14352 | -5.14344 | 0.00078 |
| ZnTPP | 3.5 | -0.06776 | -4.30095 | -4.30350 | 0.00663 |
| | 4 | -0.02966 | -4.35340 | -4.35535 | 0.00318 |
| | 4.5 | -0.01201 | -4.41854 | -4.42023 | 0.00144 |
| | 5 | -0.00433 | -4.47784 | -4.47932 | 0.00060 |
| PdTPP | 3.5 | -0.11434 | -4.31009 | -4.31320 | 0.01128 |
| | 4 | -0.05491 | -4.36771 | -4.37038 | 0.00566 |
| | 4.5 | -0.02465 | -4.43939 | -4.44171 | 0.00260 |
| | 5 | -0.01017 | -4.50604 | -4.50793 | 0.00107 |
| NiTPP | 3.5 | 0.37528 | -3.78709 | -3.79250 | 0.04632 |
| | 4 | 0.21715 | -3.85585 | -3.86165 | 0.02946 |
| | 4.5 | 0.12586 | -3.94358 | -3.94944 | 0.01828 |
| | 5 | 0.07331 | -4.02737 | -4.03328 | 0.01120 |
| PtTPP | 3.5 | 0.12920 | -4.34524 | -4.34884 | 0.01300 |
| | 4 | 0.06495 | -4.39679 | -4.39933 | 0.00695 |
| | 4.5 | 0.03085 | -4.46548 | -4.46756 | 0.00347 |
| | 5 | 0.01369 | -4.53102 | -4.53276 | 0.00159 |

Figure 1S. Linear fitting of Ln($V_{ab}$) with respect to R/2 for the exponential decay of $V_{ab}$ as given by equations (7)

## Cartesian coordinates of Porphyrin and derivatives.

The coordinates are given for the isolated monomers of each species.

**Porphyrin**

| | | | |
|---|---|---|---|
| N | -1.43165 | -1.42682 | 0.00000 |
| N | 1.43165 | 1.42682 | 0.00000 |
| C | 2.53551 | 3.47673 | 0.00000 |
| C | 1.25595 | 2.78006 | 0.00000 |
| C | 0.02189 | 3.43769 | 0.00000 |
| C | -1.24156 | 2.85203 | 0.00000 |
| C | -2.51623 | 3.50578 | 0.00000 |
| C | -3.48802 | 2.53686 | 0.00000 |
| C | 3.49072 | 2.51338 | 0.00000 |
| C | -2.83881 | 1.25981 | 0.00000 |
| C | 2.78313 | 1.23961 | 0.00000 |
| C | -3.43130 | -0.00038 | 0.00000 |
| C | 3.43130 | 0.00038 | 0.00000 |
| C | -2.78313 | -1.23961 | 0.00000 |
| C | 2.83881 | -1.25981 | 0.00000 |
| C | -3.49072 | -2.51338 | 0.00000 |
| C | 3.48802 | -2.53686 | 0.00000 |
| C | -2.53551 | -3.47673 | 0.00000 |
| C | 2.51623 | -3.50578 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -1.25595 | -2.78006 | 0.00000 |
| C | -0.02189 | -3.43769 | 0.00000 |
| C | 1.24156 | -2.85203 | 0.00000 |
| H | -0.76785 | 0.78534 | 0.00000 |
| H | 0.76785 | -0.78534 | 0.00000 |
| H | 4.51922 | 0.01345 | 0.00000 |
| H | -4.56850 | -2.63508 | 0.00000 |
| H | -4.51922 | -0.01345 | 0.00000 |
| H | -0.04211 | -4.52539 | 0.00000 |
| N | -1.49052 | 1.50454 | 0.00000 |
| N | 1.49052 | -1.50454 | 0.00000 |
| H | 0.04211 | 4.52539 | 0.00000 |
| H | -2.65189 | 4.58031 | 0.00000 |
| H | 2.66615 | 4.55349 | 0.00000 |
| H | -4.56224 | 2.67560 | 0.00000 |
| H | 4.56850 | 2.63508 | 0.00000 |
| H | 4.56224 | -2.67560 | 0.00000 |
| H | -2.66615 | -4.55349 | 0.00000 |
| H | 2.65189 | -4.58031 | 0.00000 |

**$H_2$PorphyrinF**

| | | | |
|---|---|---|---|
| N | 0.02699 | -2.02179 | 0.00000 |
| N | -0.03314 | 2.02673 | 0.00000 |
| C | -0.71470 | 4.25911 | 0.00000 |
| C | -1.11197 | 2.86433 | 0.00000 |
| C | -2.43337 | 2.41442 | 0.00000 |
| C | -2.91610 | 1.10749 | 0.00000 |
| C | -4.27102 | 0.65908 | 0.00000 |
| C | -4.24825 | -0.71553 | 0.00000 |
| C | 0.64500 | 4.24954 | 0.00000 |
| C | -2.88218 | -1.14167 | 0.00000 |
| C | 1.05129 | 2.85308 | 0.00000 |
| C | -2.39261 | -2.44856 | 0.00000 |
| C | 2.39067 | 2.44122 | 0.00000 |
| C | -1.05638 | -2.85355 | 0.00000 |
| C | 2.87889 | 1.13925 | 0.00000 |
| C | -0.64454 | -4.25164 | 0.00000 |
| C | 4.24909 | 0.71540 | 0.00000 |
| C | 0.71195 | -4.24709 | 0.00000 |
| C | 4.26901 | -0.65586 | 0.00000 |
| C | 1.11410 | -2.84653 | 0.00000 |
| C | 2.44919 | -2.42943 | 0.00000 |
| C | 2.91220 | -1.11670 | 0.00000 |
| H | -1.09672 | 0.01185 | 0.00000 |
| H | 1.09895 | -0.02967 | 0.00000 |
| H | 3.14294 | 3.22711 | 0.00000 |
| H | -1.31333 | -5.10537 | 0.00000 |
| H | -3.14501 | -3.23416 | 0.00000 |
| H | 3.21131 | -3.20565 | 0.00000 |
| N | -2.11604 | -0.00656 | 0.00000 |
| N | 2.11744 | -0.00131 | 0.00000 |
| F | -3.39980 | 3.37740 | 0.00000 |
| H | -5.13330 | 1.31206 | 0.00000 |
| H | -1.38482 | 5.10959 | 0.00000 |
| H | -5.09793 | -1.38699 | 0.00000 |
| H | 1.31688 | 5.10095 | 0.00000 |
| H | 5.09702 | 1.38921 | 0.00000 |

| | | | |
|---|---|---|---|
| H | 1.38691 | -5.09608 | 0.00000 |
| H | 5.13573 | -1.30537 | 0.00000 |

**$H_2$PorphyrinCl**

| | | | |
|---|---|---|---|
| N | 0.06253 | -2.02283 | 0.00000 |
| N | -0.08191 | 2.03132 | 0.00000 |
| C | -0.70731 | 4.27752 | 0.00000 |
| C | -1.14556 | 2.89228 | 0.00000 |
| C | -2.48467 | 2.46421 | 0.00000 |
| C | -2.94634 | 1.14282 | 0.00000 |
| C | -4.28938 | 0.65361 | 0.00000 |
| C | -4.23239 | -0.71751 | 0.00000 |
| C | 0.64946 | 4.23870 | 0.00000 |
| C | -2.85588 | -1.10973 | 0.00000 |
| C | 1.02317 | 2.83247 | 0.00000 |
| C | -2.36285 | -2.41324 | 0.00000 |
| C | 2.35691 | 2.41094 | 0.00000 |
| C | -1.03225 | -2.83641 | 0.00000 |
| C | 2.85713 | 1.11196 | 0.00000 |
| C | -0.64288 | -4.24162 | 0.00000 |
| C | 4.23477 | 0.71198 | 0.00000 |
| C | 0.71404 | -4.25897 | 0.00000 |
| C | 4.27970 | -0.65938 | 0.00000 |
| C | 1.13740 | -2.86492 | 0.00000 |
| C | 2.47538 | -2.45749 | 0.00000 |
| C | 2.93046 | -1.14148 | 0.00000 |
| H | -1.10102 | 0.12161 | 0.00000 |
| H | 1.09779 | -0.11017 | 0.00000 |
| H | 3.10853 | 3.19848 | 0.00000 |
| H | -1.32697 | -5.08331 | 0.00000 |
| H | -3.12163 | -3.19383 | 0.00000 |
| H | 3.23665 | -3.23475 | 0.00000 |
| N | -2.11857 | 0.04625 | 0.00000 |
| N | 2.11570 | -0.03947 | 0.00000 |
| Cl | -3.72577 | 3.69824 | 0.00000 |
| H | -5.16940 | 1.28203 | 0.00000 |
| H | -1.35408 | 5.14529 | 0.00000 |
| H | -5.06384 | -1.41194 | 0.00000 |
| H | 1.34206 | 5.07337 | 0.00000 |
| H | 5.06938 | 1.40270 | 0.00000 |
| H | 1.37658 | -5.11786 | 0.00000 |
| H | 5.15730 | -1.29443 | 0.00000 |

**$H_2$PorphyrinBr**

| | | | |
|---|---|---|---|
| N | 0.06299 | -2.02067 | 0.00000 |
| N | -0.08957 | 2.03767 | 0.00000 |
| C | -0.70499 | 4.28584 | 0.00000 |
| C | -1.15201 | 2.90204 | 0.00000 |
| C | -2.49022 | 2.47042 | 0.00000 |
| C | -2.95598 | 1.15098 | 0.00000 |
| C | -4.29680 | 0.65391 | 0.00000 |
| C | -4.23472 | -0.71602 | 0.00000 |
| C | 0.65078 | 4.24110 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -2.85786 | -1.10297 | 0.00000 |
| C | 1.01858 | 2.83448 | 0.00000 |
| C | -2.36305 | -2.40627 | 0.00000 |
| C | 2.35206 | 2.41085 | 0.00000 |
| C | -1.03266 | -2.83187 | 0.00000 |
| C | 2.85368 | 1.11259 | 0.00000 |
| C | -0.64604 | -4.23742 | 0.00000 |
| C | 4.23042 | 0.71373 | 0.00000 |
| C | 0.71088 | -4.25753 | 0.00000 |
| C | 4.27624 | -0.65752 | 0.00000 |
| C | 1.13689 | -2.86442 | 0.00000 |
| C | 2.47459 | -2.45683 | 0.00000 |
| C | 2.92824 | -1.14040 | 0.00000 |
| H | -1.10757 | 0.13493 | 0.00000 |
| H | 1.09481 | -0.10854 | 0.00000 |
| H | 3.10288 | 3.19888 | 0.00000 |
| H | -1.33064 | -5.07883 | 0.00000 |
| H | -3.12190 | -3.18666 | 0.00000 |
| H | 5.15497 | -1.29091 | 0.00000 |
| N | -2.12496 | 0.05561 | 0.00000 |
| N | 2.11273 | -0.03916 | 0.00000 |
| Br | -3.85339 | 3.82565 | 0.00000 |
| H | -5.18104 | 1.27641 | 0.00000 |
| H | -1.34518 | 5.15849 | 0.00000 |
| H | -5.06510 | -1.41164 | 0.00000 |
| H | 1.34566 | 5.07393 | 0.00000 |
| H | 5.06592 | 1.40329 | 0.00000 |
| H | 1.37038 | -5.11875 | 0.00000 |
| H | 3.23696 | -3.23246 | 0.00000 |

**$H_2$PorphyrinI**

| | | | |
|---|---|---|---|
| N | 0.07161 | -2.01903 | 0.00000 |
| N | -0.10700 | 2.04023 | 0.00000 |
| C | -0.70530 | 4.29142 | 0.00000 |
| C | -1.16586 | 2.91045 | 0.00000 |
| C | -2.50989 | 2.49030 | 0.00000 |
| C | -2.96599 | 1.16550 | 0.00000 |
| C | -4.30364 | 0.65442 | 0.00000 |
| C | -4.23118 | -0.71404 | 0.00000 |
| C | 0.64911 | 4.23890 | 0.00000 |
| C | -2.85034 | -1.09025 | 0.00000 |
| C | 1.00740 | 2.82920 | 0.00000 |
| C | -2.35565 | -2.39250 | 0.00000 |
| C | 2.33887 | 2.40241 | 0.00000 |
| C | -1.02783 | -2.82442 | 0.00000 |
| C | 2.84263 | 1.10578 | 0.00000 |
| C | -0.64791 | -4.23215 | 0.00000 |
| C | 4.22250 | 0.71401 | 0.00000 |
| C | 0.70853 | -4.25913 | 0.00000 |
| C | 4.27577 | -0.65674 | 0.00000 |
| C | 1.14090 | -2.86804 | 0.00000 |
| C | 2.47919 | -2.46367 | 0.00000 |
| C | 2.92970 | -1.14591 | 0.00000 |
| H | -1.11045 | 0.17200 | 0.00000 |

| | | | |
|---|---|---|---|
| H | 1.09041 | -0.13102 | 0.00000 |
| H | 3.09040 | 3.18950 | 0.00000 |
| H | -1.33703 | -5.06968 | 0.00000 |
| H | -3.11715 | -3.17005 | 0.00000 |
| H | 5.15712 | -1.28610 | 0.00000 |
| N | -2.12702 | 0.07490 | 0.00000 |
| N | 2.10796 | -0.04924 | 0.00000 |
| I | -4.01237 | 3.98615 | 0.00000 |
| H | -5.19226 | 1.27051 | 0.00000 |
| H | -1.33949 | 5.16843 | 0.00000 |
| H | -5.05421 | -1.41782 | 0.00000 |
| H | 1.34986 | 5.06633 | 0.00000 |
| H | 5.05273 | 1.40953 | 0.00000 |
| H | 1.36428 | -5.12309 | 0.00000 |
| H | 3.24120 | -3.23948 | 0.00000 |

**$H_2$PorphyrinF$_4$**

| | | | |
|---|---|---|---|
| N | 0.02048 | -2.03259 | 0.00000 |
| N | -0.02060 | 2.03168 | 0.00000 |
| C | -0.71450 | 4.25841 | 0.00000 |
| C | -1.10496 | 2.86250 | 0.00000 |
| C | -2.42627 | 2.40931 | 0.00000 |
| C | -2.91036 | 1.10202 | 0.00000 |
| C | -4.26481 | 0.65470 | 0.00000 |
| C | -4.25099 | -0.72125 | 0.00000 |
| C | 0.64650 | 4.26644 | 0.00000 |
| C | -2.88769 | -1.14199 | 0.00000 |
| C | 1.05362 | 2.87504 | 0.00000 |
| C | -2.38137 | -2.44097 | 0.00000 |
| C | 2.38110 | 2.43988 | 0.00000 |
| C | -1.05395 | -2.87602 | 0.00000 |
| C | 2.88732 | 1.14103 | 0.00000 |
| C | -0.64665 | -4.26730 | 0.00000 |
| C | 4.25048 | 0.72012 | 0.00000 |
| C | 0.71436 | -4.25921 | 0.00000 |
| C | 4.26415 | -0.65579 | 0.00000 |
| C | 1.10489 | -2.86329 | 0.00000 |
| C | 2.42630 | -2.41027 | 0.00000 |
| C | 2.91040 | -1.10292 | 0.00000 |
| H | -1.09237 | 0.00292 | 0.00000 |
| H | 1.09221 | -0.00461 | 0.00000 |
| F | 3.33281 | 3.41628 | 0.00000 |
| H | -1.31147 | -5.12194 | 0.00000 |
| F | -3.33310 | -3.41739 | 0.00000 |
| F | 3.39256 | -3.37186 | 0.00000 |
| N | -2.11072 | -0.01202 | 0.00000 |
| N | 2.11054 | 0.01084 | 0.00000 |
| F | -3.39263 | 3.37077 | 0.00000 |
| H | -5.12663 | 1.30829 | 0.00000 |
| H | -1.38960 | 5.10496 | 0.00000 |
| H | -5.09943 | -1.39212 | 0.00000 |
| H | 1.31151 | 5.12089 | 0.00000 |
| H | 5.09892 | 1.39093 | 0.00000 |
| H | 1.38939 | -5.10584 | 0.00000 |
| H | 5.12595 | -1.30941 | 0.00000 |

**$H_2$PorphyrinCl$_4$**

| | | | |
|---|---|---|---|
| N | 0.01744 | -2.03989 | 0.00000 |
| N | -0.01748 | 2.03968 | 0.00000 |
| C | -0.71198 | 4.26420 | 0.00000 |
| C | -1.10710 | 2.86775 | 0.00000 |
| C | -2.43916 | 2.42256 | 0.00000 |
| C | -2.90967 | 1.10404 | 0.00000 |
| C | -4.26316 | 0.65187 | 0.00000 |
| C | -4.25116 | -0.71894 | 0.00000 |
| C | 0.64333 | 4.27445 | 0.00000 |
| C | -2.88966 | -1.14782 | 0.00000 |
| C | 1.05953 | 2.88398 | 0.00000 |
| C | -2.39819 | -2.45876 | 0.00000 |
| C | 2.39827 | 2.45929 | 0.00000 |
| C | -1.05954 | -2.88415 | 0.00000 |
| C | 2.89021 | 1.14853 | 0.00000 |
| C | -0.64318 | -4.27461 | 0.00000 |
| C | 4.25116 | 0.71958 | 0.00000 |
| C | 0.71216 | -4.26436 | 0.00000 |
| C | 4.26288 | -0.65147 | 0.00000 |
| C | 1.10719 | -2.86779 | 0.00000 |
| C | 2.43908 | -2.42231 | 0.00000 |
| C | 2.90932 | -1.10345 | 0.00000 |
| H | -1.09400 | -0.00219 | 0.00000 |
| H | 1.09395 | 0.00383 | 0.00000 |
| Cl | 3.62512 | 3.70835 | 0.00000 |
| H | -1.30236 | -5.13209 | 0.00000 |
| Cl | -3.62539 | -3.70773 | 0.00000 |
| Cl | 3.68529 | -3.65151 | 0.00000 |
| N | -2.11180 | -0.01472 | 0.00000 |
| N | 2.11176 | 0.01553 | 0.00000 |
| Cl | -3.68566 | 3.65157 | 0.00000 |
| H | -5.12516 | 1.30378 | 0.00000 |
| H | -1.38413 | 5.11165 | 0.00000 |
| H | -5.10175 | -1.38556 | 0.00000 |
| H | 1.30249 | 5.13199 | 0.00000 |
| H | 5.10229 | 1.38555 | 0.00000 |
| H | 1.38448 | -5.11169 | 0.00000 |
| H | 5.12485 | -1.30334 | 0.00000 |

**$H_2$PorphyrinBr$_4$**

| | | | |
|---|---|---|---|
| N | 0.01643 | -2.04635 | 0.00000 |
| N | -0.01658 | 2.04689 | 0.00000 |
| C | -0.71168 | 4.27072 | 0.00000 |
| C | -1.10839 | 2.87364 | 0.00000 |
| C | -2.43788 | 2.42095 | 0.00000 |
| C | -2.91294 | 1.10445 | 0.00000 |
| C | -4.26599 | 0.64974 | 0.00000 |
| C | -4.25487 | -0.71891 | 0.00000 |
| C | 0.64154 | 4.28197 | 0.00000 |
| C | -2.89441 | -1.15143 | 0.00000 |
| C | 1.06137 | 2.89156 | 0.00000 |
| C | -2.39823 | -2.46015 | 0.00000 |
| C | 2.39808 | 2.46068 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -1.06152 | -2.89101 | 0.00000 |
| C | 2.89429 | 1.15195 | 0.00000 |
| C | -0.64172 | -4.28147 | 0.00000 |
| C | 4.25462 | 0.71937 | 0.00000 |
| C | 0.71146 | -4.27029 | 0.00000 |
| C | 4.26561 | -0.64932 | 0.00000 |
| C | 1.10823 | -2.87313 | 0.00000 |
| C | 2.43759 | -2.42034 | 0.00000 |
| C | 2.91256 | -1.10381 | 0.00000 |
| H | -1.09834 | -0.00828 | 0.00000 |
| H | 1.09799 | 0.00928 | 0.00000 |
| Br | 3.74719 | 3.83224 | 0.00000 |
| H | -1.29634 | -5.14261 | 0.00000 |
| Br | -3.74701 | -3.83210 | 0.00000 |
| Br | 3.80894 | -3.76998 | 0.00000 |
| N | -2.11656 | -0.01709 | 0.00000 |
| N | 2.11620 | 0.01769 | 0.00000 |
| Br | -3.80912 | 3.77070 | 0.00000 |
| H | -5.13031 | 1.29864 | 0.00000 |
| H | -1.38081 | 5.12063 | 0.00000 |
| H | -5.10856 | -1.38173 | 0.00000 |
| H | 1.29629 | 5.14299 | 0.00000 |
| H | 5.10840 | 1.38207 | 0.00000 |
| H | 1.38028 | -5.12046 | 0.00000 |
| H | 5.12994 | -1.29821 | 0.00000 |

**$H_2$PorphyrinI$_4$**

| | | | |
|---|---|---|---|
| N | 0.01695 | -2.04889 | 0.00000 |
| N | -0.01666 | 2.04903 | 0.00000 |
| C | -0.71042 | 4.27247 | 0.00000 |
| C | -1.11104 | 2.87480 | 0.00000 |
| C | -2.44477 | 2.42826 | 0.00000 |
| C | -2.91225 | 1.10719 | 0.00000 |
| C | -4.26607 | 0.64842 | 0.00000 |
| C | -4.25473 | -0.71836 | 0.00000 |
| C | 0.64086 | 4.28351 | 0.00000 |
| C | -2.89352 | -1.15454 | 0.00000 |
| C | 1.06409 | 2.89257 | 0.00000 |
| C | -2.40461 | -2.46774 | 0.00000 |
| C | 2.40475 | 2.46798 | 0.00000 |
| C | -1.06379 | -2.89248 | 0.00000 |
| C | 2.89371 | 1.15470 | 0.00000 |
| C | -0.64028 | -4.28338 | 0.00000 |
| C | 4.25486 | 0.71820 | 0.00000 |
| C | 0.71096 | -4.27224 | 0.00000 |
| C | 4.26601 | -0.64855 | 0.00000 |
| C | 1.11139 | -2.87458 | 0.00000 |
| C | 2.44479 | -2.42810 | 0.00000 |
| C | 2.91218 | -1.10705 | 0.00000 |
| H | -1.09837 | -0.00850 | 0.00000 |
| H | 1.09845 | 0.00882 | 0.00000 |
| I | 3.89558 | 3.98509 | 0.00000 |
| H | -1.29366 | -5.14516 | 0.00000 |

| | | | |
|---|---|---|---|
| I | -3.89645 | -3.98382 | 0.00000 |
| I | 3.96054 | -3.92019 | 0.00000 |
| N | -2.11671 | -0.01717 | 0.00000 |
| N | 2.11679 | 0.01740 | 0.00000 |
| I | -3.96043 | 3.92044 | 0.00000 |
| H | -5.13087 | 1.29628 | 0.00000 |
| H | -1.37789 | 5.12342 | 0.00000 |
| H | -5.10862 | -1.38054 | 0.00000 |
| H | 1.29440 | 5.14520 | 0.00000 |
| H | 5.10888 | 1.38018 | 0.00000 |
| H | 1.37852 | -5.12310 | 0.00000 |
| H | 5.13068 | -1.29657 | 0.00000 |

**ZnPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.44805 | 1.44803 | 0.00000 |
| N | 1.44805 | -1.44803 | 0.00000 |
| C | 3.48429 | -2.51984 | 0.00000 |
| C | 2.80534 | -1.24684 | 0.00000 |
| C | 3.42950 | 0.00000 | 0.00000 |
| C | 2.80534 | 1.24684 | 0.00000 |
| C | 3.48429 | 2.51984 | 0.00000 |
| C | 2.51999 | 3.48417 | 0.00000 |
| C | 2.51999 | -3.48417 | 0.00000 |
| C | 1.24695 | 2.80535 | 0.00000 |
| C | 1.24695 | -2.80535 | 0.00000 |
| C | 0.00000 | 3.42936 | 0.00000 |
| C | 0.00000 | -3.42936 | 0.00000 |
| C | -1.24695 | 2.80535 | 0.00000 |
| C | -1.24695 | -2.80535 | 0.00000 |
| C | -2.51999 | 3.48417 | 0.00000 |
| C | -2.51999 | -3.48417 | 0.00000 |
| C | -3.48429 | 2.51984 | 0.00000 |
| C | -3.48429 | -2.51984 | 0.00000 |
| C | -2.80534 | 1.24684 | 0.00000 |
| C | -3.42950 | 0.00000 | 0.00000 |
| C | -2.80534 | -1.24684 | 0.00000 |
| H | -4.56019 | 2.65211 | 0.00000 |
| H | -4.56019 | -2.65211 | 0.00000 |
| H | 0.00000 | -4.51739 | 0.00000 |
| H | -2.65239 | 4.56001 | 0.00000 |
| H | 0.00000 | 4.51739 | 0.00000 |
| H | -4.51763 | 0.00000 | 0.00000 |
| N | 1.44805 | 1.44803 | 0.00000 |
| N | -1.44805 | -1.44803 | 0.00000 |
| H | 4.51763 | 0.00000 | 0.00000 |
| H | 4.56019 | 2.65211 | 0.00000 |
| H | 4.56019 | -2.65211 | 0.00000 |
| H | 2.65239 | 4.56001 | 0.00000 |
| H | 2.65239 | -4.56001 | 0.00000 |
| H | -2.65239 | -4.56001 | 0.00000 |
| Zn | 0.00000 | 0.00000 | 0.00000 |

**NiPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.38309 | 1.38301 | 0.00000 |
| N | 1.38309 | -1.38301 | 0.00000 |

| | | | |
|---|---|---|---|
| C | 3.43514 | -2.47457 | 0.00000 |
| C | 2.75329 | -1.21171 | 0.00000 |
| C | 3.40612 | 0.00000 | 0.00000 |
| C | 2.75329 | 1.21171 | 0.00000 |
| C | 3.43514 | 2.47457 | 0.00000 |
| C | 2.47473 | 3.43484 | 0.00000 |
| C | 2.47473 | -3.43484 | 0.00000 |
| C | 1.21178 | 2.75311 | 0.00000 |
| C | 1.21178 | -2.75311 | 0.00000 |
| C | 0.00000 | 3.40590 | 0.00000 |
| C | 0.00000 | -3.40590 | 0.00000 |
| C | -1.21178 | 2.75311 | 0.00000 |
| C | -1.21178 | -2.75311 | 0.00000 |
| C | -2.47473 | 3.43484 | 0.00000 |
| C | -2.47473 | -3.43484 | 0.00000 |
| C | -3.43514 | 2.47457 | 0.00000 |
| C | -3.43514 | -2.47457 | 0.00000 |
| C | -2.75329 | 1.21171 | 0.00000 |
| C | -3.40612 | 0.00000 | 0.00000 |
| C | -2.75329 | -1.21171 | 0.00000 |
| H | -4.51255 | 2.58780 | 0.00000 |
| H | -4.51255 | -2.58780 | 0.00000 |
| H | 0.00000 | -4.49225 | 0.00000 |
| H | -2.58788 | 4.51219 | 0.00000 |
| H | 0.00000 | 4.49225 | 0.00000 |
| H | -4.49249 | 0.00000 | 0.00000 |
| N | 1.38309 | 1.38301 | 0.00000 |
| N | -1.38309 | -1.38301 | 0.00000 |
| H | 4.49249 | 0.00000 | 0.00000 |
| H | 4.51255 | 2.58780 | 0.00000 |
| H | 4.51255 | -2.58780 | 0.00000 |
| H | 2.58788 | 4.51219 | 0.00000 |
| H | 2.58788 | -4.51219 | 0.00000 |
| H | -2.58788 | -4.51219 | 0.00000 |
| Ni | 0.00000 | 0.00000 | 0.00000 |

**FePorphyrin**

| | | | |
|---|---|---|---|
| N | -1.39731 | 1.39601 | 0.00000 |
| N | 1.39731 | -1.39601 | 0.00000 |
| C | 3.44821 | -2.48577 | 0.00000 |
| C | 2.77136 | -1.22134 | 0.00000 |
| C | 3.41632 | 0.00000 | 0.00000 |
| C | 2.77136 | 1.22134 | 0.00000 |
| C | 3.44821 | 2.48577 | 0.00000 |
| C | 2.48520 | 3.44822 | 0.00000 |
| C | 2.48520 | -3.44822 | 0.00000 |
| C | 1.22133 | 2.76982 | 0.00000 |
| C | 1.22133 | -2.76982 | 0.00000 |
| C | 0.00000 | 3.41540 | 0.00000 |
| C | 0.00000 | -3.41540 | 0.00000 |
| C | -1.22133 | 2.76982 | 0.00000 |
| C | -1.22133 | -2.76982 | 0.00000 |
| C | -2.48520 | 3.44822 | 0.00000 |
| C | -2.48520 | -3.44822 | 0.00000 |
| C | -3.44821 | 2.48577 | 0.00000 |
| C | -3.44821 | -2.48577 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -2.77136 | 1.22134 | 0.00000 |
| C | -3.41632 | 0.00000 | 0.00000 |
| C | -2.77136 | -1.22134 | 0.00000 |
| H | -4.52488 | 2.60907 | 0.00000 |
| H | -4.52488 | -2.60907 | 0.00000 |
| H | 0.00000 | -4.50244 | 0.00000 |
| H | -2.60726 | 4.52494 | 0.00000 |
| H | 0.00000 | 4.50244 | 0.00000 |
| H | -4.50328 | 0.00000 | 0.00000 |
| N | 1.39731 | 1.39601 | 0.00000 |
| N | -1.39731 | -1.39601 | 0.00000 |
| H | 4.50328 | 0.00000 | 0.00000 |
| H | 4.52488 | 2.60907 | 0.00000 |
| H | 4.52488 | -2.60907 | 0.00000 |
| H | 2.60726 | 4.52494 | 0.00000 |
| H | 2.60726 | -4.52494 | 0.00000 |
| H | -2.60726 | -4.52494 | 0.00000 |
| Fe | 0.00000 | 0.00000 | 0.00000 |

**CdPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.52272 | 1.51837 | 0.00000 |
| N | 1.52272 | -1.51837 | 0.00000 |
| C | 3.53474 | -2.56974 | 0.00000 |
| C | 2.86323 | -1.28640 | 0.00000 |
| C | 3.46327 | 0.00000 | 0.00000 |
| C | 2.86323 | 1.28640 | 0.00000 |
| C | 3.53474 | 2.56974 | 0.00000 |
| C | 2.56179 | 3.53965 | 0.00000 |
| C | 2.56179 | -3.53965 | 0.00000 |
| C | 1.28376 | 2.86701 | 0.00000 |
| C | 1.28376 | -2.86701 | 0.00000 |
| C | 0.00000 | 3.45678 | 0.00000 |
| C | 0.00000 | -3.45678 | 0.00000 |
| C | -1.28376 | 2.86701 | 0.00000 |
| C | -1.28376 | -2.86701 | 0.00000 |
| C | -2.56179 | 3.53965 | 0.00000 |
| C | -2.56179 | -3.53965 | 0.00000 |
| C | -3.53474 | 2.56974 | 0.00000 |
| C | -3.53474 | -2.56974 | 0.00000 |
| C | -2.86323 | 1.28640 | 0.00000 |
| C | -3.46327 | 0.00000 | 0.00000 |
| C | -2.86323 | -1.28640 | 0.00000 |
| H | -4.60846 | 2.71816 | 0.00000 |
| H | -4.60846 | -2.71816 | 0.00000 |
| H | 0.00000 | -4.54616 | 0.00000 |
| H | -2.70782 | 4.61381 | 0.00000 |
| H | 0.00000 | 4.54616 | 0.00000 |
| H | -4.55181 | 0.00000 | 0.00000 |
| N | 1.52272 | 1.51837 | 0.00000 |
| N | -1.52272 | -1.51837 | 0.00000 |
| H | 4.55181 | 0.00000 | 0.00000 |
| H | 4.60846 | 2.71816 | 0.00000 |
| H | 4.60846 | -2.71816 | 0.00000 |
| H | 2.70782 | 4.61381 | 0.00000 |
| H | 2.70782 | -4.61381 | 0.00000 |
| H | -2.70782 | -4.61381 | 0.00000 |
| Cd | 0.00000 | 0.00000 | 0.00000 |

**TiPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.44974392 | 1.44974392 | 0.00000000 |
| N | 1.44974392 | -1.44974392 | 0.00000000 |
| C | 3.48842299 | -2.51915183 | 0.00000000 |
| C | 2.83065754 | -1.24816598 | 0.00000000 |
| C | 3.45049027 | 0.00000000 | 0.00000000 |
| C | 2.83065754 | 1.24816598 | 0.00000000 |
| C | 3.48842299 | 2.51915183 | 0.00000000 |
| C | 2.51915183 | 3.48842299 | 0.00000000 |
| C | 2.51915183 | -3.48842299 | 0.00000000 |
| C | 1.24816598 | 2.83065754 | 0.00000000 |
| C | 1.24816598 | -2.83065754 | 0.00000000 |
| C | 0.00000000 | 3.45049027 | 0.00000000 |
| C | 0.00000000 | -3.45049027 | 0.00000000 |
| C | -1.24816598 | 2.83065754 | 0.00000000 |
| C | -1.24816598 | -2.83065754 | 0.00000000 |
| C | -2.51915183 | 3.48842299 | 0.00000000 |
| C | -2.51915183 | -3.48842299 | 0.00000000 |
| C | -3.48842299 | 2.51915183 | 0.00000000 |
| C | -3.48842299 | -2.51915183 | 0.00000000 |
| C | -2.83065754 | 1.24816598 | 0.00000000 |
| C | -3.45049027 | 0.00000000 | 0.00000000 |
| C | -2.83065754 | -1.24816598 | 0.00000000 |
| H | -4.56382784 | 2.65695180 | 0.00000000 |
| H | -4.56382784 | -2.65695180 | 0.00000000 |
| H | 0.00000000 | -4.53839220 | 0.00000000 |
| H | -2.65695180 | 4.56382784 | 0.00000000 |
| H | 0.00000000 | 4.53839220 | 0.00000000 |
| H | -4.53839220 | 0.00000000 | 0.00000000 |
| N | 1.44974392 | 1.44974392 | 0.00000000 |
| N | -1.44974392 | -1.44974392 | 0.00000000 |
| H | 4.53839220 | 0.00000000 | 0.00000000 |
| H | 4.56382784 | 2.65695180 | 0.00000000 |
| H | 4.56382784 | -2.65695180 | 0.00000000 |
| H | 2.65695180 | 4.56382784 | 0.00000000 |
| H | 2.65695180 | -4.56382784 | 0.00000000 |
| H | -2.65695180 | -4.56382784 | 0.00000000 |
| Ti | 0.00000000 | 0.00000000 | 0.00000000 |

**PdPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.43352 | 1.43326 | 0.00000 |
| N | 1.43352 | -1.43326 | 0.00000 |
| C | 3.46930 | -2.50721 | 0.00000 |
| C | 2.79374 | -1.23414 | 0.00000 |
| C | 3.42404 | 0.00000 | 0.00000 |
| C | 2.79374 | 1.23414 | 0.00000 |
| C | 3.46930 | 2.50721 | 0.00000 |
| C | 2.50697 | 3.46943 | 0.00000 |
| C | 2.50697 | -3.46943 | 0.00000 |
| C | 1.23417 | 2.79354 | 0.00000 |
| C | 1.23417 | -2.79354 | 0.00000 |
| C | 0.00000 | 3.42367 | 0.00000 |
| C | 0.00000 | -3.42367 | 0.00000 |
| C | -1.23417 | 2.79354 | 0.00000 |
| C | -1.23417 | -2.79354 | 0.00000 |
| C | -2.50697 | 3.46943 | 0.00000 |

| | | | |
|---|---|---|---|
| C | -2.50697 | -3.46943 | 0.00000 |
| C | -3.46930 | 2.50721 | 0.00000 |
| C | -3.46930 | -2.50721 | 0.00000 |
| C | -2.79374 | 1.23414 | 0.00000 |
| C | -3.42404 | 0.00000 | 0.00000 |
| C | -2.79374 | -1.23414 | 0.00000 |
| H | -4.54546 | 2.63304 | 0.00000 |
| H | -4.54546 | -2.63304 | 0.00000 |
| H | 0.00000 | -4.51080 | 0.00000 |
| H | -2.63262 | 4.54566 | 0.00000 |
| H | 0.00000 | 4.51080 | 0.00000 |
| H | -4.51116 | 0.00000 | 0.00000 |
| N | 1.43352 | 1.43326 | 0.00000 |
| N | -1.43352 | -1.43326 | 0.00000 |
| H | 4.51116 | 0.00000 | 0.00000 |
| H | 4.54546 | 2.63304 | 0.00000 |
| H | 4.54546 | -2.63304 | 0.00000 |
| H | 2.63262 | 4.54566 | 0.00000 |
| H | 2.63262 | -4.54566 | 0.00000 |
| H | -2.63262 | -4.54566 | 0.00000 |
| Pd | 0.00000 | 0.00000 | 0.00000 |

**PtPorphyrin**

| | | | |
|---|---|---|---|
| N | -1.43091 | 1.43067 | 0.00000 |
| N | 1.43091 | -1.43067 | 0.00000 |
| C | 3.46737 | -2.50561 | 0.00000 |
| C | 2.79400 | -1.23285 | 0.00000 |
| C | 3.42499 | 0.00000 | 0.00000 |
| C | 2.79400 | 1.23285 | 0.00000 |
| C | 3.46737 | 2.50561 | 0.00000 |
| C | 2.50546 | 3.46745 | 0.00000 |
| C | 2.50546 | -3.46745 | 0.00000 |
| C | 1.23289 | 2.79380 | 0.00000 |
| C | 1.23289 | -2.79380 | 0.00000 |
| C | 0.00000 | 3.42459 | 0.00000 |
| C | 0.00000 | -3.42459 | 0.00000 |
| C | -1.23289 | 2.79380 | 0.00000 |
| C | -1.23289 | -2.79380 | 0.00000 |
| C | -2.50546 | 3.46745 | 0.00000 |
| C | -2.50546 | -3.46745 | 0.00000 |
| C | -3.46737 | 2.50561 | 0.00000 |
| C | -3.46737 | -2.50561 | 0.00000 |
| C | -2.79400 | 1.23285 | 0.00000 |
| C | -3.42499 | 0.00000 | 0.00000 |
| C | -2.79400 | -1.23285 | 0.00000 |
| H | -4.54334 | 2.62964 | 0.00000 |
| H | -4.54334 | -2.62964 | 0.00000 |
| H | 0.00000 | -4.51183 | 0.00000 |
| H | -2.62938 | 4.54347 | 0.00000 |
| H | 0.00000 | 4.51183 | 0.00000 |
| H | -4.51226 | 0.00000 | 0.00000 |
| N | 1.43091 | 1.43067 | 0.00000 |
| N | -1.43091 | -1.43067 | 0.00000 |
| H | 4.51226 | 0.00000 | 0.00000 |
| H | 4.54334 | 2.62964 | 0.00000 |
| H | 4.54334 | -2.62964 | 0.00000 |
| H | 2.62938 | 4.54347 | 0.00000 |

| | | | |
|---|---|---|---|
| H | 2.62938 | -4.54347 | 0.00000 |
| H | -2.62938 | -4.54347 | 0.00000 |
| Pt | 0.00000 | 0.00000 | 0.00000 |

**TPP**

| | | | |
|---|---|---|---|
| N | -0.23721500 | -2.00496400 | 0.00000000 |
| N | 0.23201500 | 2.02156600 | 0.00000000 |
| C | -0.18834600 | 4.30708600 | 0.00000000 |
| C | -0.75434500 | 2.96912900 | 0.00000000 |
| C | -2.14262000 | 2.72418300 | 0.00000000 |
| C | -2.74190500 | 1.45806100 | 0.00000000 |
| C | -4.14396100 | 1.17403800 | 0.00000000 |
| C | -4.30297000 | -0.18565300 | 0.00000000 |
| C | 1.15809000 | 4.15276300 | 0.00000000 |
| C | -3.00356300 | -0.78414200 | 0.00000000 |
| C | 1.40671000 | 2.72146300 | 0.00000000 |
| C | -2.70745000 | -2.15414400 | 0.00000000 |
| C | 2.70366700 | 2.17020500 | 0.00000000 |
| C | -1.41087300 | -2.70570300 | 0.00000000 |
| C | 3.00021000 | 0.79945600 | 0.00000000 |
| C | -1.16244900 | -4.13622200 | 0.00000000 |
| C | 4.29958500 | 0.19957700 | 0.00000000 |
| C | 0.18321400 | -4.29038200 | 0.00000000 |
| C | 4.14098700 | -1.16052700 | 0.00000000 |
| C | 0.74851200 | -2.95280500 | 0.00000000 |
| C | 2.13654500 | -2.71048100 | 0.00000000 |
| C | 2.73836600 | -1.44470300 | 0.00000000 |
| H | -1.08345900 | 0.12477400 | 0.00000000 |
| H | 1.08056900 | -0.11017700 | 0.00000000 |
| H | 4.91945600 | -1.91070900 | 0.00000000 |
| H | -1.91744900 | -4.90625600 | 0.00000000 |
| H | 3.15246200 | -4.00129100 | 2.15566100 |
| H | 3.97276200 | 3.24068300 | -2.14510400 |
| N | -2.09406300 | 0.24638500 | 0.00000000 |
| N | 2.09123000 | -0.23179000 | 0.00000000 |
| H | -3.99878400 | -3.18503200 | 2.15063400 |
| H | -4.92234500 | 1.92525700 | 0.00000000 |
| H | -0.74982500 | 5.22875700 | 0.00000000 |
| H | -5.23322600 | -0.73754300 | 0.00000000 |
| H | 1.91381700 | 4.92355300 | 0.00000000 |
| H | 5.23045000 | 0.75026700 | 0.00000000 |
| H | 0.74520000 | -5.21186700 | 0.00000000 |
| C | 3.86365900 | 3.11552900 | -0.00003700 |
| C | 4.41600300 | 3.56563800 | 1.20463200 |
| C | 5.47936100 | 4.46886400 | 1.20561700 |
| C | 6.00552400 | 4.93319000 | 0.00010600 |
| C | 5.46419300 | 4.48693400 | -1.20551300 |
| C | 4.40084700 | 3.58375300 | -1.20465000 |
| H | 3.99968300 | 3.20866200 | 2.14519300 |
| H | 5.89360600 | 4.81278800 | 2.15130800 |
| H | 6.83218100 | 5.64120100 | 0.00020400 |
| H | 5.86674200 | 4.84476700 | -2.15109000 |
| C | 3.06690100 | -3.88218000 | 0.00926000 |
| C | 3.52785300 | -4.43751100 | -1.18969500 |
| C | 4.41098200 | -5.51756300 | -1.17933200 |
| C | 4.84540900 | -6.05600100 | 0.03187500 |
| C | 4.39012900 | -5.50978400 | 1.23191300 |
| C | 3.50702100 | -4.42994100 | 1.21969500 |

| | | | |
|---|---|---|---|
| H | 3.18971000 | -4.01504900 | -2.13446200 |
| H | 4.76063400 | -5.93695500 | -2.12056600 |
| H | 5.53609800 | -6.89704800 | 0.04061700 |
| H | 4.72344800 | -5.92275900 | 2.18193500 |
| C | -3.87400600 | -3.09151900 | 0.00472300 |
| C | -4.42916900 | -3.54556900 | -1.19711000 |
| C | -5.51256000 | -4.42464000 | -1.19252300 |
| C | -6.05602300 | -4.86084600 | 0.01579300 |
| C | -5.51048400 | -4.41228100 | 1.21863500 |
| C | -4.42708100 | -3.53332400 | 1.21218600 |
| H | -4.00250800 | -3.20701300 | -2.13983200 |
| H | -5.93072000 | -4.76971000 | -2.13605200 |
| H | -6.90023800 | -5.54778200 | 0.02007100 |
| H | -5.92695800 | -4.74759500 | 2.16643800 |
| C | -3.07458200 | 3.89563700 | -0.00360200 |
| C | -3.52185900 | 4.45556700 | 1.19864400 |
| C | -4.40609100 | 5.53485100 | 1.19504500 |
| C | -4.85575700 | 6.06857200 | -0.01266800 |
| C | -4.41453700 | 5.51802000 | -1.21594000 |
| C | -3.53034000 | 4.43881300 | -1.21044800 |
| H | -3.17233900 | 4.03735800 | 2.14114500 |
| H | -4.74481600 | 5.95737600 | 2.13895600 |
| H | -5.54723500 | 6.90909300 | -0.01613900 |
| H | -4.75970700 | 5.92728900 | -2.16334700 |
| H | -3.18733800 | 4.00737700 | -2.14940400 |

***Meso*-Tetra-*para*-methoxyphenylporphyrin**

| | | | |
|---|---|---|---|
| N | -0.23721500 | -2.00496400 | 0.00000000 |
| N | 0.23201500 | 2.02156600 | 0.00000000 |
| C | -0.18834600 | 4.30708600 | 0.00000000 |
| C | -0.75434500 | 2.96912900 | 0.00000000 |
| C | -2.14262000 | 2.72418300 | 0.00000000 |
| C | -2.74190500 | 1.45806100 | 0.00000000 |
| C | -4.14396100 | 1.17403800 | 0.00000000 |
| C | -4.30297000 | -0.18565300 | 0.00000000 |
| C | 1.15809000 | 4.15276300 | 0.00000000 |
| C | -3.00356300 | -0.78414200 | 0.00000000 |
| C | 1.40671000 | 2.72146300 | 0.00000000 |
| C | -2.70745000 | -2.15414400 | 0.00000000 |
| C | 2.70366700 | 2.17020500 | 0.00000000 |
| C | -1.41087300 | -2.70570300 | 0.00000000 |
| C | 3.00021000 | 0.79945600 | 0.00000000 |
| C | -1.16244900 | -4.13622200 | 0.00000000 |
| C | 4.29958500 | 0.19957700 | 0.00000000 |
| C | 0.18321400 | -4.29038200 | 0.00000000 |
| C | 4.14098700 | -1.16052700 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 0.74851200 | -2.95280500 | 0.00000000 |
| C | 2.13654500 | -2.71048100 | 0.00000000 |
| C | 2.73836600 | -1.44470300 | 0.00000000 |
| H | -1.08345900 | 0.12477400 | 0.00000000 |
| H | 1.08056900 | -0.11017700 | 0.00000000 |
| H | 4.91945600 | -1.91070900 | 0.00000000 |
| H | -1.91744900 | -4.90625600 | 0.00000000 |
| H | 3.12688800 | -4.05557500 | 2.15420200 |
| H | 4.05034900 | 3.26497700 | -2.10012100 |
| N | -2.09406300 | 0.24638500 | 0.00000000 |
| N | 2.09123000 | -0.23179000 | 0.00000000 |
| H | -3.99201500 | -3.20144300 | 2.15730500 |
| H | -4.92234500 | 1.92525700 | 0.00000000 |
| H | -0.74982500 | 5.22875700 | 0.00000000 |
| H | -5.23322600 | -0.73754300 | 0.00000000 |
| H | 1.91381700 | 4.92355300 | 0.00000000 |
| H | 5.23045000 | 0.75026700 | 0.00000000 |
| H | 0.74520000 | -5.21186700 | 0.00000000 |
| C | 3.87024500 | 3.10520000 | 0.03600000 |
| C | 4.40610500 | 3.53071300 | 1.26157200 |
| C | 5.48430900 | 4.40469200 | 1.31065600 |
| C | 6.05872200 | 4.87692900 | 0.12233900 |
| C | 5.54116500 | 4.46076300 | -1.10968300 |
| C | 4.45242900 | 3.58339100 | -1.13884400 |
| H | 3.96410800 | 3.16841400 | 2.18899000 |
| H | 5.89811000 | 4.73588700 | 2.26159400 |
| H | 8.53075600 | 6.88653900 | -0.60335400 |
| H | 5.96903900 | 4.80918900 | -2.04620100 |
| C | 3.05375500 | -3.89259000 | 0.00510500 |
| C | 3.50945600 | -4.45140800 | -1.19042500 |
| C | 4.34825400 | -5.57013600 | -1.20105700 |
| C | 4.74920400 | -6.14414200 | 0.01123000 |
| C | 4.30817100 | -5.58690200 | 1.22033500 |
| C | 3.47161900 | -4.47720300 | 1.21066000 |
| H | 3.19545100 | -4.01197500 | -2.13680500 |
| H | 4.67599800 | -5.98031700 | -2.15298400 |
| H | 6.58112600 | -8.72289800 | -0.80985000 |
| H | 4.62764200 | -6.04280100 | 2.15571600 |
| C | -3.87486300 | -3.08994200 | 0.00713100 |
| C | -4.43816100 | -3.55069800 | -1.18418900 |
| C | -5.51975700 | -4.43752800 | -1.18594400 |
| C | -6.04669400 | -4.88626400 | 0.03056900 |
| C | -5.49047800 | -4.43223900 | 1.23545600 |
| C | -4.42100600 | -3.54579900 | 1.21697800 |
| H | -4.02643900 | -3.21105300 | -2.13403000 |
| H | -5.93365400 | -4.76981400 | -2.13494500 |
| H | -8.17451600 | -5.36626300 | -1.59686400 |
| H | -5.91054700 | -4.78887400 | 2.17441400 |
| C | -3.06501100 | 3.90163600 | 0.00945800 |
| C | -3.47734900 | 4.47865200 | 1.21199700 |
| C | -4.33228800 | 5.58500800 | 1.23637200 |
| C | -4.78698700 | 6.13185500 | 0.03113300 |
| C | -4.38266800 | 5.56135200 | -1.18493100 |
| C | -3.53375200 | 4.46158900 | -1.18861500 |
| H | -3.12318900 | 4.05845600 | 2.15280600 |
| H | -4.63002700 | 6.00572900 | 2.19348100 |
| H | -5.19993700 | 8.18809700 | 1.74459300 |
| H | -4.74378100 | 5.99700400 | -2.11497800 |
| H | -3.22208800 | 4.02613200 | -2.13729100 |

| | | | |
|---|---|---|---|
| O | 5.56341100 | -7.24420300 | 0.11855500 |
| C | 5.97013800 | -7.86430400 | -1.09920600 |
| H | 5.10227200 | -8.21483000 | -1.67703700 |
| H | 6.56973900 | -7.18180800 | -1.71904900 |
| O | -7.09232300 | -5.76804400 | 0.14924200 |
| C | -7.70871000 | -6.20603200 | -1.05984800 |
| H | -6.98874600 | -6.70690200 | -1.72351600 |
| H | -8.48013500 | -6.92042100 | -0.76111100 |
| O | -5.62258600 | 7.21710000 | -0.06455400 |
| C | -6.05151000 | 7.81122300 | 1.15874800 |
| H | -6.69299400 | 8.64880200 | 0.87345700 |
| H | -6.62768800 | 7.10065200 | 1.76926900 |
| O | 7.11650500 | 5.74011500 | 0.27086700 |
| C | 7.73929300 | 6.20521000 | -0.92392800 |
| H | 8.18032500 | 5.37479600 | -1.49469700 |
| H | 7.02961000 | 6.74908200 | -1.56392200 |

***Meso*-Tetra-*para*-ethoxyphenylporphyrin**

| | | | |
|---|---|---|---|
| N | 0.26278500 | -1.50496400 | 0.00000000 |
| N | 0.73201500 | 2.52156600 | 0.00000000 |
| C | 0.31165400 | 4.80708600 | 0.00000000 |
| C | -0.25434500 | 3.46912900 | 0.00000000 |
| C | -1.64262000 | 3.22418300 | 0.00000000 |
| C | -2.24190500 | 1.95806100 | 0.00000000 |
| C | -3.64396100 | 1.67403800 | 0.00000000 |
| C | -3.80297000 | 0.31434700 | 0.00000000 |
| C | 1.65809000 | 4.65276300 | 0.00000000 |
| C | -2.50356300 | -0.28414200 | 0.00000000 |
| C | 1.90671000 | 3.22146300 | 0.00000000 |
| C | -2.20745000 | -1.65414400 | 0.00000000 |
| C | 3.20366700 | 2.67020500 | 0.00000000 |
| C | -0.91087300 | -2.20570300 | 0.00000000 |
| C | 3.50021000 | 1.29945600 | 0.00000000 |
| C | -0.66244900 | -3.63622200 | 0.00000000 |
| C | 4.79958500 | 0.69957700 | 0.00000000 |
| C | 0.68321400 | -3.79038200 | 0.00000000 |
| C | 4.64098700 | -0.66052700 | 0.00000000 |
| C | 1.24851200 | -2.45280500 | 0.00000000 |
| C | 2.63654500 | -2.21048100 | 0.00000000 |
| C | 3.23836600 | -0.94470300 | 0.00000000 |
| H | -0.58345900 | 0.62477400 | 0.00000000 |
| H | 1.58056900 | 0.38982300 | 0.00000000 |
| H | 5.41945600 | -1.41070900 | 0.00000000 |
| H | -1.41744900 | -4.40625600 | 0.00000000 |
| H | 3.68501800 | -3.54327600 | -2.12377900 |
| H | 4.37824600 | 3.68313900 | 2.21377900 |
| N | -1.59406300 | 0.74638500 | 0.00000000 |
| N | 2.59123000 | 0.26821000 | 0.00000000 |
| H | -3.58060500 | -2.71986100 | 2.10351300 |
| H | -4.42234500 | 2.42525700 | 0.00000000 |
| H | -0.23893400 | 5.73920400 | -0.03269900 |
| H | -4.73322600 | -0.23754300 | 0.00000000 |
| H | 2.41381700 | 5.42355300 | 0.00000000 |
| H | 5.73045000 | 1.25026700 | 0.00000000 |
| H | 1.24520000 | -4.71186700 | 0.18470900 |
| C | 4.36115000 | 3.61372100 | 0.06726100 |
| C | 4.98648800 | 4.09086800 | -1.09261900 |

| | | | |
|---|---|---|---|
| C | 6.04914000 | 4.98164100 | -1.02061400 |
| C | 6.51496600 | 5.42365500 | 0.22517100 |
| C | 5.91057000 | 4.94800400 | 1.39382400 |
| C | 4.84817900 | 4.04630800 | 1.30194100 |
| H | 4.62547200 | 3.76220400 | -2.06537800 |
| H | 6.53044700 | 5.35570600 | -1.92105400 |
| H | 9.96491100 | 7.31685000 | 0.63500900 |
| H | 6.25386000 | 5.27058200 | 2.37226400 |
| C | 3.56224600 | -3.38400800 | 0.01416500 |
| C | 4.00434900 | -3.93451200 | 1.22556100 |
| C | 4.87120500 | -5.01804300 | 1.24813700 |
| C | 5.32501300 | -5.58161300 | 0.04763100 |
| C | 4.89431600 | -5.04493200 | -1.17099600 |
| C | 4.01871900 | -3.95625600 | -1.17337500 |
| H | 3.65948400 | -3.50216200 | 2.16300500 |
| H | 5.21387200 | -5.44448500 | 2.18793300 |
| H | 8.44832800 | -7.97382900 | 0.02697200 |
| H | 5.22912900 | -5.46321700 | -2.11555300 |
| C | -3.37332100 | -2.58883300 | -0.03653900 |
| C | -3.89027300 | -3.03386400 | -1.25411700 |
| C | -4.97279900 | -3.91466600 | -1.31049200 |
| C | -5.55860500 | -4.36569400 | -0.12257000 |
| C | -5.04910600 | -3.92655400 | 1.10738900 |
| C | -3.97140100 | -3.05213300 | 1.14351000 |
| H | -3.43635400 | -2.68827500 | -2.18097400 |
| H | -5.34637000 | -4.24058600 | -2.27651500 |
| H | -7.97341700 | -7.46304700 | -0.29724100 |
| H | -5.51236400 | -4.28598700 | 2.02320100 |
| C | -2.55969100 | 4.40388300 | 0.02913200 |
| C | -3.01127000 | 5.00697900 | -1.15274500 |
| C | -3.85652000 | 6.10777600 | -1.11908500 |
| C | -4.27315100 | 6.63868600 | 0.10939200 |
| C | -3.83426900 | 6.04724900 | 1.29918900 |
| C | -2.98948200 | 4.93657200 | 1.24492100 |
| H | -2.68864300 | 4.60564700 | -2.11142800 |
| H | -4.20580600 | 6.57614200 | -2.03604600 |
| H | -5.90752300 | 10.22103700 | 0.27162600 |
| H | -4.13933600 | 6.43988600 | 2.26445600 |
| H | -2.64853200 | 4.48135900 | 2.17316300 |
| O | 6.17637200 | -6.64219300 | 0.17094300 |
| O | 7.55390900 | 6.30915600 | 0.19645600 |
| O | -5.10102600 | 7.72273200 | 0.04322400 |
| O | -6.61767500 | -5.22528300 | -0.05848900 |
| C | 6.70931500 | -7.23116000 | -1.01967700 |
| H | 7.25419100 | -6.46670100 | -1.59480500 |
| H | 5.88729400 | -7.60986100 | -1.64634000 |
| C | 7.63393300 | -8.35631800 | -0.59858000 |
| H | 7.08700100 | -9.11650100 | -0.02999400 |
| H | 8.07087300 | -8.83259400 | -1.48441600 |
| C | 8.00568400 | 6.86962600 | 1.43366500 |
| H | 8.35462800 | 6.06742300 | 2.10162200 |
| H | 7.16846300 | 7.38560700 | 1.92853000 |
| C | 9.12931600 | 7.83662600 | 1.11680200 |
| H | 8.78032200 | 8.63047200 | 0.44671200 |
| H | 9.49467700 | 8.29931700 | 2.04154300 |
| C | -5.51302900 | 8.34207400 | 1.26651300 |
| H | -4.62620800 | 8.69282700 | 1.81671400 |
| H | -6.03744000 | 7.60787500 | 1.89698200 |
| C | -6.42676200 | 9.49761300 | 0.91020000 |

| | | | |
|---|---|---|---|
| H | -7.31413700 | 9.13873700 | 0.37689600 |
| H | -6.75393600 | 10.01006000 | 1.82277900 |
| C | -7.17512800 | -5.71365200 | -1.28315700 |
| H | -6.40058300 | -6.24911900 | -1.85350300 |
| H | -7.52534800 | -4.86627900 | -1.89269100 |
| C | -8.32322800 | -6.63704700 | -0.92661900 |
| H | -9.10502000 | -6.09359300 | -0.38382600 |
| H | -8.76229600 | -7.05788900 | -1.83895600 |

**Tetra-*meso*-Pyridineporphyrin**

| | | | |
|---|---|---|---|
| N | -0.23721500 | -2.00496400 | 0.00000000 |
| N | 0.23201500 | 2.02156600 | 0.00000000 |
| C | -0.18834600 | 4.30708600 | 0.00000000 |
| C | -0.75434500 | 2.96912900 | 0.00000000 |
| C | -2.14262000 | 2.72418300 | 0.00000000 |
| C | -2.74190500 | 1.45806100 | 0.00000000 |
| C | -4.14396100 | 1.17403800 | 0.00000000 |
| C | -4.30297000 | -0.18565300 | 0.00000000 |
| C | 1.15809000 | 4.15276300 | 0.00000000 |
| C | -3.00356300 | -0.78414200 | 0.00000000 |
| C | 1.40671000 | 2.72146300 | 0.00000000 |
| C | -2.70745000 | -2.15414400 | 0.00000000 |
| C | 2.70366700 | 2.17020500 | 0.00000000 |
| C | -1.41087300 | -2.70570300 | 0.00000000 |
| C | 3.00021000 | 0.79945600 | 0.00000000 |
| C | -1.16244900 | -4.13622200 | 0.00000000 |
| C | 4.29958500 | 0.19957700 | 0.00000000 |
| C | 0.18321400 | -4.29038200 | 0.00000000 |
| C | 4.14098700 | -1.16052700 | 0.00000000 |
| C | 0.74851200 | -2.95280500 | 0.00000000 |
| C | 2.13654500 | -2.71048100 | 0.00000000 |
| C | 2.73836600 | -1.44470300 | 0.00000000 |
| H | -1.08345900 | 0.12477400 | 0.00000000 |
| H | 1.08056900 | -0.11017700 | 0.00000000 |
| H | 4.91945600 | -1.91070900 | 0.00000000 |
| H | -1.91744900 | -4.90625600 | 0.00000000 |
| H | 1.91381700 | 4.92355300 | 0.00000000 |
| H | 5.23045000 | 0.75026700 | 0.00000000 |
| N | -2.09406300 | 0.24638500 | 0.00000000 |
| N | 2.09123000 | -0.23179000 | 0.00000000 |
| H | 0.74520000 | -5.21186700 | 0.00000000 |
| H | -4.92234500 | 1.92525700 | 0.00000000 |
| H | -0.74982500 | 5.22875700 | 0.00000000 |
| H | -5.23322600 | -0.73754300 | 0.00000000 |
| C | 3.87027500 | 3.10608800 | 0.00000000 |
| C | 4.43831200 | 3.56170400 | -1.19332300 |
| C | 5.52474600 | 4.43464700 | -1.13938800 |
| N | 6.07378200 | 4.87522500 | 0.00000000 |
| C | 5.52474600 | 4.43464700 | 1.13938800 |
| C | 4.43831200 | 3.56170400 | 1.19332300 |
| H | 4.03556400 | 3.24080400 | -2.15265100 |
| H | 5.97652400 | 4.79870700 | -2.06254200 |
| H | 5.97652400 | 4.79870700 | 2.06254200 |
| H | 4.03556400 | 3.24080400 | 2.15265100 |
| C | 3.06081300 | -3.88663500 | 0.00000000 |
| C | 3.51119700 | -4.45901500 | -1.19330200 |
| C | 4.37492600 | -5.55264900 | -1.13934600 |

| | | | |
|---|---|---|---|
| N | 4.81122600 | -6.10511400 | 0.00000000 |
| C | 4.37492600 | -5.55264900 | 1.13934600 |
| C | 3.51119700 | -4.45901500 | 1.19330200 |
| H | 3.19108400 | -4.05552300 | -2.15257900 |
| H | 4.73440500 | -6.00827300 | -2.06247000 |
| H | 4.73440500 | -6.00827300 | 2.06247000 |
| H | 3.19108400 | -4.05552300 | 2.15257900 |
| C | -3.87462700 | -3.08966300 | 0.00000000 |
| C | -4.44293300 | -3.54498900 | -1.19331600 |
| C | -5.53011100 | -4.41704500 | -1.13938700 |
| N | -6.07947700 | -4.85713500 | 0.00000000 |
| C | -5.53011100 | -4.41704500 | 1.13938700 |
| C | -4.44293300 | -3.54498900 | 1.19331600 |
| H | -4.03995600 | -3.22453200 | -2.15267400 |
| H | -5.98240400 | -4.78057600 | -2.06248600 |
| H | -5.98240400 | -4.78057600 | 2.06248600 |
| H | -4.03995600 | -3.22453200 | 2.15267400 |
| C | -3.06685300 | 3.90055600 | 0.00000000 |
| C | -3.51695500 | 4.47316900 | -1.19324500 |
| C | -4.37733200 | 5.56938300 | -1.13933600 |
| N | -4.81207800 | 6.12318700 | 0.00000000 |
| C | -4.37733200 | 5.56938300 | 1.13933600 |
| C | -3.51695500 | 4.47316900 | 1.19324500 |
| H | -3.19751600 | 4.06934100 | -2.15263400 |
| H | -4.73528700 | 6.02606100 | -2.06252300 |
| H | -4.73528700 | 6.02606100 | 2.06252300 |
| H | -3.19751600 | 4.06934100 | 2.15263400 |

**ZnTPP**

| | | | |
|---|---|---|---|
| N | 1.44053400 | 1.42561700 | 0.00000000 |
| N | -1.43976500 | -1.42692500 | 0.00000000 |
| C | -2.53822200 | -3.47477600 | 0.00000000 |
| C | -1.26079100 | -2.78293000 | 0.00000000 |
| C | -0.02336700 | -3.45827400 | 0.00000000 |
| C | 1.23522100 | -2.84332400 | 0.00000000 |
| C | 2.50780600 | -3.49674500 | 0.00000000 |
| C | 3.48087000 | -2.53383800 | 0.00000000 |
| C | -3.49370000 | -2.51364800 | 0.00000000 |
| C | 2.83942100 | -1.25509200 | 0.00000000 |
| C | -2.79436600 | -1.24032000 | 0.00000000 |
| C | 3.46338600 | 0.00000000 | 0.00000000 |
| C | -3.46338600 | 0.00000000 | 0.00000000 |
| C | 2.79485100 | 1.24031800 | 0.00000000 |
| C | -2.83929100 | 1.25594400 | 0.00000000 |
| C | 3.49385000 | 2.51291300 | 0.00000000 |
| C | -3.47984700 | 2.53575600 | 0.00000000 |
| C | 2.53887500 | 3.47343200 | 0.00000000 |
| C | -2.50684600 | 3.49924200 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | 1.26222800 | 2.78144400 | 0.00000000 |
| C | 0.02663000 | 3.45868600 | 0.00000000 |
| C | -1.23372400 | 2.84558800 | 0.00000000 |
| H | -0.01730700 | -5.11307000 | -2.15266100 |
| H | -0.01168200 | -7.59635300 | -2.17054900 |
| H | -2.64664200 | 4.57127000 | 0.00000000 |
| H | 4.56437600 | 2.64311300 | 0.00000000 |
| H | 0.05272600 | 5.10794200 | 2.15528300 |
| H | -5.12808300 | -0.04270100 | -2.14527100 |
| N | 1.48557700 | -1.49233200 | 0.00000000 |
| N | -1.48540400 | 1.49407000 | 0.00000000 |
| H | 5.11508400 | 0.01452500 | 2.15389100 |
| H | 2.64688800 | -4.56953000 | 0.00000000 |
| H | -2.67499600 | -4.54530400 | 0.00000000 |
| H | 4.55211700 | -2.68346200 | 0.00000000 |
| H | -4.56526600 | -2.64398400 | 0.00000000 |
| H | -4.55082100 | 2.68669700 | 0.00000000 |
| H | 2.67513600 | 4.54413100 | 0.00000000 |
| C | -4.96190700 | -0.02440500 | 0.00182200 |
| C | -5.67442200 | -0.03676900 | 1.20786800 |
| C | -7.07027100 | -0.07780300 | 1.21026900 |
| C | -7.77329500 | -0.10575000 | 0.00395900 |
| C | -7.07168800 | -0.09034500 | -1.20332100 |
| C | -5.67594200 | -0.04998000 | -1.20299600 |
| H | -5.12547300 | -0.01957700 | 2.14940200 |
| H | -7.60810300 | -0.09045800 | 2.15763200 |
| H | -8.86237600 | -0.14087100 | 0.00465700 |
| H | -7.61068800 | -0.11218800 | -2.15009500 |
| C | 0.04447600 | 4.95710400 | 0.00708400 |
| C | 0.03594400 | 5.67786400 | -1.19376700 |
| C | 0.03437900 | 7.07440000 | -1.18614400 |
| C | 0.03964000 | 7.76940600 | 0.02502400 |
| C | 0.04737600 | 7.05902300 | 1.22742000 |
| C | 0.04984300 | 5.66280200 | 1.21695600 |
| H | 0.02803300 | 5.13511400 | -2.13903700 |
| H | 0.02659100 | 7.61910400 | -2.12985900 |
| H | 0.03611300 | 8.85904100 | 0.03197500 |
| H | 0.04953200 | 7.59147700 | 2.17801900 |
| C | 4.96194300 | 0.01781600 | 0.00577500 |
| C | 5.68171800 | 0.03082200 | -1.19570000 |
| C | 7.07808400 | 0.05230800 | -1.18941700 |
| C | 7.77429300 | 0.06025300 | 0.02126400 |
| C | 7.06497900 | 0.04605900 | 1.22427000 |
| C | 5.66883800 | 0.02465600 | 1.21496500 |
| H | 5.13834000 | 0.02577500 | -2.14057700 |
| H | 7.62176100 | 0.06345900 | -2.13363400 |
| H | 8.86380800 | 0.07775800 | 0.02723800 |
| H | 7.59818900 | 0.05218700 | 2.17449700 |
| C | -0.03951100 | -4.95735900 | -0.00477300 |
| C | -0.04629800 | -5.67658200 | 1.19724500 |
| C | -0.04145200 | -7.07313700 | 1.19215300 |
| C | -0.02964800 | -7.77048300 | -0.01768300 |
| C | -0.02265500 | -7.06210900 | -1.22100100 |
| C | -0.02677200 | -5.66571100 | -1.21312600 |
| H | -0.05239400 | -5.13267300 | 2.14184100 |
| H | -0.04488000 | -7.61632700 | 2.13695700 |
| H | -0.02425900 | -8.86014400 | -0.02260100 |
| Zn | 0.00353600 | 0.00745400 | 0.00000000 |

**PdTPP**

| | | | |
|---|---|---|---|
| N | 1.44053400 | 1.42561700 | 0.00000000 |
| N | -1.43976500 | -1.42692500 | 0.00000000 |
| C | -2.53822200 | -3.47477600 | 0.00000000 |
| C | -1.26079100 | -2.78293000 | 0.00000000 |
| C | -0.02336700 | -3.45827400 | 0.00000000 |
| C | 1.23522100 | -2.84332400 | 0.00000000 |
| C | 2.50780600 | -3.49674500 | 0.00000000 |
| C | 3.48087000 | -2.53383800 | 0.00000000 |
| C | -3.49370000 | -2.51364800 | 0.00000000 |
| C | 2.83942100 | -1.25509200 | 0.00000000 |
| C | -2.79436600 | -1.24032000 | 0.00000000 |
| C | 3.46338600 | 0.00000000 | 0.00000000 |
| C | -3.46338600 | 0.00000000 | 0.00000000 |
| C | 2.79485100 | 1.24031800 | 0.00000000 |
| C | -2.83929100 | 1.25594400 | 0.00000000 |
| C | 3.49385000 | 2.51291300 | 0.00000000 |
| C | -3.47984700 | 2.53575600 | 0.00000000 |
| C | 2.53887500 | 3.47343200 | 0.00000000 |
| C | -2.50684600 | 3.49924200 | 0.00000000 |
| C | 1.26222800 | 2.78144400 | 0.00000000 |
| C | 0.02663000 | 3.45868600 | 0.00000000 |
| C | -1.23372400 | 2.84558800 | 0.00000000 |
| H | -0.03084900 | -5.11605500 | -2.15055600 |
| H | -0.02257200 | -7.59952700 | -2.16455600 |
| H | -2.64664200 | 4.57127000 | 0.00000000 |
| H | 4.56437600 | 2.64311300 | 0.00000000 |
| H | 0.04556800 | 5.10877800 | 2.15671600 |
| H | -5.12572800 | -0.02048500 | -2.14586100 |
| N | 1.48557700 | -1.49233200 | 0.00000000 |
| N | -1.48540400 | 1.49407000 | 0.00000000 |
| H | 5.11630400 | 0.01382200 | 2.15322700 |
| H | 2.64688800 | -4.56953000 | 0.00000000 |
| H | -2.67499600 | -4.54530400 | 0.00000000 |
| H | 4.55211700 | -2.68346200 | 0.00000000 |
| H | -4.56526600 | -2.64398400 | 0.00000000 |
| H | -4.55082100 | 2.68669700 | 0.00000000 |
| H | 2.67513600 | 4.54413100 | 0.00000000 |
| C | -4.96161300 | -0.01923100 | 0.00171000 |
| C | -5.67402700 | -0.02908200 | 1.20746100 |
| C | -7.07035500 | -0.05416900 | 1.20853900 |
| C | -7.77286200 | -0.06794300 | 0.00156400 |
| C | -7.07053200 | -0.05429000 | -1.20536700 |
| C | -5.67434500 | -0.02893200 | -1.20418900 |
| H | -5.12549700 | -0.02086100 | 2.14921300 |
| H | -7.60902500 | -0.06321000 | 2.15565000 |
| H | -8.86209100 | -0.08843600 | 0.00054200 |
| H | -7.60995000 | -0.06428500 | -2.15225300 |
| C | 0.04040600 | 4.95746000 | 0.00826100 |
| C | 0.03358500 | 5.67763300 | -1.19297400 |
| C | 0.03046600 | 7.07426300 | -1.18563000 |
| C | 0.03318400 | 7.76958100 | 0.02534400 |
| C | 0.04019600 | 7.05951700 | 1.22802100 |
| C | 0.04332700 | 5.66302600 | 1.21830000 |
| H | 0.02876700 | 5.13505500 | -2.13814800 |
| H | 0.02416100 | 7.61856300 | -2.12932800 |
| H | 0.02908100 | 8.85902900 | 0.03194100 |

| | | | |
|---|---|---|---|
| H | 0.04150300 | 7.59244700 | 2.17816800 |
| C | 4.96231800 | 0.01672500 | 0.00500400 |
| C | 5.68133700 | 0.02831100 | -1.19694700 |
| C | 7.07789900 | 0.04685700 | -1.19098500 |
| C | 7.77463300 | 0.05333100 | 0.01941400 |
| C | 7.06576500 | 0.04102900 | 1.22275700 |
| C | 5.66939200 | 0.02272700 | 1.21412800 |
| H | 5.13808400 | 0.02402700 | -2.14167600 |
| H | 7.62136000 | 0.05640100 | -2.13507900 |
| H | 8.86414700 | 0.06805600 | 0.02488000 |
| H | 7.59958800 | 0.04582200 | 2.17242100 |
| C | -0.04020000 | -4.95756400 | -0.00253400 |
| C | -0.04633300 | -5.67450900 | 1.20078900 |
| C | -0.04114200 | -7.07120300 | 1.19742300 |
| C | -0.03139900 | -7.77021500 | -0.01149300 |
| C | -0.03018900 | -7.06374300 | -1.21600000 |
| C | -0.03551700 | -5.66715800 | -1.21035000 |
| H | -0.05002100 | -5.12939700 | 2.14455000 |
| H | -0.04227100 | -7.61304800 | 2.14260700 |
| H | -0.02417900 | -8.85975600 | -0.01504100 |
| Pd | 0.00353600 | 0.00745400 | 0.00000000 |

**NiTPP**

| | | | |
|---|---|---|---|
| N | 1.44053400 | 1.42561700 | 0.00000000 |
| N | -1.43976500 | -1.42692500 | 0.00000000 |
| C | -2.53822200 | -3.47477600 | 0.00000000 |
| C | -1.26079100 | -2.78293000 | 0.00000000 |
| C | -0.02336700 | -3.45827400 | 0.00000000 |
| C | 1.23522100 | -2.84332400 | 0.00000000 |
| C | 2.50780600 | -3.49674500 | 0.00000000 |
| C | 3.48087000 | -2.53383800 | 0.00000000 |
| C | -3.49370000 | -2.51364800 | 0.00000000 |
| C | 2.83942100 | -1.25509200 | 0.00000000 |
| C | -2.79436600 | -1.24032000 | 0.00000000 |
| C | 3.46338600 | 0.00000000 | 0.00000000 |
| C | -3.46338600 | 0.00000000 | 0.00000000 |
| C | 2.79485100 | 1.24031800 | 0.00000000 |
| C | -2.83929100 | 1.25594400 | 0.00000000 |
| C | 3.49385000 | 2.51291300 | 0.00000000 |
| C | -3.47984700 | 2.53575600 | 0.00000000 |
| C | 2.53887500 | 3.47343200 | 0.00000000 |
| C | -2.50684600 | 3.49924200 | 0.00000000 |
| C | 1.26222800 | 2.78144400 | 0.00000000 |
| C | 0.02663000 | 3.45868600 | 0.00000000 |
| C | -1.23372400 | 2.84558800 | 0.00000000 |
| H | -0.02761900 | -5.11299100 | -2.15318700 |
| H | -0.02518700 | -7.59647000 | -2.17136900 |
| H | -2.64664200 | 4.57127000 | 0.00000000 |
| H | 4.56437600 | 2.64311300 | 0.00000000 |
| H | 0.05201300 | 5.10982700 | 2.15455800 |
| H | -5.12995900 | -0.02743800 | -2.14483300 |
| N | 1.48557700 | -1.49233200 | 0.00000000 |
| N | -1.48540400 | 1.49407000 | 0.00000000 |
| H | 5.11318800 | 0.01509800 | 2.15553700 |
| H | 2.64688800 | -4.56953000 | 0.00000000 |
| H | -2.67499600 | -4.54530400 | 0.00000000 |
| H | 4.55211700 | -2.68346200 | 0.00000000 |

| | | | |
|---|---|---|---|
| H | -4.56526600 | -2.64398400 | 0.00000000 |
| H | -4.55082100 | 2.68669700 | 0.00000000 |
| H | 2.67513600 | 4.54413100 | 0.00000000 |
| C | -4.96213700 | -0.02171600 | 0.00264500 |
| C | -5.67299400 | -0.03311200 | 1.20965800 |
| C | -7.06903400 | -0.06757900 | 1.21323200 |
| C | -7.77349200 | -0.08856900 | 0.00728700 |
| C | -7.07315300 | -0.07246000 | -1.20105600 |
| C | -5.67707500 | -0.03749400 | -1.20215600 |
| H | -5.12282000 | -0.02002000 | 2.15050500 |
| H | -7.60598600 | -0.07961800 | 2.16120000 |
| H | -8.86255000 | -0.11777900 | 0.00908500 |
| H | -7.61378600 | -0.08894100 | -2.14696400 |
| C | 0.04544400 | 4.95760700 | 0.00624200 |
| C | 0.04100400 | 5.67717600 | -1.19558400 |
| C | 0.04408900 | 7.07380100 | -1.18903600 |
| C | 0.05063000 | 7.76998000 | 0.02211000 |
| C | 0.05454700 | 7.06043100 | 1.22523700 |
| C | 0.05163700 | 5.66399400 | 1.21590500 |
| H | 0.03349700 | 5.13374100 | -2.14041200 |
| H | 0.03976700 | 7.61777800 | -2.13327100 |
| H | 0.05175400 | 8.85952200 | 0.02813900 |
| H | 0.05786600 | 7.59373500 | 2.17518900 |
| C | 4.96262900 | 0.01920800 | 0.00700400 |
| C | 5.68382300 | 0.03417100 | -1.19385700 |
| C | 7.08034200 | 0.05980900 | -1.18572700 |
| C | 7.77527700 | 0.06985400 | 0.02602700 |
| C | 7.06428600 | 0.05287100 | 1.22837000 |
| C | 5.66801300 | 0.02719200 | 1.21732300 |
| H | 5.14181000 | 0.02772700 | -2.13946300 |
| H | 7.62527400 | 0.07235500 | -2.12911300 |
| H | 8.86472100 | 0.09057000 | 0.03339300 |
| H | 7.59648300 | 0.05991000 | 2.17917200 |
| C | -0.04150400 | -4.95776700 | -0.00480100 |
| C | -0.04924600 | -5.67671100 | 1.19753000 |
| C | -0.04721200 | -7.07341300 | 1.19226900 |
| C | -0.03829900 | -7.77078200 | -0.01796000 |
| C | -0.03316100 | -7.06230500 | -1.22167600 |
| C | -0.03496200 | -5.66569400 | -1.21374500 |
| H | -0.05306400 | -5.13274900 | 2.14206800 |
| H | -0.05009900 | -7.61658600 | 2.13682900 |
| H | -0.03436200 | -8.86033200 | -0.02311900 |
| Ni | 0.00089200 | 0.00147600 | 0.00000000 |

**PtTPP**

| | | | |
|---|---|---|---|
| N | 1.44053400 | 1.42561700 | 0.00000000 |
| N | -1.43976500 | -1.42692500 | 0.00000000 |
| C | -2.53822200 | -3.47477600 | 0.00000000 |
| C | -1.26079100 | -2.78293000 | 0.00000000 |
| C | -0.02336700 | -3.45827400 | 0.00000000 |
| C | 1.23522100 | -2.84332400 | 0.00000000 |
| C | 2.50780600 | -3.49674500 | 0.00000000 |
| C | 3.48087000 | -2.53383800 | 0.00000000 |
| C | -3.49370000 | -2.51364800 | 0.00000000 |
| C | 2.83942100 | -1.25509200 | 0.00000000 |
| C | -2.79436600 | -1.24032000 | 0.00000000 |
| C | 3.46338600 | 0.00000000 | 0.00000000 |

| | | | |
|---|---|---|---|
| C | -3.46338600 | 0.00000000 | 0.00000000 |
| C | 2.79485100 | 1.24031800 | 0.00000000 |
| C | -2.83929100 | 1.25594400 | 0.00000000 |
| C | 3.49385000 | 2.51291300 | 0.00000000 |
| C | -3.47984700 | 2.53575600 | 0.00000000 |
| C | 2.53887500 | 3.47343200 | 0.00000000 |
| C | -2.50684600 | 3.49924200 | 0.00000000 |
| C | 1.26222800 | 2.78144400 | 0.00000000 |
| C | 0.02663000 | 3.45868600 | 0.00000000 |
| C | -1.23372400 | 2.84558800 | 0.00000000 |
| H | -0.02983700 | -5.12411700 | -2.14372000 |
| H | -0.02360700 | -7.60793700 | -2.14507500 |
| H | -2.64664200 | 4.57127000 | 0.00000000 |
| H | 4.56437600 | 2.64311300 | 0.00000000 |
| H | 0.04353100 | 5.09593500 | 2.16257600 |
| H | -5.11668100 | -0.01931900 | -2.15117600 |
| N | 1.48557700 | -1.49233200 | 0.00000000 |
| N | -1.48540400 | 1.49407000 | 0.00000000 |
| H | 5.12377900 | 0.00942700 | 2.14739100 |
| H | 2.64688800 | -4.56953000 | 0.00000000 |
| H | -2.67499600 | -4.54530400 | 0.00000000 |
| H | 4.55211700 | -2.68346200 | 0.00000000 |
| H | -4.56526600 | -2.64398400 | 0.00000000 |
| H | -4.55082100 | 2.68669700 | 0.00000000 |
| H | 2.67513600 | 4.54413100 | 0.00000000 |
| C | -4.96104100 | -0.01740500 | -0.00324600 |
| C | -5.67721400 | -0.02439400 | 1.20010100 |
| C | -7.07361400 | -0.04393700 | 1.19589900 |
| C | -7.77178100 | -0.05471600 | -0.01350600 |
| C | -7.06501500 | -0.04523100 | -1.21799000 |
| C | -5.66878500 | -0.02556200 | -1.21173300 |
| H | -5.13197900 | -0.01749600 | 2.14352200 |
| H | -7.61572500 | -0.05114500 | 2.14067900 |
| H | -8.86114800 | -0.07067400 | -0.01755700 |
| H | -7.60023400 | -0.05341200 | -2.16682100 |
| C | 0.04308200 | 4.95652400 | 0.01344700 |
| C | 0.04112200 | 5.68195800 | -1.18436200 |
| C | 0.04178000 | 7.07840100 | -1.16942000 |
| C | 0.04368900 | 7.76718400 | 0.04522300 |
| C | 0.04552100 | 7.05134900 | 1.24423000 |
| C | 0.04496800 | 5.65514700 | 1.22725400 |
| H | 0.03721500 | 5.14412600 | -2.13206800 |
| H | 0.03918300 | 7.62797800 | -2.11010400 |
| H | 0.04287700 | 8.85669200 | 0.05728100 |
| H | 0.04528700 | 7.57913200 | 2.19709300 |
| C | 4.96161800 | 0.01682800 | -0.00013400 |
| C | 5.67495400 | 0.03285200 | -1.20520200 |
| C | 7.07135300 | 0.05316600 | -1.20475200 |
| C | 7.77272100 | 0.05721100 | 0.00267000 |
| C | 7.06919500 | 0.04085800 | 1.20875500 |
| C | 5.67293200 | 0.02081800 | 1.20624400 |
| H | 5.12773900 | 0.03097300 | -2.14745900 |
| H | 7.61108300 | 0.06636300 | -2.15099800 |
| H | 8.86219100 | 0.07364700 | 0.00369200 |
| H | 7.60711800 | 0.04428700 | 2.15617100 |
| C | -0.03954500 | -4.95630900 | 0.00340200 |
| C | -0.04275400 | -5.66615900 | 1.21062200 |
| C | -0.03804500 | -7.06261300 | 1.21410200 |
| C | -0.03096000 | -7.76708900 | 0.00864900 |

| | | | |
|---|---|---|---|
| C | -0.03039900 | -7.06719200 | -1.19925700 |
| C | -0.03470300 | -5.67074000 | -1.20107400 |
| H | -0.04423300 | -5.11601500 | 2.15129300 |
| H | -0.03728100 | -7.59976900 | 2.16196700 |
| H | -0.02434900 | -8.85665000 | 0.01063600 |
| Pt | -0.00010400 | 0.00029100 | 0.00000000 |