

Supplementary Materials for

Ambipolar Charge Transport in Organic Semiconductors: How Intramolecular Reorganization Energy Is Controlled by Diradical Character

Table S1. Diradical characters and the linear combinations of HOMO and LUMO of the open-shell broken-symmetry (BS) structure for the library of investigated molecules. BS orbitals are expressed as linear combination of closed-shell frontier molecular orbitals (H_{cs} and L_{cs}). Only the α orbitals are considered. Calculations from RB3LYP and UB3LYP levels of theory together with 6-311G* basis set. Diradical character are evaluated at PUHF/6-311G* level.

| Molecule | y_0^{PUHF} | H_α | | L_α | |
|---------------------|--------------|------------|----------|------------|----------|
| | | H_{cs} | L_{cs} | H_{cs} | L_{cs} |
| FF | 0.523 | 0.90 | 0.25 | -0.23 | 0.90 |
| DFPy | 0.541 | 0.92 | -0.38 | 0.35 | 0.93 |
| DFFU | 0.555 | 0.89 | -0.43 | 0.40 | 0.91 |
| DFTTh | 0.570 | 0.88 | -0.46 | 0.43 | 0.90 |
| DFTThSO2 | 0.591 | 0.86 | -0.49 | 0.46 | 0.88 |
| 2TIO | 0.633 | -0.91 | 0.41 | -0.39 | -0.92 |
| EsQ4 | 0.634 | 0.89 | -0.44 | 0.43 | 0.90 |
| A-IIDBT | 0.641 | -0.91 | 0.34 | -0.32 | -0.90 |
| QDTBDT | 0.659 | 0.88 | -0.46 | 0.43 | 0.90 |
| DIA _n | 0.681 | 0.85 | 0.45 | 0.42 | -0.86 |
| S-IIDBT | 0.691 | -0.91 | 0.35 | 0.33 | 0.92 |
| NZ | 0.742 | 0.86 | -0.51 | 0.48 | 0.87 |
| Ph2-IDPL | 0.757 | 0.90 | -0.43 | -0.39 | -0.92 |
| BT-DIA _n | 0.774 | 0.87 | -0.47 | -0.46 | -0.88 |
| TPQ | 0.846 | 0.76 | -0.59 | 0.56 | 0.82 |
| BISPHE | 0.847 | 0.84 | -0.53 | -0.51 | -0.86 |

Table S2. Diradical characters and reorganization energies of the investigated library of diradicals. Diradical characters are evaluated at the optimized geometries of the BS structures at PUHF/6-311G* level of theory. The reorganization energies are calculated both considering the CS (λ_{CS}) and the BS neutral PES (λ_{BS}) for hole and electron transports. Calculations carried out at RB3LYP and UB3LYP levels of theory with 6-311G* basis set.

| Molecule | y_0^{PUHF} @ geo BS | $\lambda_{CS}(\text{hole})$ | $\lambda_{CS}(\text{ele.})$ | $\lambda_{BS}(\text{hole})$ | $\lambda_{BS}(\text{ele.})$ |
|---------------------|--------------------------|-----------------------------|-----------------------------|-----------------------------|-----------------------------|
| EsQ2 | - | 0.201 | 0.489 | - | - |
| EsQ3 | - | 0.183 | 0.429 | - | - |
| A-IDBT | - | 0.204 | 0.131 | - | - |
| S-IDBT | - | 0.285 | 0.197 | - | - |
| FF | 0.523 | 0.227 | 0.219 | 0.147 | 0.158 |
| DFPy | 0.541 | 0.210 | 0.216 | 0.104 | 0.114 |
| DFFU | 0.555 | 0.212 | 0.222 | 0.101 | 0.113 |
| DFTTh | 0.570 | 0.190 | 0.237 | 0.093 | 0.136 |
| DFTThSO2 | 0.591 | 0.258 | 0.209 | 0.123 | 0.102 |
| 2TIO | 0.633 | 0.115 | 0.327 | 0.056 | 0.113 |
| EsQ4 | 0.634 | 0.168 | 0.382 | 0.108 | 0.171 |
| A-IIDBT | 0.641 | 0.219 | 0.086 | 0.148 | 0.100 |
| QDTBDT | 0.659 | 0.068 | 0.244 | 0.050 | 0.080 |
| DIA _n | 0.681 | 0.189 | 0.169 | 0.069 | 0.104 |
| S-IIDBT | 0.691 | 0.194 | 0.088 | 0.126 | 0.078 |
| NZ | 0.742 | 0.119 | 0.127 | 0.032 | 0.037 |
| Ph2-IDPL | 0.757 | 0.110 | 0.032 | 0.042 | 0.032 |
| BT-DIA _n | 0.774 | 0.177 | 0.082 | 0.090 | 0.131 |
| TPQ | 0.846 | 0.049 | 0.225 | 0.073 | 0.031 |
| BISPHE | 0.847 | 0.077 | 0.023 | 0.014 | 0.035 |

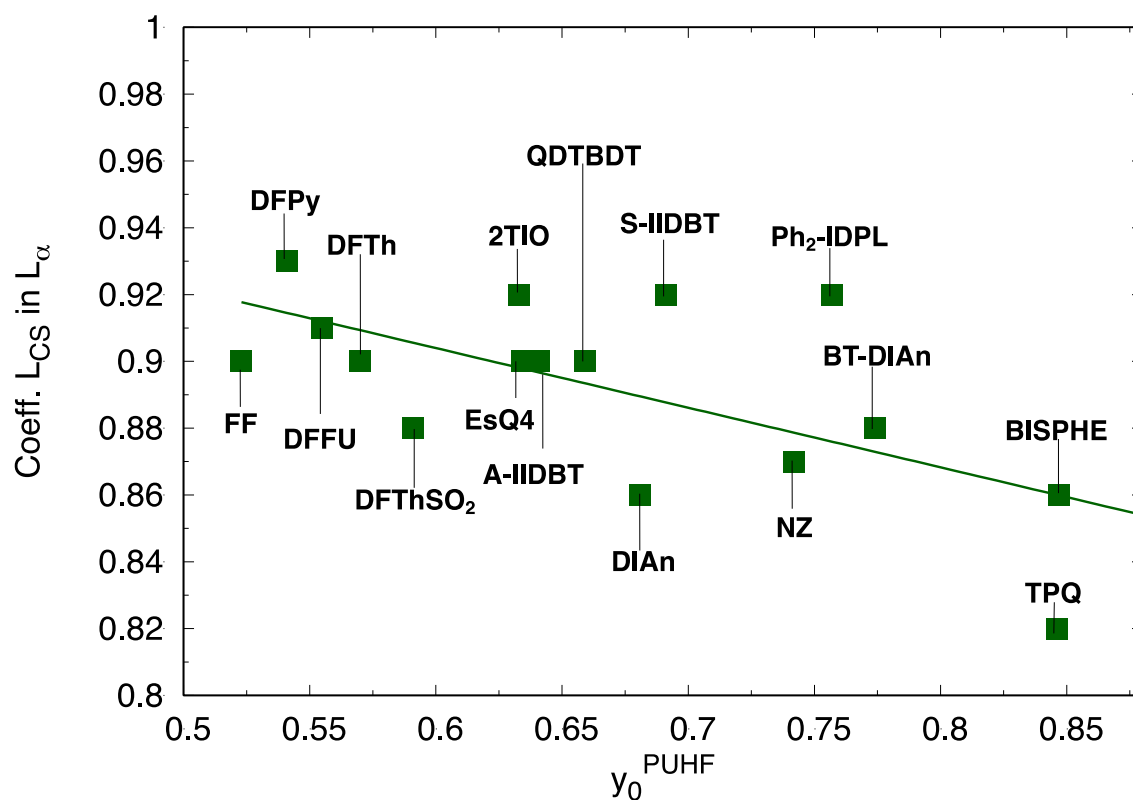


Figure S1. Contribution of the L_{CS} to the L_α BS orbitals (from RB3LYP/6-311G* and UB3LYP/6-311G* calculations), as a function of the computed diradical index y_0^{PUHF} , for the library of investigated diradicals.

OPTIMIZED GEOMETRIES

2TIO-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 0.005386 | 0.690801 | 0.000000 |
| C | -1.110131 | 1.575529 | 0.000000 |
| C | -0.782625 | 2.900058 | 0.000000 |
| C | 0.620480 | 3.170901 | 0.000000 |
| S | 1.504122 | 1.633515 | 0.000000 |
| H | -2.130484 | 1.211689 | 0.000000 |
| H | -1.522274 | 3.688765 | 0.000000 |
| C | -0.005386 | -0.690801 | 0.000000 |
| C | 1.110131 | -1.575529 | 0.000000 |
| S | -1.504122 | -1.633515 | 0.000000 |
| C | 0.782625 | -2.900058 | 0.000000 |
| H | 2.130484 | -1.211689 | 0.000000 |
| C | -0.620480 | -3.170901 | 0.000000 |
| H | 1.522274 | -3.688765 | 0.000000 |
| C | 1.258635 | 4.407898 | 0.000000 |
| C | 2.697914 | 4.520721 | 0.000000 |
| C | 0.502695 | 5.640337 | 0.000000 |
| C | 3.322137 | 5.720406 | 0.000000 |
| H | 3.293225 | 3.612248 | 0.000000 |
| C | 1.110131 | 6.848933 | 0.000000 |
| H | -0.580569 | 5.594522 | 0.000000 |
| C | 2.572385 | 6.984948 | 0.000000 |
| H | 4.403845 | 5.799023 | 0.000000 |
| H | 0.539045 | 7.771003 | 0.000000 |
| C | -1.258635 | -4.407898 | 0.000000 |
| C | -0.502695 | -5.640337 | 0.000000 |
| C | -2.697914 | -4.520721 | 0.000000 |
| C | -1.110131 | -6.848933 | 0.000000 |
| H | 0.580569 | -5.594522 | 0.000000 |
| C | -3.322137 | -5.720406 | 0.000000 |
| H | -3.293225 | -3.612248 | 0.000000 |
| C | -2.572385 | -6.984948 | 0.000000 |
| H | -0.539045 | -7.771003 | 0.000000 |
| H | -4.403845 | -5.799023 | 0.000000 |
| O | -3.132599 | -8.078824 | 0.000000 |
| O | 3.132599 | 8.078824 | 0.000000 |

2TIO-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|-----------|----------|----------|
| C | -0.003198 | 0.701142 | 0.000000 |
|---|-----------|----------|----------|

| | | | |
|---|-----------|-----------|----------|
| C | -1.113571 | 1.568483 | 0.000000 |
| C | -0.786940 | 2.907353 | 0.000000 |
| C | 0.602113 | 3.174733 | 0.000000 |
| S | 1.486793 | 1.643707 | 0.000000 |
| H | -2.133193 | 1.202522 | 0.000000 |
| H | -1.529890 | 3.693163 | 0.000000 |
| C | 0.003198 | -0.701142 | 0.000000 |
| C | 1.113571 | -1.568483 | 0.000000 |
| S | -1.486793 | -1.643707 | 0.000000 |
| C | 0.786940 | -2.907353 | 0.000000 |
| H | 2.133193 | -1.202522 | 0.000000 |
| C | -0.602113 | -3.174733 | 0.000000 |
| H | 1.529890 | -3.693163 | 0.000000 |
| C | 1.253224 | 4.423597 | 0.000000 |
| C | 2.686950 | 4.528656 | 0.000000 |
| C | 0.501585 | 5.651587 | 0.000000 |
| C | 3.317516 | 5.729915 | 0.000000 |
| H | 3.280213 | 3.618900 | 0.000000 |
| C | 1.113571 | 6.862279 | 0.000000 |
| H | -0.581822 | 5.608637 | 0.000000 |
| C | 2.572804 | 6.992664 | 0.000000 |
| H | 4.399626 | 5.803698 | 0.000000 |
| H | 0.544001 | 7.785390 | 0.000000 |
| C | -1.253224 | -4.423597 | 0.000000 |
| C | -0.501585 | -5.651587 | 0.000000 |
| C | -2.686950 | -4.528656 | 0.000000 |
| C | -1.113571 | -6.862279 | 0.000000 |
| H | 0.581822 | -5.608637 | 0.000000 |
| C | -3.317516 | -5.729915 | 0.000000 |
| H | -3.280213 | -3.618900 | 0.000000 |
| C | -2.572804 | -6.992664 | 0.000000 |
| H | -0.544001 | -7.785390 | 0.000000 |
| H | -4.399626 | -5.803698 | 0.000000 |
| O | -3.137541 | -8.088678 | 0.000000 |
| O | 3.137541 | 8.088678 | 0.000000 |

2TIO-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | -0.000719 | 0.704466 | 0.000000 |
| C | -1.118874 | 1.567187 | 0.000000 |
| C | -0.789035 | 2.902474 | 0.000000 |
| C | 0.604072 | 3.156222 | 0.000000 |
| S | 1.483393 | 1.629719 | 0.000000 |
| H | -2.139155 | 1.204452 | 0.000000 |
| H | -1.529749 | 3.689842 | 0.000000 |
| C | 0.000719 | -0.704466 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | 1.118874 | -1.567187 | 0.000000 |
| S | -1.483393 | -1.629719 | 0.000000 |
| C | 0.789035 | -2.902474 | 0.000000 |
| H | 2.139155 | -1.204452 | 0.000000 |
| C | -0.604072 | -3.156222 | 0.000000 |
| H | 1.529749 | -3.689842 | 0.000000 |
| C | 1.261956 | 4.403682 | 0.000000 |
| C | 2.701174 | 4.488789 | 0.000000 |
| C | 0.503246 | 5.630833 | 0.000000 |
| C | 3.337728 | 5.683188 | 0.000000 |
| H | 3.286352 | 3.574860 | 0.000000 |
| C | 1.118874 | 6.836866 | 0.000000 |
| H | -0.578902 | 5.588535 | 0.000000 |
| C | 2.586235 | 6.950046 | 0.000000 |
| H | 4.419187 | 5.757732 | 0.000000 |
| H | 0.559145 | 7.765235 | 0.000000 |
| C | -1.261956 | -4.403682 | 0.000000 |
| C | -0.503246 | -5.630833 | 0.000000 |
| C | -2.701174 | -4.488789 | 0.000000 |
| C | -1.118874 | -6.836866 | 0.000000 |
| H | 0.578902 | -5.588535 | 0.000000 |
| C | -3.337728 | -5.683188 | 0.000000 |
| H | -3.286352 | -3.574860 | 0.000000 |
| C | -2.586235 | -6.950046 | 0.000000 |
| H | -0.559145 | -7.765235 | 0.000000 |
| H | -4.419187 | -5.757732 | 0.000000 |
| O | -3.152660 | -8.035922 | 0.000000 |
| O | 3.152660 | 8.035922 | 0.000000 |

2TIO-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 0.007680 | 0.706374 | 0.000000 |
| C | -1.065190 | 1.598947 | 0.000000 |
| C | -0.701624 | 2.943183 | 0.000000 |
| C | 0.680008 | 3.180188 | 0.000000 |
| S | 1.522917 | 1.620685 | 0.000000 |
| H | -2.095368 | 1.261343 | 0.000000 |
| H | -1.427026 | 3.746501 | 0.000000 |
| C | -0.007680 | -0.706374 | 0.000000 |
| C | 1.065190 | -1.598947 | 0.000000 |
| S | -1.522917 | -1.620685 | 0.000000 |
| C | 0.701624 | -2.943183 | 0.000000 |
| H | 2.095368 | -1.261343 | 0.000000 |
| C | -0.680008 | -3.180188 | 0.000000 |
| H | 1.427026 | -3.746501 | 0.000000 |
| C | 1.379946 | 4.418576 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | 2.805879 | 4.490920 | 0.000000 |
| C | 0.680008 | 5.666066 | 0.000000 |
| C | 3.476257 | 5.680688 | 0.000000 |
| H | 3.377772 | 3.566034 | 0.000000 |
| C | 1.332192 | 6.864983 | 0.000000 |
| H | -0.406127 | 5.661266 | 0.000000 |
| C | 2.786253 | 6.964231 | 0.000000 |
| H | 4.561899 | 5.712072 | 0.000000 |
| H | 0.781959 | 7.801580 | 0.000000 |
| C | -1.379946 | -4.418576 | 0.000000 |
| C | -0.680008 | -5.666066 | 0.000000 |
| C | -2.805879 | -4.490920 | 0.000000 |
| C | -1.332192 | -6.864983 | 0.000000 |
| H | 0.406127 | -5.661266 | 0.000000 |
| C | -3.476257 | -5.680688 | 0.000000 |
| H | -3.377772 | -3.566034 | 0.000000 |
| C | -2.786253 | -6.964231 | 0.000000 |
| H | -0.781959 | -7.801580 | 0.000000 |
| H | -4.561899 | -5.712072 | 0.000000 |
| O | -3.388319 | -8.053958 | 0.000000 |
| O | 3.388319 | 8.053958 | 0.000000 |

EsQ2-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 0.001327 | 0.685668 | 0.000000 |
| C | 1.144818 | 1.551244 | 0.000000 |
| C | 0.837620 | 2.871411 | 0.000000 |
| C | -0.577569 | 3.147996 | 0.000000 |
| S | -1.499964 | 1.647560 | 0.000000 |
| H | 2.158569 | 1.169440 | 0.000000 |
| H | 1.564145 | 3.673690 | 0.000000 |
| C | -0.001327 | -0.685668 | 0.000000 |
| C | -1.144818 | -1.551244 | 0.000000 |
| S | 1.499964 | -1.647560 | 0.000000 |
| C | -0.837620 | -2.871411 | 0.000000 |
| H | -2.158569 | -1.169440 | 0.000000 |
| C | 0.577569 | -3.147996 | 0.000000 |
| H | -1.564145 | -3.673690 | 0.000000 |
| C | 1.144818 | -4.403705 | 0.000000 |
| C | 2.611207 | -4.564090 | 0.000000 |
| O | 3.382918 | -3.626393 | 0.000000 |
| C | 0.309177 | -5.552361 | 0.000000 |
| N | -0.400643 | -6.465892 | 0.000000 |
| O | 2.985258 | -5.849495 | 0.000000 |
| C | 4.403115 | -6.094256 | 0.000000 |
| H | 4.505917 | -7.175988 | 0.000000 |

| | | | |
|---|-----------|-----------|-----------|
| H | 4.862662 | -5.662008 | 0.889216 |
| H | 4.862662 | -5.662008 | -0.889216 |
| C | -1.144818 | 4.403705 | 0.000000 |
| C | -0.309177 | 5.552361 | 0.000000 |
| N | 0.400643 | 6.465892 | 0.000000 |
| C | -2.611207 | 4.564090 | 0.000000 |
| O | -3.382918 | 3.626393 | 0.000000 |
| O | -2.985258 | 5.849495 | 0.000000 |
| C | -4.403115 | 6.094256 | 0.000000 |
| H | -4.862662 | 5.662008 | 0.889216 |
| H | -4.862662 | 5.662008 | -0.889216 |
| H | -4.505917 | 7.175988 | 0.000000 |

EsQ2-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 0.005070 | 0.702231 | 0.000000 |
| C | 1.154134 | 1.546164 | 0.000000 |
| C | 0.844613 | 2.874208 | 0.000000 |
| C | -0.565342 | 3.133747 | 0.000000 |
| S | -1.483056 | 1.629620 | 0.000000 |
| H | 2.167665 | 1.165168 | 0.000000 |
| H | 1.571890 | 3.676205 | 0.000000 |
| C | -0.005070 | -0.702231 | 0.000000 |
| C | -1.154134 | -1.546164 | 0.000000 |
| S | 1.483056 | -1.629620 | 0.000000 |
| C | -0.844613 | -2.874208 | 0.000000 |
| H | -2.167665 | -1.165168 | 0.000000 |
| C | 0.565342 | -3.133747 | 0.000000 |
| H | -1.571890 | -3.676205 | 0.000000 |
| C | 1.154134 | -4.384179 | 0.000000 |
| C | 2.649111 | -4.523943 | 0.000000 |
| O | 3.374347 | -3.555324 | 0.000000 |
| C | 0.345625 | -5.544875 | 0.000000 |
| N | -0.339080 | -6.478212 | 0.000000 |
| O | 3.021342 | -5.788866 | 0.000000 |
| C | 4.449156 | -6.054103 | 0.000000 |
| H | 4.532338 | -7.135968 | 0.000000 |
| H | 4.902099 | -5.624324 | 0.892289 |
| H | 4.902099 | -5.624324 | -0.892289 |
| C | -1.154134 | 4.384179 | 0.000000 |
| C | -0.345625 | 5.544875 | 0.000000 |
| N | 0.339080 | 6.478212 | 0.000000 |
| C | -2.649111 | 4.523943 | 0.000000 |
| O | -3.374347 | 3.555324 | 0.000000 |
| O | -3.021342 | 5.788866 | 0.000000 |
| C | -4.449156 | 6.054103 | 0.000000 |

| | | | |
|---|-----------|----------|-----------|
| H | -4.902099 | 5.624324 | 0.892289 |
| H | -4.902099 | 5.624324 | -0.892289 |
| H | -4.532338 | 7.135968 | 0.000000 |

EsQ2-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | -0.013478 | 0.703875 | 0.000000 |
| C | 1.064512 | 1.598554 | 0.000000 |
| C | 0.696270 | 2.935662 | 0.000000 |
| C | -0.696270 | 3.152860 | 0.000000 |
| S | -1.544312 | 1.606277 | 0.000000 |
| H | 2.095648 | 1.264251 | 0.000000 |
| H | 1.397134 | 3.760888 | 0.000000 |
| C | 0.013478 | -0.703875 | 0.000000 |
| C | -1.064512 | -1.598554 | 0.000000 |
| S | 1.544312 | -1.606277 | 0.000000 |
| C | -0.696270 | -2.935662 | 0.000000 |
| H | -2.095648 | -1.264251 | 0.000000 |
| C | 0.696270 | -3.152860 | 0.000000 |
| H | -1.397134 | -3.760888 | 0.000000 |
| C | 1.355856 | -4.402230 | 0.000000 |
| C | 2.798585 | -4.490445 | 0.000000 |
| O | 3.565339 | -3.539318 | 0.000000 |
| C | 0.575300 | -5.582158 | 0.000000 |
| N | -0.099855 | -6.526262 | 0.000000 |
| O | 3.250952 | -5.779862 | 0.000000 |
| C | 4.668911 | -5.925548 | 0.000000 |
| H | 4.851473 | -6.999244 | 0.000000 |
| H | 5.111791 | -5.465558 | 0.886305 |
| H | 5.111791 | -5.465558 | -0.886305 |
| C | -1.355856 | 4.402230 | 0.000000 |
| C | -0.575300 | 5.582158 | 0.000000 |
| N | 0.099855 | 6.526262 | 0.000000 |
| C | -2.798585 | 4.490445 | 0.000000 |
| O | -3.565339 | 3.539318 | 0.000000 |
| O | -3.250952 | 5.779862 | 0.000000 |
| C | -4.668911 | 5.925548 | 0.000000 |
| H | -5.111791 | 5.465558 | 0.886305 |
| H | -5.111791 | 5.465558 | -0.886305 |
| H | -4.851473 | 6.999244 | 0.000000 |

EsQ3-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|----------|----------|----------|
| C | 0.000000 | 5.145672 | 0.573910 |
| C | 0.000000 | 4.569588 | 1.890830 |
| C | 0.000000 | 3.209952 | 1.902166 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.000000 | 2.616428 | 0.604335 |
| S | 0.000000 | 3.880418 | -0.651430 |
| H | 0.000000 | 5.193326 | 2.775289 |
| H | 0.000000 | 2.618930 | 2.810417 |
| C | 0.000000 | 1.274708 | 0.292937 |
| C | 0.000000 | 0.680880 | -1.007614 |
| S | 0.000000 | -0.000000 | 1.525848 |
| C | -0.000000 | -0.680880 | -1.007614 |
| H | 0.000000 | 1.281547 | -1.908770 |
| C | -0.000000 | -1.274708 | 0.292937 |
| H | -0.000000 | -1.281547 | -1.908770 |
| C | -0.000000 | -2.616428 | 0.604335 |
| C | -0.000000 | -3.209952 | 1.902166 |
| S | -0.000000 | -3.880418 | -0.651430 |
| C | -0.000000 | -4.569588 | 1.890830 |
| H | -0.000000 | -2.618930 | 2.810417 |
| C | -0.000000 | -5.145672 | 0.573910 |
| H | -0.000000 | -5.193326 | 2.775289 |
| C | 0.000000 | 6.497385 | 0.287451 |
| C | 0.000000 | 7.437821 | 1.350703 |
| N | 0.000000 | 8.174661 | 2.243072 |
| C | 0.000000 | 6.965887 | -1.107379 |
| O | 0.000000 | 6.215526 | -2.063692 |
| O | 0.000000 | 8.303207 | -1.201206 |
| C | 0.000000 | 8.840857 | -2.534619 |
| H | -0.888999 | 8.515764 | -3.075950 |
| H | 0.000000 | 9.920163 | -2.407585 |
| H | 0.888999 | 8.515764 | -3.075950 |
| C | -0.000000 | -6.497385 | 0.287451 |
| C | -0.000000 | -7.437821 | 1.350703 |
| N | -0.000000 | -8.174661 | 2.243072 |
| C | -0.000000 | -6.965887 | -1.107379 |
| O | -0.000000 | -6.215526 | -2.063692 |
| O | -0.000000 | -8.303207 | -1.201206 |
| C | -0.000000 | -8.840857 | -2.534619 |
| H | -0.000000 | -9.920163 | -2.407585 |
| H | -0.888999 | -8.515764 | -3.075950 |
| H | 0.888999 | -8.515764 | -3.075950 |

EsQ3-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|----------|----------|-----------|
| C | 0.000000 | 5.126937 | 0.589969 |
| C | 0.000000 | 4.545366 | 1.900489 |
| C | 0.000000 | 3.181551 | 1.894946 |
| C | 0.000000 | 2.621799 | 0.585832 |
| S | 0.000000 | 3.871131 | -0.650470 |

| | | | |
|---|-----------|-----------|-----------|
| H | 0.000000 | 5.157661 | 2.793248 |
| H | 0.000000 | 2.578919 | 2.794745 |
| C | 0.000000 | 1.259263 | 0.251110 |
| C | 0.000000 | 0.687323 | -1.042806 |
| S | 0.000000 | -0.000000 | 1.473561 |
| C | -0.000000 | -0.687323 | -1.042806 |
| H | 0.000000 | 1.285951 | -1.945052 |
| C | -0.000000 | -1.259263 | 0.251110 |
| H | -0.000000 | -1.285951 | -1.945052 |
| C | -0.000000 | -2.621799 | 0.585832 |
| C | -0.000000 | -3.181551 | 1.894946 |
| S | -0.000000 | -3.871131 | -0.650470 |
| C | -0.000000 | -4.545366 | 1.900489 |
| H | -0.000000 | -2.578919 | 2.794745 |
| C | -0.000000 | -5.126937 | 0.589969 |
| H | -0.000000 | -5.157661 | 2.793248 |
| C | 0.000000 | 6.477378 | 0.308872 |
| C | 0.000000 | 7.418426 | 1.367802 |
| N | 0.000000 | 8.162552 | 2.253796 |
| C | 0.000000 | 6.957900 | -1.106957 |
| O | 0.000000 | 6.188718 | -2.042651 |
| O | 0.000000 | 8.278351 | -1.181033 |
| C | 0.000000 | 8.856922 | -2.509640 |
| H | -0.891626 | 8.541623 | -3.050119 |
| H | 0.000000 | 9.930227 | -2.348475 |
| H | 0.891626 | 8.541623 | -3.050119 |
| C | -0.000000 | -6.477378 | 0.308872 |
| C | -0.000000 | -7.418426 | 1.367802 |
| N | -0.000000 | -8.162552 | 2.253796 |
| C | -0.000000 | -6.957900 | -1.106957 |
| O | -0.000000 | -6.188718 | -2.042651 |
| O | -0.000000 | -8.278351 | -1.181033 |
| C | -0.000000 | -8.856922 | -2.509640 |
| H | -0.000000 | -9.930227 | -2.348475 |
| H | -0.891626 | -8.541623 | -3.050119 |
| H | 0.891626 | -8.541623 | -3.050119 |

EsQ3-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|----------|-----------|
| C | -0.000000 | 5.181882 | 0.593383 |
| C | -0.000000 | 4.605710 | 1.880925 |
| C | -0.000000 | 3.219743 | 1.881940 |
| C | -0.000000 | 2.642789 | 0.607363 |
| S | -0.000000 | 3.914746 | -0.632224 |
| H | -0.000000 | 5.217072 | 2.774279 |
| H | -0.000000 | 2.626507 | 2.789652 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.000000 | 1.277586 | 0.258907 |
| C | -0.000000 | 0.695497 | -1.014524 |
| S | -0.000000 | -0.000000 | 1.485235 |
| C | -0.000000 | -0.695497 | -1.014524 |
| H | -0.000000 | 1.292191 | -1.918786 |
| C | -0.000000 | -1.277586 | 0.258907 |
| H | -0.000000 | -1.292191 | -1.918786 |
| C | -0.000000 | -2.642789 | 0.607363 |
| C | -0.000000 | -3.219743 | 1.881940 |
| S | -0.000000 | -3.914746 | -0.632224 |
| C | -0.000000 | -4.605710 | 1.880925 |
| H | -0.000000 | -2.626507 | 2.789652 |
| C | -0.000000 | -5.181882 | 0.593383 |
| H | -0.000000 | -5.217072 | 2.774279 |
| C | -0.000000 | 6.559003 | 0.286319 |
| C | -0.000000 | 7.492609 | 1.349207 |
| N | -0.000000 | 8.224346 | 2.249906 |
| C | -0.000000 | 7.020144 | -1.084682 |
| O | -0.000000 | 6.297461 | -2.069543 |
| O | -0.000000 | 8.380410 | -1.187062 |
| C | -0.000000 | 8.890667 | -2.519086 |
| H | -0.886529 | 8.561497 | -3.065527 |
| H | -0.000000 | 9.974610 | -2.415411 |
| H | 0.886529 | 8.561497 | -3.065527 |
| C | -0.000000 | -6.559003 | 0.286319 |
| C | -0.000000 | -7.492609 | 1.349207 |
| N | -0.000000 | -8.224346 | 2.249906 |
| C | -0.000000 | -7.020144 | -1.084682 |
| O | -0.000000 | -6.297461 | -2.069543 |
| O | -0.000000 | -8.380410 | -1.187062 |
| C | -0.000000 | -8.890667 | -2.519086 |
| H | -0.000000 | -9.974610 | -2.415411 |
| H | -0.886529 | -8.561497 | -3.065527 |
| H | 0.886529 | -8.561497 | -3.065527 |

EsQ4-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|----------|----------|
| C | 0.705879 | 7.061770 | 0.000000 |
| C | 1.968386 | 6.380605 | 0.000000 |
| C | 1.867005 | 5.021930 | 0.000000 |
| C | 0.528236 | 4.538559 | 0.000000 |
| S | -0.618439 | 5.900302 | 0.000000 |
| H | 2.901613 | 6.928634 | 0.000000 |
| H | 2.724255 | 4.358914 | 0.000000 |
| C | 0.102958 | 3.223779 | 0.000000 |
| C | -1.237389 | 2.739971 | 0.000000 |

| | | | |
|---|-----------|------------|-----------|
| S | 1.226017 | 1.852445 | 0.000000 |
| C | -1.347409 | 1.377833 | 0.000000 |
| H | -2.087317 | 3.411006 | 0.000000 |
| C | -0.106090 | 0.684040 | 0.000000 |
| H | -2.296304 | 0.855190 | 0.000000 |
| C | 0.106090 | -0.684040 | 0.000000 |
| C | 1.347409 | -1.377833 | 0.000000 |
| S | -1.226017 | -1.852445 | 0.000000 |
| C | 1.237389 | -2.739971 | 0.000000 |
| H | 2.296304 | -0.855190 | 0.000000 |
| C | -0.102958 | -3.223779 | 0.000000 |
| H | 2.087317 | -3.411006 | 0.000000 |
| C | -0.528236 | -4.538559 | 0.000000 |
| C | -1.867005 | -5.021930 | 0.000000 |
| S | 0.618439 | -5.900302 | 0.000000 |
| C | -1.968386 | -6.380605 | 0.000000 |
| H | -2.724255 | -4.358914 | 0.000000 |
| C | -0.705879 | -7.061770 | 0.000000 |
| H | -2.901613 | -6.928634 | 0.000000 |
| C | -0.528236 | -8.434548 | 0.000000 |
| C | 0.528236 | 8.434548 | 0.000000 |
| C | -0.822292 | 9.013402 | 0.000000 |
| O | -1.837868 | 8.344399 | 0.000000 |
| O | -0.808518 | 10.355334 | 0.000000 |
| C | -2.094218 | 10.997056 | 0.000000 |
| H | -2.660356 | 10.716508 | 0.888846 |
| H | -1.881993 | 12.062999 | 0.000000 |
| H | -2.660356 | 10.716508 | -0.888846 |
| C | 1.664132 | 9.284879 | 0.000000 |
| N | 2.614449 | 9.945731 | 0.000000 |
| C | 0.822292 | -9.013402 | 0.000000 |
| O | 1.837868 | -8.344399 | 0.000000 |
| O | 0.808518 | -10.355334 | 0.000000 |
| C | 2.094218 | -10.997056 | 0.000000 |
| H | 2.660356 | -10.716508 | 0.888846 |
| H | 1.881993 | -12.062999 | 0.000000 |
| H | 2.660356 | -10.716508 | -0.888846 |
| C | -1.664132 | -9.284879 | 0.000000 |
| N | -2.614449 | -9.945731 | 0.000000 |

EsQ4-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|----------|----------|----------|
| C | 0.704876 | 7.072148 | 0.000000 |
| C | 1.960009 | 6.394005 | 0.000000 |
| C | 1.854647 | 5.026668 | 0.000000 |
| C | 0.523213 | 4.553968 | 0.000000 |

| | | | |
|---|-----------|------------|-----------|
| S | -0.619203 | 5.909411 | 0.000000 |
| H | 2.895444 | 6.938268 | 0.000000 |
| H | 2.710858 | 4.362538 | 0.000000 |
| C | 0.081763 | 3.224699 | 0.000000 |
| C | -1.243391 | 2.747675 | 0.000000 |
| S | 1.204400 | 1.860791 | 0.000000 |
| C | -1.349917 | 1.369127 | 0.000000 |
| H | -2.097233 | 3.413683 | 0.000000 |
| C | -0.117845 | 0.694001 | 0.000000 |
| H | -2.298032 | 0.845261 | 0.000000 |
| C | 0.117845 | -0.694001 | 0.000000 |
| C | 1.349917 | -1.369127 | 0.000000 |
| S | -1.204400 | -1.860791 | 0.000000 |
| C | 1.243391 | -2.747675 | 0.000000 |
| H | 2.298032 | -0.845261 | 0.000000 |
| C | -0.081763 | -3.224699 | 0.000000 |
| H | 2.097233 | -3.413683 | 0.000000 |
| C | -0.523213 | -4.553968 | 0.000000 |
| C | -1.854647 | -5.026668 | 0.000000 |
| S | 0.619203 | -5.909411 | 0.000000 |
| C | -1.960009 | -6.394005 | 0.000000 |
| H | -2.710858 | -4.362538 | 0.000000 |
| C | -0.704876 | -7.072148 | 0.000000 |
| H | -2.895444 | -6.938268 | 0.000000 |
| C | -0.523213 | -8.450263 | 0.000000 |
| C | 0.523213 | 8.450263 | 0.000000 |
| C | -0.827615 | 9.030590 | 0.000000 |
| O | -1.843882 | 8.363433 | 0.000000 |
| O | -0.810823 | 10.372394 | 0.000000 |
| C | -2.095374 | 11.016924 | 0.000000 |
| H | -2.661924 | 10.737426 | 0.888890 |
| H | -1.880795 | 12.082371 | 0.000000 |
| H | -2.661924 | 10.737426 | -0.888890 |
| C | 1.657256 | 9.300788 | 0.000000 |
| N | 2.607053 | 9.963074 | 0.000000 |
| C | 0.827615 | -9.030590 | 0.000000 |
| O | 1.843882 | -8.363433 | 0.000000 |
| O | 0.810823 | -10.372394 | 0.000000 |
| C | 2.095374 | -11.016924 | 0.000000 |
| H | 2.661924 | -10.737426 | 0.888890 |
| H | 1.880795 | -12.082371 | 0.000000 |
| H | 2.661924 | -10.737426 | -0.888890 |
| C | -1.657256 | -9.300788 | 0.000000 |
| N | -2.607053 | -9.963074 | 0.000000 |

EsQ4-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|------------|-----------|
| C | 0.695106 | 7.044387 | 0.000000 |
| C | 1.956607 | 6.362946 | 0.000000 |
| C | 1.847381 | 5.003297 | 0.000000 |
| C | 0.501249 | 4.541971 | 0.000000 |
| S | -0.637137 | 5.885589 | 0.000000 |
| H | 2.893264 | 6.905573 | 0.000000 |
| H | 2.699236 | 4.334461 | 0.000000 |
| C | 0.064736 | 3.210540 | 0.000000 |
| C | -1.263128 | 2.733230 | 0.000000 |
| S | 1.191456 | 1.857419 | 0.000000 |
| C | -1.363310 | 1.358729 | 0.000000 |
| H | -2.119953 | 3.395294 | 0.000000 |
| C | -0.119782 | 0.694867 | 0.000000 |
| H | -2.308337 | 0.830012 | 0.000000 |
| C | 0.119782 | -0.694867 | 0.000000 |
| C | 1.363310 | -1.358729 | 0.000000 |
| S | -1.191456 | -1.857419 | 0.000000 |
| C | 1.263128 | -2.733230 | 0.000000 |
| H | 2.308337 | -0.830012 | 0.000000 |
| C | -0.064736 | -3.210540 | 0.000000 |
| H | 2.119953 | -3.395294 | 0.000000 |
| C | -0.501249 | -4.541971 | 0.000000 |
| C | -1.847381 | -5.003297 | 0.000000 |
| S | 0.637137 | -5.885589 | 0.000000 |
| C | -1.956607 | -6.362946 | 0.000000 |
| H | -2.699236 | -4.334461 | 0.000000 |
| C | -0.695106 | -7.044387 | 0.000000 |
| H | -2.893264 | -6.905573 | 0.000000 |
| C | -0.519478 | -8.412278 | 0.000000 |
| C | 0.519478 | 8.412278 | 0.000000 |
| C | -0.850724 | 8.999883 | 0.000000 |
| O | -1.847381 | 8.310212 | 0.000000 |
| O | -0.824361 | 10.325168 | 0.000000 |
| C | -2.104965 | 10.998842 | 0.000000 |
| H | -2.668765 | 10.725206 | 0.891155 |
| H | -1.866202 | 12.057811 | 0.000000 |
| H | -2.668765 | 10.725206 | -0.891155 |
| C | 1.649826 | 9.267661 | 0.000000 |
| N | 2.592695 | 9.938070 | 0.000000 |
| C | 0.850724 | -8.999883 | 0.000000 |
| O | 1.847381 | -8.310212 | 0.000000 |
| O | 0.824361 | -10.325168 | 0.000000 |
| C | 2.104965 | -10.998842 | 0.000000 |
| H | 2.668765 | -10.725206 | 0.891155 |
| H | 1.866202 | -12.057811 | 0.000000 |
| H | 2.668765 | -10.725206 | -0.891155 |

| | | | |
|---|-----------|-----------|----------|
| C | -1.649826 | -9.267661 | 0.000000 |
| N | -2.592695 | -9.938070 | 0.000000 |

EsQ4-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 0.717468 | 7.105114 | 0.000000 |
| C | 1.957113 | 6.430416 | 0.000000 |
| C | 1.849543 | 5.049160 | 0.000000 |
| C | 0.533949 | 4.574257 | 0.000000 |
| S | -0.602994 | 5.937840 | 0.000000 |
| H | 2.895282 | 6.970339 | 0.000000 |
| H | 2.708578 | 4.387270 | 0.000000 |
| C | 0.078686 | 3.239782 | 0.000000 |
| C | -1.236499 | 2.761310 | 0.000000 |
| S | 1.199619 | 1.870721 | 0.000000 |
| C | -1.343797 | 1.372681 | 0.000000 |
| H | -2.091192 | 3.426662 | 0.000000 |
| C | -0.123180 | 0.696167 | 0.000000 |
| H | -2.293432 | 0.850436 | 0.000000 |
| C | 0.123180 | -0.696167 | 0.000000 |
| C | 1.343797 | -1.372681 | 0.000000 |
| S | -1.199619 | -1.870721 | 0.000000 |
| C | 1.236499 | -2.761310 | 0.000000 |
| H | 2.293432 | -0.850436 | 0.000000 |
| C | -0.078686 | -3.239782 | 0.000000 |
| H | 2.091192 | -3.426662 | 0.000000 |
| C | -0.533949 | -4.574257 | 0.000000 |
| C | -1.849543 | -5.049160 | 0.000000 |
| S | 0.602994 | -5.937840 | 0.000000 |
| C | -1.957113 | -6.430416 | 0.000000 |
| H | -2.708578 | -4.387270 | 0.000000 |
| C | -0.717468 | -7.105114 | 0.000000 |
| H | -2.895282 | -6.970339 | 0.000000 |
| C | -0.518831 | -8.500861 | 0.000000 |
| C | 0.518831 | 8.500861 | 0.000000 |
| C | -0.813630 | 9.066447 | 0.000000 |
| O | -1.849543 | 8.419380 | 0.000000 |
| O | -0.811271 | 10.429001 | 0.000000 |
| C | -2.100269 | 11.041376 | 0.000000 |
| H | -2.669982 | 10.755265 | 0.886678 |
| H | -1.912540 | 12.113803 | 0.000000 |
| H | -2.669982 | 10.755265 | -0.886678 |
| C | 1.650819 | 9.349420 | 0.000000 |
| N | 2.605459 | 10.008970 | 0.000000 |
| C | 0.813630 | -9.066447 | 0.000000 |
| O | 1.849543 | -8.419380 | 0.000000 |

| | | | |
|---|-----------|------------|-----------|
| O | 0.811271 | -10.429001 | 0.000000 |
| C | 2.100269 | -11.041376 | 0.000000 |
| H | 2.669982 | -10.755265 | 0.886678 |
| H | 1.912540 | -12.113803 | 0.000000 |
| H | 2.669982 | -10.755265 | -0.886678 |
| C | -1.650819 | -9.349420 | 0.000000 |
| N | -2.605459 | -10.008970 | 0.000000 |

QDTBDT-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 0.124501 | 5.278037 | 0.000000 |
| C | -1.199774 | 4.712430 | 0.000000 |
| C | -1.129356 | 3.337904 | 0.000000 |
| C | 0.176456 | 2.774722 | 0.000000 |
| S | 1.391734 | 4.022302 | 0.000000 |
| C | 0.219646 | 1.390250 | 0.000000 |
| C | -1.117845 | 0.831635 | 0.000000 |
| S | -2.370958 | 2.091705 | 0.000000 |
| C | 1.343192 | 0.513479 | 0.000000 |
| C | 1.117845 | -0.831635 | 0.000000 |
| C | -0.219646 | -1.390250 | 0.000000 |
| C | -1.343192 | -0.513479 | 0.000000 |
| C | -0.176456 | -2.774722 | 0.000000 |
| C | 1.129356 | -3.337904 | 0.000000 |
| S | 2.370958 | -2.091705 | 0.000000 |
| C | 1.199774 | -4.712430 | 0.000000 |
| C | -0.124501 | -5.278037 | 0.000000 |
| S | -1.391734 | -4.022302 | 0.000000 |
| C | 2.477404 | -5.498949 | 0.000000 |
| C | -0.513652 | -6.611209 | 0.000000 |
| C | -1.893155 | -6.954373 | 0.000000 |
| N | -3.022144 | -7.210028 | 0.000000 |
| C | -2.477404 | 5.498949 | 0.000000 |
| C | 0.513652 | 6.611209 | 0.000000 |
| C | 1.893155 | 6.954373 | 0.000000 |
| N | 3.022144 | 7.210028 | 0.000000 |
| C | -0.400531 | 7.697600 | 0.000000 |
| N | -1.117845 | 8.605911 | 0.000000 |
| C | 0.400531 | -7.697600 | 0.000000 |
| N | 1.117845 | -8.605911 | 0.000000 |
| H | 2.348415 | 0.920476 | 0.000000 |
| H | -2.348415 | -0.920476 | 0.000000 |
| H | 2.557777 | -6.144813 | 0.877224 |
| H | 2.557777 | -6.144813 | -0.877224 |
| H | 3.337683 | -4.827645 | 0.000000 |
| H | -2.557777 | 6.144813 | -0.877224 |

| | | | |
|---|-----------|----------|----------|
| H | -3.337683 | 4.827645 | 0.000000 |
| H | -2.557777 | 6.144813 | 0.877224 |

QDTBDT-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 0.079608 | 5.288577 | 0.000000 |
| C | -1.230549 | 4.718004 | 0.000000 |
| C | -1.147525 | 3.331508 | 0.000000 |
| C | 0.152603 | 2.790822 | 0.000000 |
| S | 1.355333 | 4.045234 | 0.000000 |
| C | 0.209801 | 1.387677 | 0.000000 |
| C | -1.116294 | 0.827887 | 0.000000 |
| S | -2.378743 | 2.074813 | 0.000000 |
| C | 1.332795 | 0.528482 | 0.000000 |
| C | 1.116294 | -0.827887 | 0.000000 |
| C | -0.209801 | -1.387677 | 0.000000 |
| C | -1.332795 | -0.528482 | 0.000000 |
| C | -0.152603 | -2.790822 | 0.000000 |
| C | 1.147525 | -3.331508 | 0.000000 |
| S | 2.378743 | -2.074813 | 0.000000 |
| C | 1.230549 | -4.718004 | 0.000000 |
| C | -0.079608 | -5.288577 | 0.000000 |
| S | -1.355333 | -4.045234 | 0.000000 |
| C | 2.518909 | -5.487184 | 0.000000 |
| C | -0.461770 | -6.634442 | 0.000000 |
| C | -1.836244 | -6.989546 | 0.000000 |
| N | -2.962869 | -7.257620 | 0.000000 |
| C | -2.518909 | 5.487184 | 0.000000 |
| C | 0.461770 | 6.634442 | 0.000000 |
| C | 1.836244 | 6.989546 | 0.000000 |
| N | 2.962869 | 7.257620 | 0.000000 |
| C | -0.461770 | 7.709894 | 0.000000 |
| N | -1.191007 | 8.609515 | 0.000000 |
| C | 0.461770 | -7.709894 | 0.000000 |
| N | 1.191007 | -8.609515 | 0.000000 |
| H | 2.336072 | 0.940334 | 0.000000 |
| H | -2.336072 | -0.940334 | 0.000000 |
| H | 2.608159 | -6.131937 | 0.877222 |
| H | 2.608159 | -6.131937 | -0.877222 |
| H | 3.370273 | -4.804755 | 0.000000 |
| H | -2.608159 | 6.131937 | -0.877222 |
| H | -3.370273 | 4.804755 | 0.000000 |
| H | -2.608159 | 6.131937 | 0.877222 |

QDTBDT-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 0.115787 | 5.264127 | 0.000000 |
| C | -1.213122 | 4.707214 | 0.000000 |
| C | -1.138707 | 3.325178 | 0.000000 |
| C | 0.171133 | 2.782330 | 0.000000 |
| S | 1.385792 | 4.011981 | 0.000000 |
| C | 0.216495 | 1.380044 | 0.000000 |
| C | -1.118648 | 0.834342 | 0.000000 |
| S | -2.376121 | 2.080998 | 0.000000 |
| C | 1.339963 | 0.520594 | 0.000000 |
| C | 1.118648 | -0.834342 | 0.000000 |
| C | -0.216495 | -1.380044 | 0.000000 |
| C | -1.339963 | -0.520594 | 0.000000 |
| C | -0.171133 | -2.782330 | 0.000000 |
| C | 1.138707 | -3.325178 | 0.000000 |
| S | 2.376121 | -2.080998 | 0.000000 |
| C | 1.213122 | -4.707214 | 0.000000 |
| C | -0.115787 | -5.264127 | 0.000000 |
| S | -1.385792 | -4.011981 | 0.000000 |
| C | 2.488394 | -5.489701 | 0.000000 |
| C | -0.503667 | -6.597183 | 0.000000 |
| C | -1.882752 | -6.944473 | 0.000000 |
| N | -3.010550 | -7.201736 | 0.000000 |
| C | -2.488394 | 5.489701 | 0.000000 |
| C | 0.503667 | 6.597183 | 0.000000 |
| C | 1.882752 | 6.944473 | 0.000000 |
| N | 3.010550 | 7.201736 | 0.000000 |
| C | -0.414357 | 7.679430 | 0.000000 |
| N | -1.138707 | 8.581314 | 0.000000 |
| C | 0.414357 | -7.679430 | 0.000000 |
| N | 1.138707 | -8.581314 | 0.000000 |
| H | 2.344111 | 0.929844 | 0.000000 |
| H | -2.344111 | -0.929844 | 0.000000 |
| H | 2.565533 | -6.136269 | 0.877576 |
| H | 2.565533 | -6.136269 | -0.877576 |
| H | 3.349943 | -4.821570 | 0.000000 |
| H | -2.565533 | 6.136269 | -0.877576 |
| H | -3.349943 | 4.821570 | 0.000000 |
| H | -2.565533 | 6.136269 | 0.877576 |

QDTBDT-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|----------|----------|
| C | 0.070343 | 5.319670 | 0.000000 |
| C | -1.220867 | 4.742416 | 0.000000 |
| C | -1.134221 | 3.346491 | 0.000000 |
| C | 0.152565 | 2.803387 | 0.000000 |
| S | 1.346846 | 4.075618 | 0.000000 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.213413 | 1.395257 | 0.000000 |
| C | -1.107296 | 0.830254 | 0.000000 |
| S | -2.367378 | 2.084438 | 0.000000 |
| C | 1.328262 | 0.527924 | 0.000000 |
| C | 1.107296 | -0.830254 | 0.000000 |
| C | -0.213413 | -1.395257 | 0.000000 |
| C | -1.328262 | -0.527924 | 0.000000 |
| C | -0.152565 | -2.803387 | 0.000000 |
| C | 1.134221 | -3.346491 | 0.000000 |
| S | 2.367378 | -2.084438 | 0.000000 |
| C | 1.220867 | -4.742416 | 0.000000 |
| C | -0.070343 | -5.319670 | 0.000000 |
| S | -1.346846 | -4.075618 | 0.000000 |
| C | 2.518169 | -5.502797 | 0.000000 |
| C | -0.460058 | -6.681008 | 0.000000 |
| C | -1.829606 | -7.034942 | 0.000000 |
| N | -2.957521 | -7.310652 | 0.000000 |
| C | -2.518169 | 5.502797 | 0.000000 |
| C | 0.460058 | 6.681008 | 0.000000 |
| C | 1.829606 | 7.034942 | 0.000000 |
| N | 2.957521 | 7.310652 | 0.000000 |
| C | -0.460058 | 7.754233 | 0.000000 |
| N | -1.188532 | 8.658445 | 0.000000 |
| C | 0.460058 | -7.754233 | 0.000000 |
| N | 1.188532 | -8.658445 | 0.000000 |
| H | 2.334373 | 0.934116 | 0.000000 |
| H | -2.334373 | -0.934116 | 0.000000 |
| H | 2.616769 | -6.147819 | 0.876496 |
| H | 2.616769 | -6.147819 | -0.876496 |
| H | 3.363584 | -4.811118 | 0.000000 |
| H | -2.616769 | 6.147819 | -0.876496 |
| H | -3.363584 | 4.811118 | 0.000000 |
| H | -2.616769 | 6.147819 | 0.876496 |

TPQ-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| N | -1.530066 | 10.618678 | 0.000000 |
| C | -0.711366 | 9.799057 | 0.000000 |
| C | 0.273999 | 8.779673 | 0.000000 |
| C | 1.629772 | 9.194416 | 0.000000 |
| N | 2.745118 | 9.507870 | 0.000000 |
| C | -0.072367 | 7.417516 | 0.000000 |
| C | -1.453748 | 7.011163 | 0.000000 |
| C | -1.816515 | 5.694111 | 0.000000 |
| C | -0.810755 | 4.693092 | 0.000000 |
| C | 0.576954 | 5.085787 | 0.000000 |

| | | | |
|---|-----------|------------|-----------|
| C | 0.939524 | 6.396146 | 0.000000 |
| H | 1.983612 | 6.690337 | 0.000000 |
| H | -2.216703 | 7.781070 | 0.000000 |
| H | -2.866133 | 5.418867 | 0.000000 |
| C | -0.866409 | 3.293652 | 0.000000 |
| C | 0.423000 | 2.747046 | 0.000000 |
| C | 1.453748 | 3.841190 | 0.000000 |
| H | 2.107272 | 3.802168 | 0.878609 |
| H | 2.107272 | 3.802168 | -0.878609 |
| C | -1.896343 | 2.199958 | 0.000000 |
| H | -2.549746 | 2.241960 | 0.878571 |
| H | -2.549746 | 2.241960 | -0.878571 |
| C | -1.023742 | 0.953962 | 0.000000 |
| C | 0.367935 | 1.344835 | 0.000000 |
| C | 1.394438 | 0.360977 | 0.000000 |
| H | 2.439109 | 0.656597 | 0.000000 |
| N | 1.530066 | -10.618678 | 0.000000 |
| C | 0.711366 | -9.799057 | 0.000000 |
| C | -0.273999 | -8.779673 | 0.000000 |
| C | -1.629772 | -9.194416 | 0.000000 |
| N | -2.745118 | -9.507870 | 0.000000 |
| C | 0.072367 | -7.417516 | 0.000000 |
| C | 1.453748 | -7.011163 | 0.000000 |
| C | 1.816515 | -5.694111 | 0.000000 |
| C | 0.810755 | -4.693092 | 0.000000 |
| C | -0.576954 | -5.085787 | 0.000000 |
| C | -0.939524 | -6.396146 | 0.000000 |
| H | -1.983612 | -6.690337 | 0.000000 |
| H | 2.216703 | -7.781070 | 0.000000 |
| H | 2.866133 | -5.418867 | 0.000000 |
| C | 0.866409 | -3.293652 | 0.000000 |
| C | -0.423000 | -2.747046 | 0.000000 |
| C | -1.453748 | -3.841190 | 0.000000 |
| H | -2.107272 | -3.802168 | -0.878609 |
| H | -2.107272 | -3.802168 | 0.878609 |
| C | 1.896343 | -2.199958 | 0.000000 |
| H | 2.549746 | -2.241960 | -0.878571 |
| H | 2.549746 | -2.241960 | 0.878571 |
| C | 1.023742 | -0.953962 | 0.000000 |
| C | -0.367935 | -1.344835 | 0.000000 |
| C | -1.394438 | -0.360977 | 0.000000 |
| H | -2.439109 | -0.656597 | 0.000000 |

TPQ-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| N | -1.519396 | 10.657430 | 0.000000 |
|---|-----------|-----------|----------|

| | | | |
|---|-----------|------------|-----------|
| C | -0.702169 | 9.835342 | 0.000000 |
| C | 0.279293 | 8.816259 | 0.000000 |
| C | 1.632661 | 9.228725 | 0.000000 |
| N | 2.748502 | 9.543073 | 0.000000 |
| C | -0.074652 | 7.437699 | 0.000000 |
| C | -1.445504 | 7.039493 | 0.000000 |
| C | -1.810061 | 5.712167 | 0.000000 |
| C | -0.808885 | 4.722379 | 0.000000 |
| C | 0.570180 | 5.107981 | 0.000000 |
| C | 0.934106 | 6.425486 | 0.000000 |
| H | 1.979103 | 6.717237 | 0.000000 |
| H | -2.211196 | 7.806913 | 0.000000 |
| H | -2.859843 | 5.438092 | 0.000000 |
| C | -0.859769 | 3.297110 | 0.000000 |
| C | 0.412962 | 2.771862 | 0.000000 |
| C | 1.445504 | 3.863503 | 0.000000 |
| H | 2.099709 | 3.823902 | 0.878504 |
| H | 2.099709 | 3.823902 | -0.878504 |
| C | -1.888653 | 2.201910 | 0.000000 |
| H | -2.542976 | 2.241638 | 0.878518 |
| H | -2.542976 | 2.241638 | -0.878518 |
| C | -1.013193 | 0.957907 | 0.000000 |
| C | 0.364462 | 1.339712 | 0.000000 |
| C | 1.384850 | 0.369475 | 0.000000 |
| H | 2.430237 | 0.663419 | 0.000000 |
| N | 1.519396 | -10.657430 | 0.000000 |
| C | 0.702169 | -9.835342 | 0.000000 |
| C | -0.279293 | -8.816259 | 0.000000 |
| C | -1.632661 | -9.228725 | 0.000000 |
| N | -2.748502 | -9.543073 | 0.000000 |
| C | 0.074652 | -7.437699 | 0.000000 |
| C | 1.445504 | -7.039493 | 0.000000 |
| C | 1.810061 | -5.712167 | 0.000000 |
| C | 0.808885 | -4.722379 | 0.000000 |
| C | -0.570180 | -5.107981 | 0.000000 |
| C | -0.934106 | -6.425486 | 0.000000 |
| H | -1.979103 | -6.717237 | 0.000000 |
| H | 2.211196 | -7.806913 | 0.000000 |
| H | 2.859843 | -5.438092 | 0.000000 |
| C | 0.859769 | -3.297110 | 0.000000 |
| C | -0.412962 | -2.771862 | 0.000000 |
| C | -1.445504 | -3.863503 | 0.000000 |
| H | -2.099709 | -3.823902 | -0.878504 |
| H | -2.099709 | -3.823902 | 0.878504 |
| C | 1.888653 | -2.201910 | 0.000000 |
| H | 2.542976 | -2.241638 | -0.878518 |
| H | 2.542976 | -2.241638 | 0.878518 |

| | | | |
|---|-----------|-----------|----------|
| C | 1.013193 | -0.957907 | 0.000000 |
| C | -0.364462 | -1.339712 | 0.000000 |
| C | -1.384850 | -0.369475 | 0.000000 |
| H | -2.430237 | -0.663419 | 0.000000 |

TPQ-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|------------|-----------|
| N | -1.525363 | 10.616907 | 0.000000 |
| C | -0.710173 | 9.794922 | 0.000000 |
| C | 0.272795 | 8.773962 | 0.000000 |
| C | 1.627905 | 9.190184 | 0.000000 |
| N | 2.742132 | 9.504321 | 0.000000 |
| C | -0.074974 | 7.406498 | 0.000000 |
| C | -1.454695 | 7.009886 | 0.000000 |
| C | -1.816581 | 5.689065 | 0.000000 |
| C | -0.804521 | 4.699529 | 0.000000 |
| C | 0.581246 | 5.082723 | 0.000000 |
| C | 0.943420 | 6.396612 | 0.000000 |
| H | 1.986580 | 6.693095 | 0.000000 |
| H | -2.218467 | 7.778757 | 0.000000 |
| H | -2.864240 | 5.410049 | 0.000000 |
| C | -0.864026 | 3.287260 | 0.000000 |
| C | 0.420413 | 2.752879 | 0.000000 |
| C | 1.454695 | 3.839457 | 0.000000 |
| H | 2.108098 | 3.796064 | 0.878529 |
| H | 2.108098 | 3.796064 | -0.878529 |
| C | -1.896085 | 2.198331 | 0.000000 |
| H | -2.549651 | 2.240744 | 0.878457 |
| H | -2.549651 | 2.240744 | -0.878457 |
| C | -1.023141 | 0.955257 | 0.000000 |
| C | 0.364963 | 1.336169 | 0.000000 |
| C | 1.393713 | 0.365641 | 0.000000 |
| H | 2.437041 | 0.663681 | 0.000000 |
| N | 1.525363 | -10.616907 | 0.000000 |
| C | 0.710173 | -9.794922 | 0.000000 |
| C | -0.272795 | -8.773962 | 0.000000 |
| C | -1.627905 | -9.190184 | 0.000000 |
| N | -2.742132 | -9.504321 | 0.000000 |
| C | 0.074974 | -7.406498 | 0.000000 |
| C | 1.454695 | -7.009886 | 0.000000 |
| C | 1.816581 | -5.689065 | 0.000000 |
| C | 0.804521 | -4.699529 | 0.000000 |
| C | -0.581246 | -5.082723 | 0.000000 |
| C | -0.943420 | -6.396612 | 0.000000 |
| H | -1.986580 | -6.693095 | 0.000000 |
| H | 2.218467 | -7.778757 | 0.000000 |

| | | | |
|---|-----------|-----------|-----------|
| H | 2.864240 | -5.410049 | 0.000000 |
| C | 0.864026 | -3.287260 | 0.000000 |
| C | -0.420413 | -2.752879 | 0.000000 |
| C | -1.454695 | -3.839457 | 0.000000 |
| H | -2.108098 | -3.796064 | -0.878529 |
| H | -2.108098 | -3.796064 | 0.878529 |
| C | 1.896085 | -2.198331 | 0.000000 |
| H | 2.549651 | -2.240744 | -0.878457 |
| H | 2.549651 | -2.240744 | 0.878457 |
| C | 1.023141 | -0.955257 | 0.000000 |
| C | -0.364963 | -1.336169 | 0.000000 |
| C | -1.393713 | -0.365641 | 0.000000 |
| H | -2.437041 | -0.663681 | 0.000000 |

TPO-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| N | 6.643221 | 8.502344 | 0.000000 |
| C | 6.622644 | 7.340565 | 0.000000 |
| C | 6.571608 | 5.929905 | 0.000000 |
| C | 7.802017 | 5.238369 | 0.000000 |
| N | 8.802928 | 4.647986 | 0.000000 |
| C | 5.324819 | 5.227500 | 0.000000 |
| C | 4.084859 | 5.931198 | 0.000000 |
| C | 2.872261 | 5.273367 | 0.000000 |
| C | 2.843178 | 3.868066 | 0.000000 |
| C | 4.078297 | 3.148369 | 0.000000 |
| C | 5.282818 | 3.800286 | 0.000000 |
| H | 6.215886 | 3.245463 | 0.000000 |
| H | 4.105366 | 7.015569 | 0.000000 |
| H | 1.948709 | 5.845248 | 0.000000 |
| C | 1.784607 | 2.910151 | 0.000000 |
| C | 2.286128 | 1.628898 | 0.000000 |
| C | 3.791270 | 1.651009 | 0.000000 |
| H | 4.219954 | 1.154088 | 0.878468 |
| H | 4.219954 | 1.154088 | -0.878468 |
| C | 0.280574 | 2.887166 | 0.000000 |
| H | -0.145576 | 3.386294 | 0.878503 |
| H | -0.145576 | 3.386294 | -0.878503 |
| C | -0.010343 | 1.392368 | 0.000000 |
| C | 1.224226 | 0.669994 | 0.000000 |
| C | 1.224226 | -0.740486 | 0.000000 |
| H | 2.159965 | -1.293079 | 0.000000 |
| N | -6.643221 | -8.502344 | 0.000000 |
| C | -6.622644 | -7.340565 | 0.000000 |
| C | -6.571608 | -5.929905 | 0.000000 |
| C | -7.802017 | -5.238369 | 0.000000 |

| | | | |
|---|-----------|-----------|-----------|
| N | -8.802928 | -4.647986 | 0.000000 |
| C | -5.324819 | -5.227500 | 0.000000 |
| C | -4.084859 | -5.931198 | 0.000000 |
| C | -2.872261 | -5.273367 | 0.000000 |
| C | -2.843178 | -3.868066 | 0.000000 |
| C | -4.078297 | -3.148369 | 0.000000 |
| C | -5.282818 | -3.800286 | 0.000000 |
| H | -6.215886 | -3.245463 | 0.000000 |
| H | -4.105366 | -7.015569 | 0.000000 |
| H | -1.948709 | -5.845248 | 0.000000 |
| C | -1.784607 | -2.910151 | 0.000000 |
| C | -2.286128 | -1.628898 | 0.000000 |
| C | -3.791270 | -1.651009 | 0.000000 |
| H | -4.219954 | -1.154088 | -0.878468 |
| H | -4.219954 | -1.154088 | 0.878468 |
| C | -0.280574 | -2.887166 | 0.000000 |
| H | 0.145576 | -3.386294 | -0.878503 |
| H | 0.145576 | -3.386294 | 0.878503 |
| C | 0.010343 | -1.392368 | 0.000000 |
| C | -1.224226 | -0.669994 | 0.000000 |
| C | -1.224226 | 0.740486 | 0.000000 |
| H | -2.159965 | 1.293079 | 0.000000 |

NZ-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 8.598774 | 0.669978 | 0.000000 |
| C | 8.641021 | -0.706928 | 0.000000 |
| C | 7.442929 | -1.471163 | 0.000000 |
| C | 6.183066 | -0.796608 | 0.000000 |
| C | 6.161408 | 0.638261 | 0.000000 |
| C | 7.368157 | 1.341289 | 0.000000 |
| H | 7.345832 | 2.426890 | 0.000000 |
| C | 4.903983 | 1.309686 | 0.000000 |
| C | 3.700516 | 0.638034 | 0.000000 |
| C | 3.677165 | -0.825765 | 0.000000 |
| C | 4.966367 | -1.543707 | 0.000000 |
| H | 4.901916 | 2.396341 | 0.000000 |
| C | 2.462110 | 1.343896 | 0.000000 |
| C | 1.241136 | 0.705524 | 0.000000 |
| C | 1.212972 | -0.752301 | 0.000000 |
| C | 2.462110 | -1.454813 | 0.000000 |
| H | 2.495051 | 2.430251 | 0.000000 |
| H | 2.404526 | -2.537831 | 0.000000 |
| C | -0.001910 | 1.406443 | 0.000000 |
| C | -1.212972 | 0.752301 | 0.000000 |
| C | -1.241136 | -0.705524 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | 0.001910 | -1.406443 | 0.000000 |
| H | 0.019078 | 2.493220 | 0.000000 |
| H | -0.019078 | -2.493220 | 0.000000 |
| C | -2.462110 | 1.454813 | 0.000000 |
| C | -3.677165 | 0.825765 | 0.000000 |
| C | -3.700516 | -0.638034 | 0.000000 |
| C | -2.462110 | -1.343896 | 0.000000 |
| H | -2.404526 | 2.537831 | 0.000000 |
| H | -2.495051 | -2.430251 | 0.000000 |
| C | -4.966367 | 1.543707 | 0.000000 |
| C | -6.183066 | 0.796608 | 0.000000 |
| C | -6.161408 | -0.638261 | 0.000000 |
| C | -4.903983 | -1.309686 | 0.000000 |
| H | -4.901916 | -2.396341 | 0.000000 |
| C | -7.368157 | -1.341289 | 0.000000 |
| C | -8.598774 | -0.669978 | 0.000000 |
| H | -9.521201 | -1.241862 | 0.000000 |
| C | -8.641021 | 0.706928 | 0.000000 |
| H | -9.593388 | 1.228051 | 0.000000 |
| C | -7.442929 | 1.471163 | 0.000000 |
| H | -7.345832 | -2.426890 | 0.000000 |
| C | -5.052212 | 2.935209 | 0.000000 |
| C | -7.465710 | 2.884937 | 0.000000 |
| C | -6.287033 | 3.597599 | 0.000000 |
| H | -4.151250 | 3.536700 | 0.000000 |
| H | -6.306808 | 4.682742 | 0.000000 |
| H | -8.422106 | 3.398852 | 0.000000 |
| H | 9.593388 | -1.228051 | 0.000000 |
| H | 9.521201 | 1.241862 | 0.000000 |
| C | 5.052212 | -2.935209 | 0.000000 |
| C | 7.465710 | -2.884937 | 0.000000 |
| C | 6.287033 | -3.597599 | 0.000000 |
| H | 6.306808 | -4.682742 | 0.000000 |
| H | 8.422106 | -3.398852 | 0.000000 |
| H | 4.151250 | -3.536700 | 0.000000 |

NZ-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|----------|-----------|----------|
| C | 8.599021 | 0.732472 | 0.000000 |
| C | 8.644066 | -0.646898 | 0.000000 |
| C | 7.447164 | -1.415337 | 0.000000 |
| C | 6.184912 | -0.745371 | 0.000000 |
| C | 6.158469 | 0.692700 | 0.000000 |
| C | 7.370353 | 1.400744 | 0.000000 |
| H | 7.345006 | 2.486198 | 0.000000 |
| C | 4.909310 | 1.357590 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | 3.691933 | 0.671587 | 0.000000 |
| C | 3.681605 | -0.786252 | 0.000000 |
| C | 4.972153 | -1.496493 | 0.000000 |
| H | 4.899160 | 2.443953 | 0.000000 |
| C | 2.465934 | 1.367402 | 0.000000 |
| C | 1.232028 | 0.714289 | 0.000000 |
| C | 1.219672 | -0.736297 | 0.000000 |
| C | 2.465934 | -1.428519 | 0.000000 |
| H | 2.488448 | 2.453899 | 0.000000 |
| H | 2.418709 | -2.511832 | 0.000000 |
| C | -0.001541 | 1.404854 | 0.000000 |
| C | -1.219672 | 0.736297 | 0.000000 |
| C | -1.232028 | -0.714289 | 0.000000 |
| C | 0.001541 | -1.404854 | 0.000000 |
| H | 0.008837 | 2.491711 | 0.000000 |
| H | -0.008837 | -2.491711 | 0.000000 |
| C | -2.465934 | 1.428519 | 0.000000 |
| C | -3.681605 | 0.786252 | 0.000000 |
| C | -3.691933 | -0.671587 | 0.000000 |
| C | -2.465934 | -1.367402 | 0.000000 |
| H | -2.418709 | 2.511832 | 0.000000 |
| H | -2.488448 | -2.453899 | 0.000000 |
| C | -4.972153 | 1.496493 | 0.000000 |
| C | -6.184912 | 0.745371 | 0.000000 |
| C | -6.158469 | -0.692700 | 0.000000 |
| C | -4.909310 | -1.357590 | 0.000000 |
| H | -4.899160 | -2.443953 | 0.000000 |
| C | -7.370353 | -1.400744 | 0.000000 |
| C | -8.599021 | -0.732472 | 0.000000 |
| H | -9.520897 | -1.305344 | 0.000000 |
| C | -8.644066 | 0.646898 | 0.000000 |
| H | -9.597639 | 1.165749 | 0.000000 |
| C | -7.447164 | 1.415337 | 0.000000 |
| H | -7.345006 | -2.486198 | 0.000000 |
| C | -5.062860 | 2.890422 | 0.000000 |
| C | -7.475718 | 2.827977 | 0.000000 |
| C | -6.298783 | 3.546692 | 0.000000 |
| H | -4.164163 | 3.495052 | 0.000000 |
| H | -6.323737 | 4.631759 | 0.000000 |
| H | -8.434143 | 3.338116 | 0.000000 |
| H | 9.597639 | -1.165749 | 0.000000 |
| H | 9.520897 | 1.305344 | 0.000000 |
| C | 5.062860 | -2.890422 | 0.000000 |
| C | 7.475718 | -2.827977 | 0.000000 |
| C | 6.298783 | -3.546692 | 0.000000 |
| H | 6.323737 | -4.631759 | 0.000000 |
| H | 8.434143 | -3.338116 | 0.000000 |

| | | | |
|---|----------|-----------|----------|
| H | 4.164163 | -3.495052 | 0.000000 |
|---|----------|-----------|----------|

NZ-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 8.574138 | 0.759058 | 0.000000 |
| C | 8.622136 | -0.623565 | 0.000000 |
| C | 7.437146 | -1.405654 | 0.000000 |
| C | 6.170659 | -0.749306 | 0.000000 |
| C | 6.137762 | 0.686383 | 0.000000 |
| C | 7.341560 | 1.412293 | 0.000000 |
| H | 7.303690 | 2.496826 | 0.000000 |
| C | 4.890881 | 1.343880 | 0.000000 |
| C | 3.678779 | 0.650597 | 0.000000 |
| C | 3.674520 | -0.808583 | 0.000000 |
| C | 4.968230 | -1.508517 | 0.000000 |
| H | 4.873869 | 2.429822 | 0.000000 |
| C | 2.459962 | 1.356581 | 0.000000 |
| C | 1.228115 | 0.705394 | 0.000000 |
| C | 1.217540 | -0.747404 | 0.000000 |
| C | 2.459962 | -1.448425 | 0.000000 |
| H | 2.488180 | 2.442092 | 0.000000 |
| H | 2.407993 | -2.530875 | 0.000000 |
| C | 0.001232 | 1.408647 | 0.000000 |
| C | -1.217540 | 0.747404 | 0.000000 |
| C | -1.228115 | -0.705394 | 0.000000 |
| C | -0.001232 | -1.408647 | 0.000000 |
| H | 0.021905 | 2.494404 | 0.000000 |
| H | -0.021905 | -2.494404 | 0.000000 |
| C | -2.459962 | 1.448425 | 0.000000 |
| C | -3.674520 | 0.808583 | 0.000000 |
| C | -3.678779 | -0.650597 | 0.000000 |
| C | -2.459962 | -1.356581 | 0.000000 |
| H | -2.407993 | 2.530875 | 0.000000 |
| H | -2.488180 | -2.442092 | 0.000000 |
| C | -4.968230 | 1.508517 | 0.000000 |
| C | -6.170659 | 0.749306 | 0.000000 |
| C | -6.137762 | -0.686383 | 0.000000 |
| C | -4.890881 | -1.343880 | 0.000000 |
| H | -4.873869 | -2.429822 | 0.000000 |
| C | -7.341560 | -1.412293 | 0.000000 |
| C | -8.574138 | -0.759058 | 0.000000 |
| H | -9.492055 | -1.335440 | 0.000000 |
| C | -8.622136 | 0.623565 | 0.000000 |
| H | -9.580768 | 1.132275 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | -7.437146 | 1.405654 | 0.000000 |
| H | -7.303690 | -2.496826 | 0.000000 |
| C | -5.074167 | 2.901941 | 0.000000 |
| C | -7.484946 | 2.817698 | 0.000000 |
| C | -6.315139 | 3.548626 | 0.000000 |
| H | -4.182202 | 3.516338 | 0.000000 |
| H | -6.349900 | 4.632267 | 0.000000 |
| H | -8.447706 | 3.317719 | 0.000000 |
| H | 9.580768 | -1.132275 | 0.000000 |
| H | 9.492055 | 1.335440 | 0.000000 |
| C | 5.074167 | -2.901941 | 0.000000 |
| C | 7.484946 | -2.817698 | 0.000000 |
| C | 6.315139 | -3.548626 | 0.000000 |
| H | 6.349900 | -4.632267 | 0.000000 |
| H | 8.447706 | -3.317719 | 0.000000 |
| H | 4.182202 | -3.516338 | 0.000000 |

NZ-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|----------|
| C | 8.615988 | 0.708740 | 0.000000 |
| C | 8.660852 | -0.673521 | 0.000000 |
| C | 7.456398 | -1.428583 | 0.000000 |
| C | 6.194432 | -0.747468 | 0.000000 |
| C | 6.170233 | 0.696699 | 0.000000 |
| C | 7.397682 | 1.389326 | 0.000000 |
| H | 7.383698 | 2.476008 | 0.000000 |
| C | 4.927201 | 1.364289 | 0.000000 |
| C | 3.703969 | 0.688576 | 0.000000 |
| C | 3.686573 | -0.772198 | 0.000000 |
| C | 4.975453 | -1.491049 | 0.000000 |
| H | 4.922852 | 2.451819 | 0.000000 |
| C | 2.471095 | 1.374266 | 0.000000 |
| C | 1.237615 | 0.723321 | 0.000000 |
| C | 1.219488 | -0.730259 | 0.000000 |
| C | 2.471095 | -1.415173 | 0.000000 |
| H | 2.489154 | 2.462210 | 0.000000 |
| H | 2.426610 | -2.499390 | 0.000000 |
| C | -0.004536 | 1.402419 | 0.000000 |
| C | -1.219488 | 0.730259 | 0.000000 |
| C | -1.237615 | -0.723321 | 0.000000 |
| C | 0.004536 | -1.402419 | 0.000000 |
| H | -0.002519 | 2.490629 | 0.000000 |
| H | 0.002519 | -2.490629 | 0.000000 |
| C | -2.471095 | 1.415173 | 0.000000 |
| C | -3.686573 | 0.772198 | 0.000000 |
| C | -3.703969 | -0.688576 | 0.000000 |

| | | | |
|---|-----------|-----------|----------|
| C | -2.471095 | -1.374266 | 0.000000 |
| H | -2.426610 | 2.499390 | 0.000000 |
| H | -2.489154 | -2.462210 | 0.000000 |
| C | -4.975453 | 1.491049 | 0.000000 |
| C | -6.194432 | 0.747468 | 0.000000 |
| C | -6.170233 | -0.696699 | 0.000000 |
| C | -4.927201 | -1.364289 | 0.000000 |
| H | -4.922852 | -2.451819 | 0.000000 |
| C | -7.397682 | -1.389326 | 0.000000 |
| C | -8.615988 | -0.708740 | 0.000000 |
| H | -9.543064 | -1.277431 | 0.000000 |
| C | -8.660852 | 0.673521 | 0.000000 |
| H | -9.611566 | 1.199222 | 0.000000 |
| C | -7.456398 | 1.428583 | 0.000000 |
| H | -7.383698 | -2.476008 | 0.000000 |
| C | -5.052806 | 2.888603 | 0.000000 |
| C | -7.467398 | 2.843156 | 0.000000 |
| C | -6.283771 | 3.551821 | 0.000000 |
| H | -4.148171 | 3.484420 | 0.000000 |
| H | -6.301320 | 4.638664 | 0.000000 |
| H | -8.422314 | 3.362502 | 0.000000 |
| H | 9.611566 | -1.199222 | 0.000000 |
| H | 9.543064 | 1.277431 | 0.000000 |
| C | 5.052806 | -2.888603 | 0.000000 |
| C | 7.467398 | -2.843156 | 0.000000 |
| C | 6.283771 | -3.551821 | 0.000000 |
| H | 6.301320 | -4.638664 | 0.000000 |
| H | 8.422314 | -3.362502 | 0.000000 |
| H | 4.148171 | -3.484420 | 0.000000 |

Ph₂-IDPL-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | -1.109102 | 0.141698 | -0.921942 |
| C | -0.943763 | -1.026085 | -0.167205 |
| C | 0.168041 | -1.169681 | 0.757752 |
| C | 0.065698 | -2.471067 | 1.380480 |
| C | 0.794772 | -3.218791 | 2.339659 |
| C | 0.366259 | -4.484461 | 2.694947 |
| C | -0.802930 | -5.099450 | 2.133790 |
| C | -1.280545 | -6.378733 | 2.459798 |
| C | -2.435981 | -6.904165 | 1.861365 |
| C | -3.136323 | -6.144570 | 0.919014 |
| C | -2.708517 | -4.854934 | 0.549458 |
| C | -3.362973 | -4.009029 | -0.404042 |
| C | -2.900210 | -2.746124 | -0.731850 |
| C | -1.730672 | -2.242780 | -0.111899 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.087597 | -3.080004 | 0.828832 |
| C | -1.535825 | -4.352441 | 1.172070 |
| C | -2.251297 | 0.289327 | -1.872751 |
| C | -3.466891 | 0.834093 | -1.444718 |
| C | -4.532407 | 0.972143 | -2.332101 |
| C | -4.396015 | 0.567246 | -3.658882 |
| C | -3.188425 | 0.023474 | -4.093512 |
| C | -2.122892 | -0.114620 | -3.206140 |
| C | -2.907761 | -8.290653 | 2.234996 |
| H | 1.686259 | -2.812931 | 2.801330 |
| H | 0.936197 | -5.044016 | 3.431512 |
| H | -0.744481 | -6.977278 | 3.192632 |
| H | -4.031115 | -6.559086 | 0.461799 |
| H | -4.261753 | -4.380470 | -0.888466 |
| H | -3.441839 | -2.157186 | -1.461577 |
| H | -3.574197 | 1.149616 | -0.412104 |
| H | -5.469609 | 1.396419 | -1.985864 |
| H | -5.225915 | 0.674718 | -4.350034 |
| H | -3.074308 | -0.294352 | -5.125109 |
| H | -1.183281 | -0.538046 | -3.545548 |
| H | -3.029952 | -8.394272 | 3.317384 |
| H | -3.866811 | -8.527504 | 1.770033 |
| H | -2.190734 | -9.055060 | 1.918009 |
| C | 1.109102 | -0.141698 | 0.921942 |
| C | 0.943763 | 1.026085 | 0.167205 |
| C | -0.168041 | 1.169681 | -0.757752 |
| C | -0.065698 | 2.471067 | -1.380480 |
| C | -0.794772 | 3.218791 | -2.339659 |
| C | -0.366259 | 4.484461 | -2.694947 |
| C | 0.802930 | 5.099450 | -2.133790 |
| C | 1.280545 | 6.378733 | -2.459798 |
| C | 2.435981 | 6.904165 | -1.861365 |
| C | 3.136323 | 6.144570 | -0.919014 |
| C | 2.708517 | 4.854934 | -0.549458 |
| C | 3.362973 | 4.009029 | 0.404042 |
| C | 2.900210 | 2.746124 | 0.731850 |
| C | 1.730672 | 2.242780 | 0.111899 |
| C | 1.087597 | 3.080004 | -0.828832 |
| C | 1.535825 | 4.352441 | -1.172070 |
| C | 2.251297 | -0.289327 | 1.872751 |
| C | 3.466891 | -0.834093 | 1.444718 |
| C | 4.532407 | -0.972143 | 2.332101 |
| C | 4.396015 | -0.567246 | 3.658882 |
| C | 3.188425 | -0.023474 | 4.093512 |
| C | 2.122892 | 0.114620 | 3.206140 |
| C | 2.907761 | 8.290653 | -2.234996 |
| H | -1.686259 | 2.812931 | -2.801330 |

| | | | |
|---|-----------|-----------|-----------|
| H | -0.936197 | 5.044016 | -3.431512 |
| H | 0.744481 | 6.977278 | -3.192632 |
| H | 4.031115 | 6.559086 | -0.461799 |
| H | 4.261753 | 4.380470 | 0.888466 |
| H | 3.441839 | 2.157186 | 1.461577 |
| H | 3.574197 | -1.149616 | 0.412104 |
| H | 5.469609 | -1.396419 | 1.985864 |
| H | 5.225915 | -0.674718 | 4.350034 |
| H | 3.074308 | 0.294352 | 5.125109 |
| H | 1.183281 | 0.538046 | 3.545548 |
| H | 3.029952 | 8.394272 | -3.317384 |
| H | 3.866811 | 8.527504 | -1.770033 |
| H | 2.190734 | 9.055060 | -1.918009 |

Ph₂-IDPL-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | -1.107512 | 0.141774 | -0.920764 |
| C | -0.940383 | -1.025057 | -0.165091 |
| C | 0.166401 | -1.167737 | 0.755540 |
| C | 0.063620 | -2.478100 | 1.382754 |
| C | 0.791462 | -3.220672 | 2.338241 |
| C | 0.362851 | -4.491215 | 2.696073 |
| C | -0.803871 | -5.104390 | 2.135854 |
| C | -1.283047 | -6.386048 | 2.461964 |
| C | -2.438545 | -6.910623 | 1.862990 |
| C | -3.138899 | -6.151124 | 0.920675 |
| C | -2.710399 | -4.859291 | 0.550464 |
| C | -3.363521 | -4.015032 | -0.401188 |
| C | -2.897543 | -2.748081 | -0.728703 |
| C | -1.732092 | -2.249088 | -0.109516 |
| C | -1.088880 | -3.085404 | 0.830843 |
| C | -1.537227 | -4.357481 | 1.173825 |
| C | -2.250277 | 0.289082 | -1.871850 |
| C | -3.466496 | 0.833341 | -1.444447 |
| C | -4.532271 | 0.971190 | -2.331608 |
| C | -4.395864 | 0.566453 | -3.658432 |
| C | -3.188068 | 0.023160 | -4.093107 |
| C | -2.122579 | -0.114526 | -3.205591 |
| C | -2.910641 | -8.297007 | 2.236234 |
| H | 1.683009 | -2.814175 | 2.799598 |
| H | 0.933709 | -5.049575 | 3.432728 |
| H | -0.747174 | -6.984726 | 3.194721 |
| H | -4.033714 | -6.565262 | 0.463265 |
| H | -4.262382 | -4.384946 | -0.886486 |
| H | -3.438596 | -2.158393 | -1.458441 |

| | | | |
|---|-----------|-----------|-----------|
| H | -3.574100 | 1.148861 | -0.411801 |
| H | -5.469609 | 1.395164 | -1.985313 |
| H | -5.225872 | 0.673722 | -4.349529 |
| H | -3.073888 | -0.294512 | -5.124766 |
| H | -1.182864 | -0.537633 | -3.545299 |
| H | -3.031826 | -8.401074 | 3.318666 |
| H | -3.870244 | -8.533208 | 1.771999 |
| H | -2.194108 | -9.061412 | 1.918285 |
| C | 1.107512 | -0.141774 | 0.920764 |
| C | 0.940383 | 1.025057 | 0.165091 |
| C | -0.166401 | 1.167737 | -0.755540 |
| C | -0.063620 | 2.478100 | -1.382754 |
| C | -0.791462 | 3.220672 | -2.338241 |
| C | -0.362851 | 4.491215 | -2.696073 |
| C | 0.803871 | 5.104390 | -2.135854 |
| C | 1.283047 | 6.386048 | -2.461964 |
| C | 2.438545 | 6.910623 | -1.862990 |
| C | 3.138899 | 6.151124 | -0.920675 |
| C | 2.710399 | 4.859291 | -0.550464 |
| C | 3.363521 | 4.015032 | 0.401188 |
| C | 2.897543 | 2.748081 | 0.728703 |
| C | 1.732092 | 2.249088 | 0.109516 |
| C | 1.088880 | 3.085404 | -0.830843 |
| C | 1.537227 | 4.357481 | -1.173825 |
| C | 2.250277 | -0.289082 | 1.871850 |
| C | 3.466496 | -0.833341 | 1.444447 |
| C | 4.532271 | -0.971190 | 2.331608 |
| C | 4.395864 | -0.566453 | 3.658432 |
| C | 3.188068 | -0.023160 | 4.093107 |
| C | 2.122579 | 0.114526 | 3.205591 |
| C | 2.910641 | 8.297007 | -2.236234 |
| H | -1.683009 | 2.814175 | -2.799598 |
| H | -0.933709 | 5.049575 | -3.432728 |
| H | 0.747174 | 6.984726 | -3.194721 |
| H | 4.033714 | 6.565262 | -0.463265 |
| H | 4.262382 | 4.384946 | 0.886486 |
| H | 3.438596 | 2.158393 | 1.458441 |
| H | 3.574100 | -1.148861 | 0.411801 |
| H | 5.469609 | -1.395164 | 1.985313 |
| H | 5.225872 | -0.673722 | 4.349529 |
| H | 3.073888 | 0.294512 | 5.124766 |
| H | 1.182864 | 0.537633 | 3.545299 |
| H | 3.031826 | 8.401074 | -3.318666 |
| H | 3.870244 | 8.533208 | -1.771999 |
| H | 2.194108 | 9.061412 | -1.918285 |

Ph₂-IDPL-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | -1.110363 | 0.142582 | -0.923346 |
| C | -0.935095 | -1.021287 | -0.163081 |
| C | 0.163655 | -1.162969 | 0.750839 |
| C | 0.060574 | -2.482816 | 1.382798 |
| C | 0.790446 | -3.216647 | 2.334916 |
| C | 0.357569 | -4.492498 | 2.692240 |
| C | -0.805399 | -5.101016 | 2.132483 |
| C | -1.284852 | -6.385581 | 2.459696 |
| C | -2.440154 | -6.915370 | 1.863755 |
| C | -3.137344 | -6.151004 | 0.921416 |
| C | -2.707291 | -4.856924 | 0.551373 |
| C | -3.359726 | -4.017016 | -0.397326 |
| C | -2.894084 | -2.744127 | -0.728204 |
| C | -1.732815 | -2.253301 | -0.107825 |
| C | -1.089973 | -3.087937 | 0.831242 |
| C | -1.537207 | -4.356812 | 1.173322 |
| C | -2.252411 | 0.289974 | -1.873952 |
| C | -3.467135 | 0.834800 | -1.442283 |
| C | -4.532130 | 0.972117 | -2.330792 |
| C | -4.394124 | 0.566979 | -3.657479 |
| C | -3.186806 | 0.023448 | -4.093640 |
| C | -2.120317 | -0.114953 | -3.207107 |
| C | -2.911247 | -8.299923 | 2.238365 |
| H | 1.681268 | -2.810727 | 2.795959 |
| H | 0.929185 | -5.049212 | 3.428478 |
| H | -0.748194 | -6.982712 | 3.192083 |
| H | -4.031794 | -6.563450 | 0.463553 |
| H | -4.258150 | -4.385028 | -0.883241 |
| H | -3.435013 | -2.155249 | -1.457303 |
| H | -3.577549 | 1.151047 | -0.410084 |
| H | -5.469332 | 1.395730 | -1.985529 |
| H | -5.223613 | 0.674232 | -4.348216 |
| H | -3.073496 | -0.293760 | -5.124920 |
| H | -1.181661 | -0.538448 | -3.549465 |
| H | -3.031175 | -8.400062 | 3.320332 |
| H | -3.869527 | -8.538341 | 1.774970 |
| H | -2.192161 | -9.060694 | 1.920611 |
| C | 1.110363 | -0.142582 | 0.923346 |
| C | 0.935095 | 1.021287 | 0.163081 |
| C | -0.163655 | 1.162969 | -0.750839 |
| C | -0.060574 | 2.482816 | -1.382798 |
| C | -0.790446 | 3.216647 | -2.334916 |
| C | -0.357569 | 4.492498 | -2.692240 |
| C | 0.805399 | 5.101016 | -2.132483 |

| | | | |
|---|-----------|-----------|-----------|
| C | 1.284852 | 6.385581 | -2.459696 |
| C | 2.440154 | 6.915370 | -1.863755 |
| C | 3.137344 | 6.151004 | -0.921416 |
| C | 2.707291 | 4.856924 | -0.551373 |
| C | 3.359726 | 4.017016 | 0.397326 |
| C | 2.894084 | 2.744127 | 0.728204 |
| C | 1.732815 | 2.253301 | 0.107825 |
| C | 1.089973 | 3.087937 | -0.831242 |
| C | 1.537207 | 4.356812 | -1.173322 |
| C | 2.252411 | -0.289974 | 1.873952 |
| C | 3.467135 | -0.834800 | 1.442283 |
| C | 4.532130 | -0.972117 | 2.330792 |
| C | 4.394124 | -0.566979 | 3.657479 |
| C | 3.186806 | -0.023448 | 4.093640 |
| C | 2.120317 | 0.114953 | 3.207107 |
| C | 2.911247 | 8.299923 | -2.238365 |
| H | -1.681268 | 2.810727 | -2.795959 |
| H | -0.929185 | 5.049212 | -3.428478 |
| H | 0.748194 | 6.982712 | -3.192083 |
| H | 4.031794 | 6.563450 | -0.463553 |
| H | 4.258150 | 4.385028 | 0.883241 |
| H | 3.435013 | 2.155249 | 1.457303 |
| H | 3.577549 | -1.151047 | 0.410084 |
| H | 5.469332 | -1.395730 | 1.985529 |
| H | 5.223613 | -0.674232 | 4.348216 |
| H | 3.073496 | 0.293760 | 5.124920 |
| H | 1.181661 | 0.538448 | 3.549465 |
| H | 3.031175 | 8.400062 | -3.320332 |
| H | 3.869527 | 8.538341 | -1.774970 |
| H | 2.192161 | 9.060694 | -1.920611 |

Ph₂-IDPL-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | -1.101832 | 0.139158 | -0.922149 |
| C | -0.944398 | -1.032318 | -0.166767 |
| C | 0.166698 | -1.172663 | 0.763104 |
| C | 0.062883 | -2.477716 | 1.390929 |
| C | 0.782512 | -3.223626 | 2.351021 |
| C | 0.356019 | -4.493238 | 2.713501 |
| C | -0.807459 | -5.109686 | 2.150479 |
| C | -1.291525 | -6.392143 | 2.478973 |
| C | -2.442431 | -6.912403 | 1.875201 |
| C | -3.144959 | -6.158094 | 0.927978 |
| C | -2.715861 | -4.868683 | 0.553424 |
| C | -3.366443 | -4.023139 | -0.401798 |
| C | -2.896544 | -2.759008 | -0.728039 |

| | | | |
|---|-----------|-----------|-----------|
| C | -1.731625 | -2.251064 | -0.110811 |
| C | -1.089133 | -3.087613 | 0.835321 |
| C | -1.538981 | -4.362765 | 1.180404 |
| C | -2.241948 | 0.283222 | -1.876759 |
| C | -3.461193 | 0.829179 | -1.459313 |
| C | -4.525443 | 0.964504 | -2.348699 |
| C | -4.387497 | 0.554942 | -3.673949 |
| C | -3.178035 | 0.009648 | -4.101643 |
| C | -2.115743 | -0.124368 | -3.209734 |
| C | -2.909859 | -8.308892 | 2.223204 |
| H | 1.673246 | -2.816960 | 2.816700 |
| H | 0.925167 | -5.049359 | 3.454879 |
| H | -0.759379 | -6.989246 | 3.217104 |
| H | -4.040641 | -6.574887 | 0.471257 |
| H | -4.265323 | -4.393850 | -0.889061 |
| H | -3.437936 | -2.171589 | -1.461190 |
| H | -3.568735 | 1.148178 | -0.427768 |
| H | -5.463863 | 1.390707 | -2.005496 |
| H | -5.216312 | 0.659908 | -4.368190 |
| H | -3.060380 | -0.312559 | -5.132373 |
| H | -1.174303 | -0.548820 | -3.542807 |
| H | -2.645237 | -8.577552 | 3.250105 |
| H | -3.994903 | -8.406588 | 2.123792 |
| H | -2.456950 | -9.061586 | 1.566189 |
| C | 1.101832 | -0.139158 | 0.922149 |
| C | 0.944398 | 1.032318 | 0.166767 |
| C | -0.166698 | 1.172663 | -0.763104 |
| C | -0.062883 | 2.477716 | -1.390929 |
| C | -0.782512 | 3.223626 | -2.351021 |
| C | -0.356019 | 4.493238 | -2.713501 |
| C | 0.807459 | 5.109686 | -2.150479 |
| C | 1.291525 | 6.392143 | -2.478973 |
| C | 2.442431 | 6.912403 | -1.875201 |
| C | 3.144959 | 6.158094 | -0.927978 |
| C | 2.715861 | 4.868683 | -0.553424 |
| C | 3.366443 | 4.023139 | 0.401798 |
| C | 2.896544 | 2.759008 | 0.728039 |
| C | 1.731625 | 2.251064 | 0.110811 |
| C | 1.089133 | 3.087613 | -0.835321 |
| C | 1.538981 | 4.362765 | -1.180404 |
| C | 2.241948 | -0.283222 | 1.876759 |
| C | 3.461193 | -0.829179 | 1.459313 |
| C | 4.525443 | -0.964504 | 2.348699 |
| C | 4.387497 | -0.554942 | 3.673949 |
| C | 3.178035 | -0.009648 | 4.101643 |
| C | 2.115743 | 0.124368 | 3.209734 |
| C | 2.909859 | 8.308892 | -2.223204 |

| | | | |
|---|-----------|-----------|-----------|
| H | -1.673246 | 2.816960 | -2.816700 |
| H | -0.925167 | 5.049359 | -3.454879 |
| H | 0.759379 | 6.989246 | -3.217104 |
| H | 4.040641 | 6.574887 | -0.471257 |
| H | 4.265323 | 4.393850 | 0.889061 |
| H | 3.437936 | 2.171589 | 1.461190 |
| H | 3.568735 | -1.148178 | 0.427768 |
| H | 5.463863 | -1.390707 | 2.005496 |
| H | 5.216312 | -0.659908 | 4.368190 |
| H | 3.060380 | 0.312559 | 5.132373 |
| H | 1.174303 | 0.548820 | 3.542807 |
| H | 2.645237 | 8.577552 | -3.250105 |
| H | 3.994903 | 8.406588 | -2.123792 |
| H | 2.456950 | 9.061586 | -1.566189 |

BISPHE-Neutral: CS-B3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 1.322393 | 5.672938 | -6.525590 |
| C | 1.935339 | 5.902888 | -5.292747 |
| C | 0.504555 | 4.563645 | -6.747064 |
| C | 1.741090 | 5.007428 | -4.224403 |
| C | 0.273563 | 3.633755 | -5.716077 |
| C | 2.318712 | 5.142270 | -2.917079 |
| C | 0.905058 | 3.881535 | -4.465288 |
| C | -0.546063 | 2.460577 | -5.829018 |
| C | 2.093467 | 4.229929 | -1.901546 |
| C | 0.694467 | 2.977755 | -3.425785 |
| C | -0.738955 | 1.578483 | -4.780615 |
| C | 1.263912 | 3.111101 | -2.137707 |
| C | -0.113343 | 1.821863 | -3.537600 |
| C | 0.796038 | 1.976069 | -1.376515 |
| C | -0.061232 | 1.173857 | -2.247608 |
| C | 1.018006 | 1.577262 | -0.074386 |
| C | -0.645221 | 0.020926 | -1.764369 |
| C | 0.424829 | 0.397504 | 0.431640 |
| H | 2.565063 | 6.777332 | -5.157991 |
| H | 0.044569 | 4.418024 | -7.719982 |
| H | 2.957947 | 5.999350 | -2.726011 |
| H | -1.031285 | 2.265035 | -6.780880 |
| H | 2.558677 | 4.386113 | -0.932927 |
| H | -1.370843 | 0.707687 | -4.927166 |
| C | -1.322393 | -5.672938 | 6.525590 |
| C | -1.935339 | -5.902888 | 5.292747 |
| C | -0.504555 | -4.563645 | 6.747064 |
| C | -1.741090 | -5.007428 | 4.224403 |

| | | | |
|---|-----------|-----------|-----------|
| C | -0.273563 | -3.633755 | 5.716077 |
| C | -2.318712 | -5.142270 | 2.917079 |
| C | -0.905058 | -3.881535 | 4.465288 |
| C | 0.546063 | -2.460577 | 5.829018 |
| C | -2.093467 | -4.229929 | 1.901546 |
| C | -0.694467 | -2.977755 | 3.425785 |
| C | 0.738955 | -1.578483 | 4.780615 |
| C | -1.263912 | -3.111101 | 2.137707 |
| C | 0.113343 | -1.821863 | 3.537600 |
| C | -0.796038 | -1.976069 | 1.376515 |
| C | 0.061232 | -1.173857 | 2.247608 |
| C | -1.018006 | -1.577262 | 0.074386 |
| C | 0.645221 | -0.020926 | 1.764369 |
| C | -0.424829 | -0.397504 | -0.431640 |
| H | -2.565063 | -6.777332 | 5.157991 |
| H | -0.044569 | -4.418024 | 7.719982 |
| H | -2.957947 | -5.999350 | 2.726011 |
| H | 1.031285 | -2.265035 | 6.780880 |
| H | -2.558677 | -4.386113 | 0.932927 |
| H | 1.370843 | -0.707687 | 4.927166 |
| H | 1.486415 | 6.376987 | -7.335297 |
| H | -1.486415 | -6.376987 | 7.335297 |
| H | 1.284695 | 0.584471 | 2.401831 |
| H | -1.653287 | -2.164886 | -0.583567 |
| H | -1.284695 | -0.584471 | -2.401831 |
| H | 1.653287 | 2.164886 | 0.583567 |

BISPHE-Neutral: BS-UB3LYP/6-311G* geometry

| | | | |
|---|-----------|----------|-----------|
| C | 1.324049 | 5.680098 | -6.533827 |
| C | 1.937146 | 5.910339 | -5.301140 |
| C | 0.506165 | 4.570921 | -6.755615 |
| C | 1.742685 | 5.013088 | -4.230234 |
| C | 0.274479 | 3.638799 | -5.722557 |
| C | 2.318816 | 5.147750 | -2.926601 |
| C | 0.906339 | 3.886937 | -4.471508 |
| C | -0.542942 | 2.468926 | -5.835389 |
| C | 2.091292 | 4.230096 | -1.907754 |
| C | 0.695851 | 2.983532 | -3.432431 |
| C | -0.735430 | 1.584032 | -4.780951 |
| C | 1.265350 | 3.117604 | -2.145486 |
| C | -0.111632 | 1.828641 | -3.545075 |
| C | 0.793921 | 1.972932 | -1.376601 |
| C | -0.059745 | 1.174019 | -2.244100 |
| C | 1.017767 | 1.578992 | -0.077959 |
| C | -0.643797 | 0.024048 | -1.766398 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.422953 | 0.395795 | 0.429777 |
| H | 2.566869 | 6.784680 | -5.166194 |
| H | 0.046101 | 4.425133 | -7.728404 |
| H | 2.958309 | 6.004170 | -2.733662 |
| H | -1.028965 | 2.271735 | -6.786457 |
| H | 2.556237 | 4.385704 | -0.938825 |
| H | -1.367240 | 0.712966 | -4.926822 |
| C | -1.324049 | -5.680098 | 6.533827 |
| C | -1.937146 | -5.910339 | 5.301140 |
| C | -0.506165 | -4.570921 | 6.755615 |
| C | -1.742685 | -5.013088 | 4.230234 |
| C | -0.274479 | -3.638799 | 5.722557 |
| C | -2.318816 | -5.147750 | 2.926601 |
| C | -0.906339 | -3.886937 | 4.471508 |
| C | 0.542942 | -2.468926 | 5.835389 |
| C | -2.091292 | -4.230096 | 1.907754 |
| C | -0.695851 | -2.983532 | 3.432431 |
| C | 0.735430 | -1.584032 | 4.780951 |
| C | -1.265350 | -3.117604 | 2.145486 |
| C | 0.111632 | -1.828641 | 3.545075 |
| C | -0.793921 | -1.972932 | 1.376601 |
| C | 0.059745 | -1.174019 | 2.244100 |
| C | -1.017767 | -1.578992 | 0.077959 |
| C | 0.643797 | -0.024048 | 1.766398 |
| C | -0.422953 | -0.395795 | -0.429777 |
| H | -2.566869 | -6.784680 | 5.166194 |
| H | -0.046101 | -4.425133 | 7.728404 |
| H | -2.958309 | -6.004170 | 2.733662 |
| H | 1.028965 | -2.271735 | 6.786457 |
| H | -2.556237 | -4.385704 | 0.938825 |
| H | 1.367240 | -0.712966 | 4.926822 |
| H | 1.488050 | 6.384130 | -7.343519 |
| H | -1.488050 | -6.384130 | 7.343519 |
| H | 1.283009 | 0.580569 | 2.404576 |
| H | -1.653091 | -2.167228 | -0.579129 |
| H | -1.283009 | -0.580569 | -2.404576 |
| H | 1.653091 | 2.167228 | 0.579129 |

BISPHE-Cation: UB3LYP/6-311G* geometry

| | | | |
|---|----------|----------|-----------|
| C | 1.323402 | 5.677307 | -6.530619 |
| C | 1.935038 | 5.904543 | -5.296519 |
| C | 0.506002 | 4.566959 | -6.749012 |
| C | 1.739392 | 5.005788 | -4.226119 |
| C | 0.275261 | 3.635333 | -5.714287 |
| C | 2.315476 | 5.142153 | -2.925651 |

| | | | |
|---|-----------|-----------|-----------|
| C | 0.905462 | 3.883187 | -4.467193 |
| C | -0.541071 | 2.468246 | -5.829115 |
| C | 2.090501 | 4.225832 | -1.902336 |
| C | 0.695497 | 2.982046 | -3.430718 |
| C | -0.736741 | 1.579315 | -4.776037 |
| C | 1.264528 | 3.116232 | -2.145231 |
| C | -0.111192 | 1.828457 | -3.543533 |
| C | 0.791705 | 1.968807 | -1.375141 |
| C | -0.058774 | 1.172825 | -2.239446 |
| C | 1.018443 | 1.579252 | -0.076481 |
| C | -0.644728 | 0.022707 | -1.766636 |
| C | 0.421805 | 0.394748 | 0.428634 |
| H | 2.564395 | 6.778324 | -5.161585 |
| H | 0.046181 | 4.421200 | -7.721179 |
| H | 2.954661 | 5.997960 | -2.732477 |
| H | -1.026968 | 2.270860 | -6.779496 |
| H | 2.555906 | 4.383247 | -0.935384 |
| H | -1.368185 | 0.709963 | -4.923988 |
| C | -1.323402 | -5.677307 | 6.530619 |
| C | -1.935038 | -5.904543 | 5.296519 |
| C | -0.506002 | -4.566959 | 6.749012 |
| C | -1.739392 | -5.005788 | 4.226119 |
| C | -0.275261 | -3.635333 | 5.714287 |
| C | -2.315476 | -5.142153 | 2.925651 |
| C | -0.905462 | -3.883187 | 4.467193 |
| C | 0.541071 | -2.468246 | 5.829115 |
| C | -2.090501 | -4.225832 | 1.902336 |
| C | -0.695497 | -2.982046 | 3.430718 |
| C | 0.736741 | -1.579315 | 4.776037 |
| C | -1.264528 | -3.116232 | 2.145231 |
| C | 0.111192 | -1.828457 | 3.543533 |
| C | -0.791705 | -1.968807 | 1.375141 |
| C | 0.058774 | -1.172825 | 2.239446 |
| C | -1.018443 | -1.579252 | 0.076481 |
| C | 0.644728 | -0.022707 | 1.766636 |
| C | -0.421805 | -0.394748 | -0.428634 |
| H | -2.564395 | -6.778324 | 5.161585 |
| H | -0.046181 | -4.421200 | 7.721179 |
| H | -2.954661 | -5.997960 | 2.732477 |
| H | 1.026968 | -2.270860 | 6.779496 |
| H | -2.555906 | -4.383247 | 0.935384 |
| H | 1.368185 | -0.709963 | 4.923988 |
| H | 1.487183 | 6.380374 | -7.339202 |
| H | -1.487183 | -6.380374 | 7.339202 |
| H | 1.283253 | 0.580691 | 2.405187 |
| H | -1.653434 | -2.167794 | -0.579227 |
| H | -1.283253 | -0.580691 | -2.405187 |

H 1.653434 2.167794 0.579227

BISPHE-Anion: UB3LYP/6-311G* geometry

| | | | |
|---|-----------|-----------|-----------|
| C | 1.325018 | 5.684219 | -6.538575 |
| C | 1.939602 | 5.917360 | -5.307069 |
| C | 0.506548 | 4.576017 | -6.763637 |
| C | 1.746338 | 5.021271 | -4.234998 |
| C | 0.273672 | 3.642826 | -5.731838 |
| C | 2.322646 | 5.154405 | -2.928196 |
| C | 0.907272 | 3.890946 | -4.476118 |
| C | -0.544937 | 2.470168 | -5.842872 |
| C | 2.092974 | 4.236159 | -1.914012 |
| C | 0.696161 | 2.984882 | -3.433980 |
| C | -0.734456 | 1.589468 | -4.787900 |
| C | 1.266419 | 3.118716 | -2.144585 |
| C | -0.112654 | 1.827810 | -3.546287 |
| C | 0.797737 | 1.981068 | -1.380734 |
| C | -0.060872 | 1.177481 | -2.253297 |
| C | 1.017372 | 1.578661 | -0.078317 |
| C | -0.643403 | 0.024369 | -1.766031 |
| C | 0.425221 | 0.397942 | 0.432103 |
| H | 2.569958 | 6.792844 | -5.172467 |
| H | 0.046183 | 4.430504 | -7.737715 |
| H | 2.962816 | 6.011919 | -2.735372 |
| H | -1.031368 | 2.273047 | -6.795164 |
| H | 2.558367 | 4.391508 | -0.943396 |
| H | -1.367130 | 0.716902 | -4.933432 |
| C | -1.325018 | -5.684219 | 6.538575 |
| C | -1.939602 | -5.917360 | 5.307069 |
| C | -0.506548 | -4.576017 | 6.763637 |
| C | -1.746338 | -5.021271 | 4.234998 |
| C | -0.273672 | -3.642826 | 5.731838 |
| C | -2.322646 | -5.154405 | 2.928196 |
| C | -0.907272 | -3.890946 | 4.476118 |
| C | 0.544937 | -2.470168 | 5.842872 |
| C | -2.092974 | -4.236159 | 1.914012 |
| C | -0.696161 | -2.984882 | 3.433980 |
| C | 0.734456 | -1.589468 | 4.787900 |
| C | -1.266419 | -3.118716 | 2.144585 |
| C | 0.112654 | -1.827810 | 3.546287 |
| C | -0.797737 | -1.981068 | 1.380734 |
| C | 0.060872 | -1.177481 | 2.253297 |
| C | -1.017372 | -1.578661 | 0.078317 |
| C | 0.643403 | -0.024369 | 1.766031 |
| C | -0.425221 | -0.397942 | -0.432103 |

| | | | |
|---|-----------|-----------|-----------|
| H | -2.569958 | -6.792844 | 5.172467 |
| H | -0.046183 | -4.430504 | 7.737715 |
| H | -2.962816 | -6.011919 | 2.735372 |
| H | 1.031368 | -2.273047 | 6.795164 |
| H | -2.558367 | -4.391508 | 0.943396 |
| H | 1.367130 | -0.716902 | 4.933432 |
| H | 1.489343 | 6.389623 | -7.349847 |
| H | -1.489343 | -6.389623 | 7.349847 |
| H | 1.283579 | 0.582039 | 2.403649 |
| H | -1.653141 | -2.166450 | -0.580782 |
| H | -1.283579 | -0.582039 | -2.403649 |
| H | 1.653141 | 2.166450 | 0.580782 |