# Supporting Information (SI)

## Chalcogen Substitution and Ionization Effects on the Fluorescence Behavior of 8-Chalcogen-Quinoline-BODIPY: A DFT and TD-DFT Investigations

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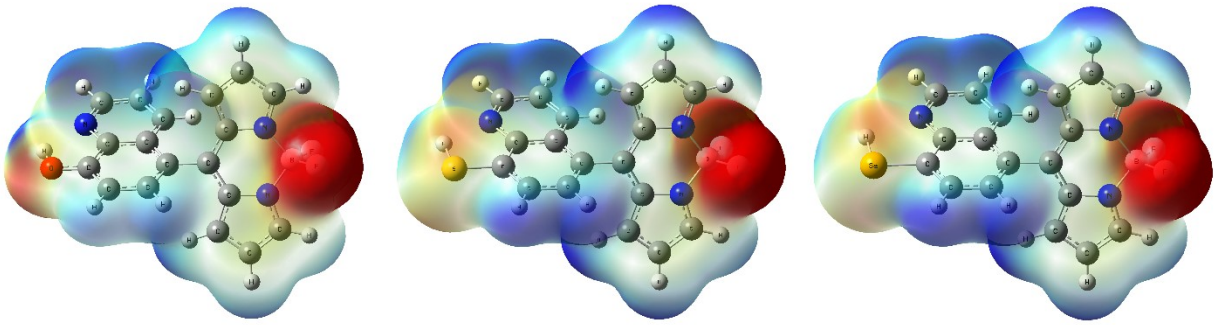


**Figure S1.** Molecular electrostatic potential (MEP) surfaces of 8-Chalcogen-Quinoline-BODIPY derivatives calculated for the ground state ($S_0$). Isosurface value: MO = 0.02 and density = 0.001.

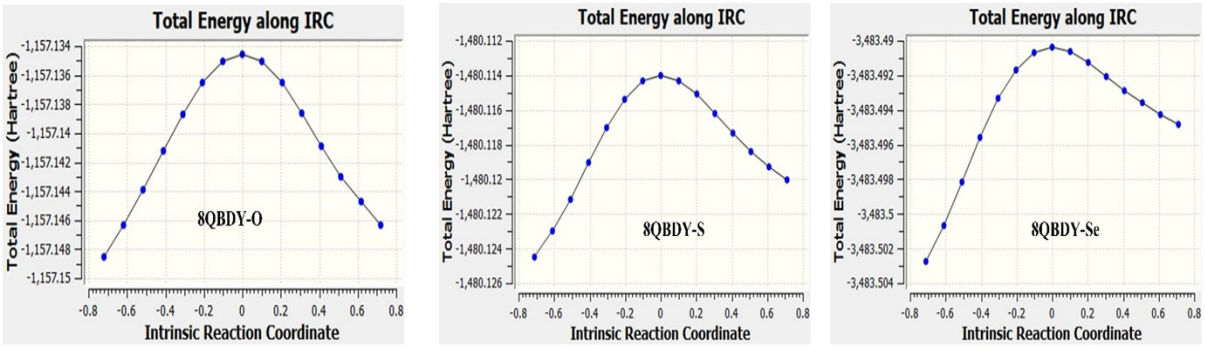


**Figure S2.** Intrinsic reaction coordinate (IRC) profiles for the ESIPT pathways of the studied 8QBDY–X derivatives in the excited state $S_1$

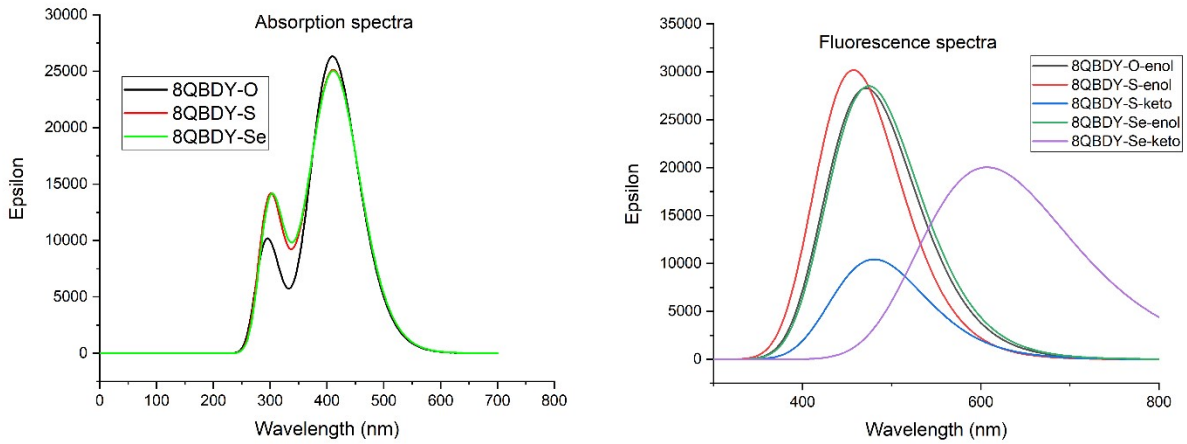


**Figure S3.** TD-DFT absorption and fluorescence spectra of neutral forms of 8QBDY–X (X = O, S, Se).

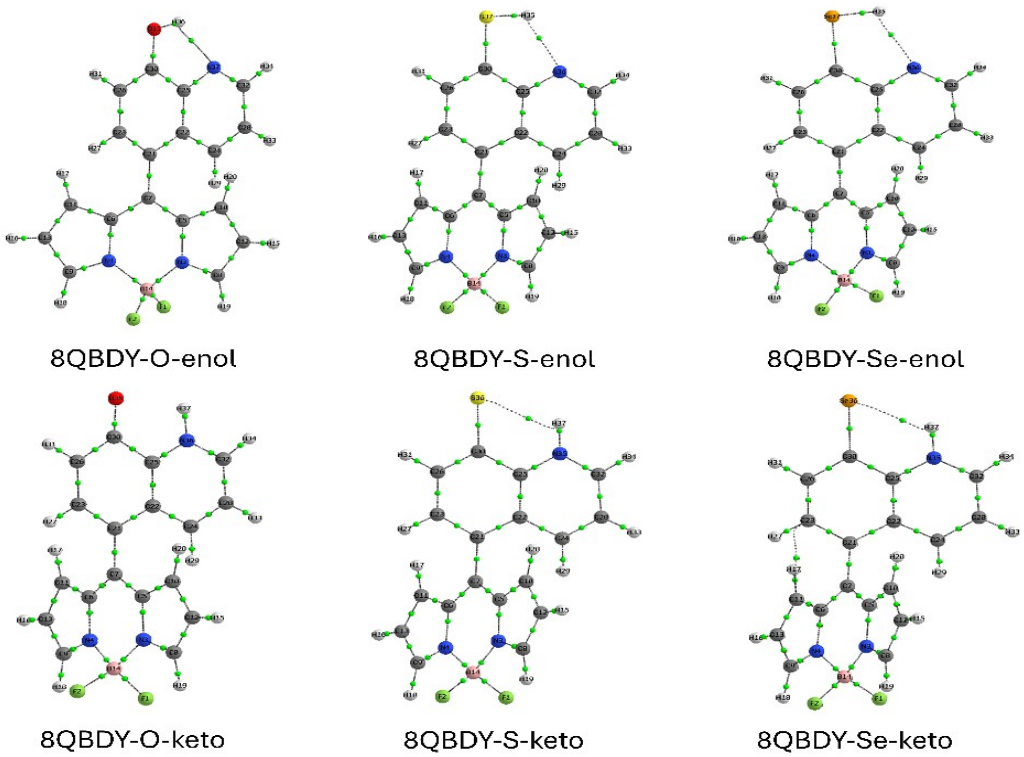


**Figure S4.** AIM topological analysis of 8QBDY–X (X = O, S, Se) derivatives at excited states ($S_1$).

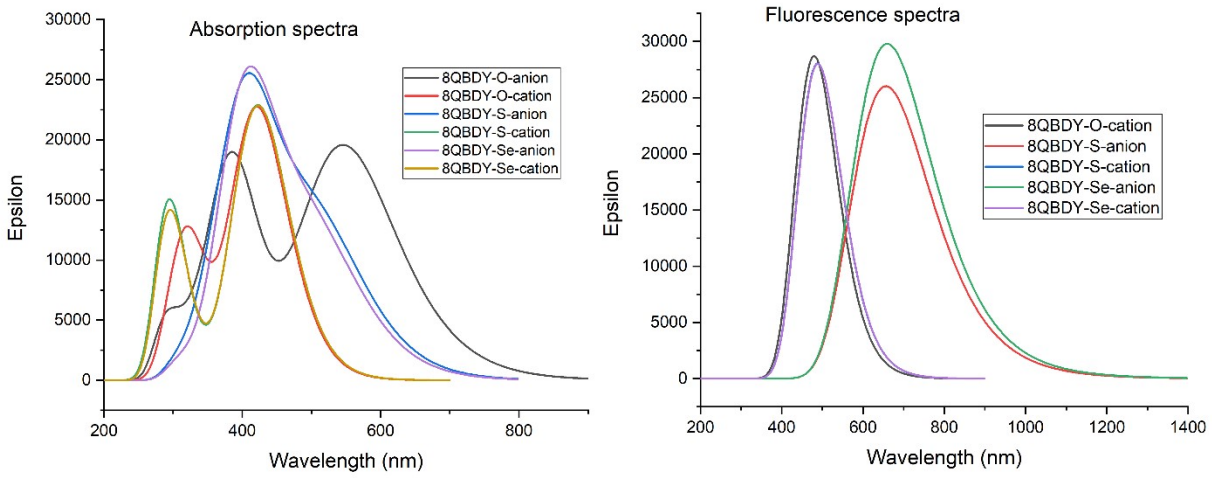


**Figure S5.** TD-DFT absorption and fluorescence spectra of the protonated and deprotonated forms of 8QBDY–X (X = O, S, Se).

**Table S1.** Dipole moment (μ, Debye) for the neutral 8QBDY-X derivatives in the ground ($S_0$) and excited ($S_1$) states.

| Systems | Forms | $\mu(S_0)$ | $\mu(S_1)$ | $\Delta\mu^{(*)}$ |
|---|---|---|---|---|
| 8QBDY-O | enol | 5.046 | 4.899 | -0.147 |
| | keto | 5.046 | 10.315 | 5.269 |
| 8QBDY-S | enol | 3.654 | 3.566 | -0.088 |
| | keto | 3.654 | 8.761 | 5.107 |
| 8QBDY-Se | enol | 3.566 | 3.537 | -0.029 |
| | keto | 3.566 | 8.699 | 5.133 |
| $^{(*)}\Delta\mu = \mu(S_1) - \mu(S_0)$ | | | | |

**Table S2.** Calculated electronic band gap ($E_{gap}$), optical band gap ($E_{opt}$), and exciton binding energy ($E_b$) for the neutral forms of 8QBDY–X (X = O, S, Se) derivatives (eV)

| **Compounds** | **$E_{HOMO}$** | **$E_{LUMO}$** | **$E_{gap}$** | **$E_{opt}$** | **$E_b$** |
|---|---|---|---|---|---|
| 8QBDY-O-enol-S1 | -7.96 | -1.64 | 6.32 | 2.63 | 3.69 |
| 8QBDY-O-keto-S1 | -7.06 | -1.75 | 5.31 | 1.80 | 3.51 |
| 8QBDY-S-enol-S1 | -8.04 | -1.64 | 6.4 | 2.71 | 3.69 |
| 8QBDY-S-keto-S1 | -7.35 | -1.69 | 5.66 | 2.58 | 3.08 |
| 8QBDY-Se-enol-S1 | -7.97 | -1.7 | 6.27 | 2.61 | 3.66 |
| 8QBDY-Se-keto-S1 | -7.15 | -1.89 | 5.26 | 2.04 | 3.22 |

**Table S3.** Second order perturbation NBO analysis (E(2), kcal/mol) for intramolecular hydrogen bonding interactions (LP(N) → σ*(X–H)) in the enol form of 8QBDY-X derivatives at the $S_0$ state.

| **Systems** | **Donor (i)** | **Acceptor (j)** | **E(2) (kcal/mol)** |
|---|---|---|---|
| 8QBDY-O-enol | LP(1) N(37) | BD*(1) O(35)–H(36) | 5.55 |
| 8QBDY-S-enol | LP(1) N(36) | BD*(1) H(35)–S(37) | 5.41 |
| 8QBDY-Se-enol | LP(1) N(36) | BD*(1) H(35)–Se(37) | 4.39 |

**Table S4.** Natural population analysis (NPA) charges on the key atoms (X, H, and N) for the studied 8QBDY-X derivatives in different forms and electronic states.

| **Systems** | **Forms** | **States** | **X(atom)** | **q(X)** | **H(atom)** | **q(H)** | **q(N)** |
|---|---|---|---|---|---|---|---|
| 8QBDY-O | enol | S0 | O(35) | -0.675 | H(36) | 0.499 | -0.510 |
| 8QBDY-O | enol | S1 | O(35) | -0.679 | H(36) | 0.497 | -0.510 |
| 8QBDY-O | keto | S1 | O(35) | -0.57 | H(37) | 0.463 | -0.411 |
| 8QBDY-S | enol | S0 | S(37) | 0.001 | H(35) | 0.181 | -0.497 |
| 8QBDY-S | enol | S1 | S(37) | -0.005 | H(35) | 0.180 | -0.498 |
| 8QBDY-S | keto | S1 | S(36) | -0.081 | H(37) | 0.447 | -0.501 |
| 8QBDY-Se | enol | S0 | Se(37) | 0.102 | H(35) | 0.130 | -0.491 |
| 8QBDY-Se | enol | S1 | Se(37) | 0.097 | H(35) | 0.129 | -0.492 |
| 8QBDY-Se | keto | S1 | Se(36) | 0.008 | H(37) | 0.443 | -0.492 |

**Table S5.** BCP parameters related to the intramolecular hydrogen bond of studied compounds for ground ($S_0$) and excited ($S_1$) states

| **Compounds** | **Contacts** | **ρ(r) (au)** | **$\nabla^2\rho(r)$ (au)** | **G(r)/\|V(r)\|** | **H(r) (au)** | **$E_{HB}$ (kcal/mol)** |
|---|---|---|---|---|---|---|
| 8QBDY-O-S0-enol | X-H...N | 0.0257 | 0.0944 | 1.0840 | 0.001697 | -6.33 |
| 8QBDY-S-S0-enol | X-H...N | 0.0230 | 0.0736 | 1.1167 | 0.00174 | -4.68 |
| 8QBDY-Se-S0-enol | X-H...N | 0.0204 | 0.0625 | 1.1319 | 0.00163 | -3.87 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 8QBDY-O-S1-enol | X-H...N | 0.0253 | 0.0933 | 1.0885 | 0.001754 | -6.21 |
| 8QBDY-S-S1-enol | X-H...N | 0.0230 | 0.0735 | 1.1162 | 0.001734 | -4.68 |
| 8QBDY-Se-S1-enol | X-H...N | 0.0202 | 0.0620 | 1.1325 | 0.001622 | -3.85 |
| 8QBDY-O-S1-keto | X...H-N | - | - | - | - | - |
| 8QBDY-S-S1-keto | X...H-N | 0.0171 | 0.0593 | 1.1759 | 0.0019 | -3.44 |
| 8QBDY-Se-S1-keto | X...H-N | 0.0186 | 0.0542 | 1.1178 | 0.0013 | -3.44 |

**Table S6.** WBI (Wiberg bond index), dipole moment (μ, Debye) for the studied 8QBDY-X derivatives in the ground ($S_0$) and excited ($S_1$) states.

| System | Form | WBI ($S_0$) | WBI ($S_1$) | μ($S_0$) | μ($S_1$) | Δμ(*) |
|---|---|---|---|---|---|---|
| 8QBDY-O | anion | 1.222 | 1.016 | 29.89 | 34.425 | 4.535 |
| | cation | 1.005 | 1.019 | 43.604 | 43.856 | 0.252 |
| 8QBDY-S | anion | 1.044 | 1.119 | 40.212 | 36.91 | -3.302 |
| | cation | 0.996 | 1.021 | 42.229 | 42.627 | 0.398 |
| 8QBDY-Se | anion | 1.035 | 1.129 | 42.006 | 37.87 | -4.136 |
| | cation | 0.996 | 1.022 | 42.277 | 42.701 | 0.425 |

(*) $\Delta\mu = \mu(S_1) - \mu(S_0)$

**Table S7.** Calculated electronic band gap ($E_{gap}$), optical band gap ($E_{opt}$), and exciton binding energy ($E_b$) for the protonated and deprotonated forms of 8QBDY–X (X = O, S, Se) derivatives (eV)

| Compounds | $E_{HOMO}$ | $E_{LUMO}$ | $E_{gap}$ | $E_{opt}$ | $E_b$ |
|---|---|---|---|---|---|
| 8QBDY-O-anion-S1 | -6.21 | -1.52 | 4.69 | 1.16 | 3.53 |
| 8QBDY-O-cation-S1 | -8.14 | -1.9 | 6.24 | 2.58 | 3.66 |
| 8QBDY-S-anion-S1 | -6.66 | -1.59 | 5.07 | 1.89 | 3.18 |
| 8QBDY-S-cation-S1 | -8.17 | -2.05 | 6.12 | 2.54 | 3.58 |
| 8QBDY-Se-anion-S1 | -6.59 | -1.64 | 4.95 | 1.88 | 3.07 |
| 8QBDY-Se-cation-S1 | -8.17 | -2.05 | 6.12 | 2.54 | 3.58 |

**Table S8.** The cartesian coordinates and energies of investigated structures in the studied media

| **Name** | | | | **8QBDY-O-enol-S0** |
|---|---|---|---|---|
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.56916400 | 1.55504500 | 0.60648700 | Zero-point correction= 0.274821 (Hartree/Particle) |
| F | 3.88530000 | 1.62308300 | -1.65642400 | Thermal correction to Energy= 0.293328 |
| N | 5.26598000 | 0.12058600 | -0.35469100 | Thermal correction to Enthalpy= 0.294272 |
| N | 2.86006500 | -0.35274300 | -0.69777000 | Thermal correction to Gibbs Free Energy= 0.226778 |
| C | 5.48240200 | -1.24187200 | -0.20549900 | Sum of electronic and zero-point Energies= -1156.983084 |
| C | 3.12701800 | -1.70214100 | -0.50849800 | Sum of electronic and thermal Energies= -1156.964577 |
| C | 4.42485400 | -2.15615600 | -0.26315200 | Sum of electronic and thermal Enthalpies= -1156.963633 |
| C | 6.45331600 | 0.73252500 | -0.32285100 | Sum of electronic and thermal Free Energies= -1157.031127 |
| C | 1.54943200 | -0.21928500 | -0.91672800 | |
| C | 6.87147300 | -1.45139400 | -0.08360600 | |
| C | 1.90783600 | -2.40601300 | -0.61441500 | |
| C | 7.47861400 | -0.20847800 | -0.15242900 | |
| C | 0.92055600 | -1.47232300 | -0.87950600 | |
| B | 3.88418000 | 0.79893200 | -0.52884100 | |

| | | | |
|---|---|---|---|
| H | 8.53294900 | 0.01137000 | -0.09840100 |
| H | -0.13231900 | -1.65328500 | -1.02630500 |
| H | 1.79226200 | -3.47306900 | -0.50445300 |
| H | 1.11207200 | 0.75451900 | -1.08063000 |
| H | 6.52639900 | 1.80493400 | -0.42686500 |
| H | 7.35005300 | -2.41192800 | 0.03157700 |
| C | 4.67981000 | -3.60264200 | -0.09940800 |
| C | 5.20981100 | -4.13205300 | 1.11666000 |
| C | 4.41325900 | -4.46172200 | -1.14283600 |
| C | 5.45898900 | -3.38138000 | 2.29330300 |
| C | 5.46750800 | -5.51764500 | 1.19738500 |
| C | 4.67519700 | -5.84113900 | -1.06820400 |
| H | 4.01075700 | -4.06060200 | -2.06573800 |
| C | 5.95122400 | -4.00945200 | 3.40392700 |
| H | 5.25874600 | -2.31706000 | 2.31138800 |
| C | 5.20119100 | -6.37004800 | 0.08297100 |
| H | 4.46981000 | -6.48534400 | -1.91361400 |
| C | 6.19794100 | -5.39854300 | 3.36113700 |
| H | 6.14969400 | -3.45852000 | 4.31418000 |
| H | 6.59490900 | -5.90851900 | 4.23341100 |
| O | 5.47021300 | -7.67559600 | 0.20339100 |
| H | 5.81939900 | -7.79210000 | 1.10288800 |
| N | 5.96066100 | -6.13216300 | 2.30127500 |

| **Name** | | | **8QBDY-O-enol-S1** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy (Hartree) |
| F | 3.56472500 | 1.47353200 | 0.75117100 |
| F | 3.85222300 | 1.72983500 | -1.49926000 |
| N | 5.24559200 | 0.12152400 | -0.34834000 |
| N | 2.85935000 | -0.32947900 | -0.70186100 |
| C | 5.46124400 | -1.24962800 | -0.19657500 |
| C | 3.10100300 | -1.69225800 | -0.50494800 |
| C | 4.39362300 | -2.17782400 | -0.21229400 |
| C | 6.43742700 | 0.73301200 | -0.33686200 |
| C | 1.56002200 | -0.17597200 | -0.99339200 |
| C | 6.86792900 | -1.46220700 | -0.09368300 |
| C | 1.86988100 | -2.38301500 | -0.68614100 |
| C | 7.46880000 | -0.22265500 | -0.17841300 |
| C | 0.91577200 | -1.43252700 | -0.99700400 |
| B | 3.86760200 | 0.80916700 | -0.44754200 |
| H | 8.52363500 | 0.00182200 | -0.14045500 |
| H | -0.13154500 | -1.59460600 | -1.20059600 |
| H | 1.73905300 | -3.44958000 | -0.59517100 |
| H | 1.14125400 | 0.80411400 | -1.16916600 |
| H | 6.51416700 | 1.80570400 | -0.43929800 |
| H | 7.34160200 | -2.42512700 | 0.01589300 |
| C | 4.65553600 | -3.62119100 | -0.06951700 |
| C | 5.20470000 | -4.15362400 | 1.13680200 |
| C | 4.39030100 | -4.48704800 | -1.10897400 |
| C | 5.47589900 | -3.39233000 | 2.30049100 |
| C | 5.48331700 | -5.53558400 | 1.21697900 |
| C | 4.65121700 | -5.86817600 | -1.03101200 |

| | |
|---|---|
| Zero-point correction= | 0.272240 (Hartree/Particle) |
| Thermal correction to Energy= | 0.291074 |
| Thermal correction to Enthalpy= | 0.292018 |
| Thermal correction to Gibbs Free Energy= | 0.223709 |
| Sum of electronic and zero-point Energies= | -1156.887062 |
| Sum of electronic and thermal Energies= | -1156.868228 |
| Sum of electronic and thermal Enthalpies= | -1156.867284 |
| Sum of electronic and thermal Free Energies= | -1156.935593 |

| | | | | |
|---|---|---|---|---|
| H | 3.98110300 | -4.09061900 | -2.03154200 | |
| C | 6.00780300 | -4.00632600 | 3.40170100 | |
| H | 5.25511900 | -2.33147200 | 2.31554800 | |
| C | 5.19872300 | -6.39319100 | 0.11139000 | |
| H | 4.43564600 | -6.51581100 | -1.87161700 | |
| C | 6.26721600 | -5.39281800 | 3.36050800 | |
| H | 6.22508200 | -3.44792600 | 4.30314600 | |
| H | 6.69165600 | -5.89294800 | 4.22562900 | |
| O | 5.47713200 | -7.69926500 | 0.23010600 | |
| H | 5.84675400 | -7.81027200 | 1.12162100 | |
| N | 6.01016100 | -6.13744900 | 2.31179500 | |
| **Name** | | | | **8QBDY-O-keto-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.78865900 | 1.75128500 | 0.31329500 | Zero-point correction= 0.273325 (Hartree/Particle) |
| F | 3.72222500 | 1.31478800 | -1.92632100 | Thermal correction to Energy= 0.292268 |
| N | 5.33868600 | 0.10974700 | -0.57372100 | Thermal correction to Enthalpy= 0.293212 |
| N | 2.91782100 | -0.39642300 | -0.40337000 | Thermal correction to Gibbs Free Energy= 0.223955 |
| C | 5.61669500 | -1.23655200 | -0.48335000 | Sum of electronic and zero-point Energies= -1156.891018 |
| C | 3.21459800 | -1.73873400 | -0.31366600 | Sum of electronic and thermal Energies= -1156.872075 |
| C | 4.56250000 | -2.18320400 | -0.37807600 | Sum of electronic and thermal Enthalpies= -1156.871131 |
| C | 6.52630100 | 0.77959100 | -0.63161500 | Sum of electronic and thermal Free Energies= -1156.940388 |
| C | 1.56556300 | -0.25764400 | -0.28236100 | |
| C | 7.00293100 | -1.40898700 | -0.48359600 | |
| C | 2.02585900 | -2.44955900 | -0.13231300 | |
| C | 7.57160700 | -0.11871800 | -0.57874300 | |
| C | 0.98264800 | -1.49641700 | -0.11433400 | |
| B | 3.93425800 | 0.72918500 | -0.65276600 | |
| H | 8.62200100 | 0.12899700 | -0.60216200 | |
| H | -0.07217400 | -1.68885600 | 0.01044800 | |
| H | 1.94187100 | -3.52081400 | -0.02426100 | |
| H | 1.10966500 | 0.71974000 | -0.32422200 | |
| H | 6.54447200 | 1.85616500 | -0.70604000 | |
| H | 7.52093600 | -2.35430700 | -0.41778700 | |
| C | 4.86733100 | -3.59499900 | -0.24504800 | |
| C | 5.08620800 | -4.16565900 | 1.06212200 | |
| C | 4.95885200 | -4.44825100 | -1.37995700 | |
| C | 5.02377300 | -3.42303600 | 2.25651600 | |
| C | 5.37674100 | -5.52158400 | 1.15800300 | |
| C | 5.24144300 | -5.77726600 | -1.29701300 | |
| H | 4.79108200 | -3.99680900 | -2.35019400 | |
| C | 5.24631200 | -4.04209900 | 3.47053100 | |
| H | 4.79958600 | -2.36456200 | 2.20880000 | |
| C | 5.47245100 | -6.41878400 | -0.02125700 | |
| H | 5.30300600 | -6.39940900 | -2.18015100 | |
| C | 5.53226600 | -5.39927800 | 3.50394200 | |
| H | 5.20260300 | -3.49037900 | 4.39821400 | |
| H | 5.71834900 | -5.95214500 | 4.41268800 | |
| O | 5.73145500 | -7.60196700 | 0.14691200 | |
| N | 5.58635200 | -6.08035000 | 2.36006000 | |
| H | 5.79445600 | -7.07911600 | 2.35342200 | |

| **Name** | | | | **8QBDY-O-anion-S0** | |
|---|---|---|---|---|---|
| Cartesian Coordinates | | | | Energy (Hartree) | |
| F | 3.38665800 | 1.53166600 | 0.51715400 | Zero-point correction= | 0.261331 (Hartree/Particle) |
| F | 4.03852900 | 1.64169900 | -1.66984100 | Thermal correction to Energy= | 0.278664 |
| N | 5.21369800 | 0.11433800 | -0.21100200 | Thermal correction to Enthalpy= | 0.279608 |
| N | 2.89729500 | -0.35785300 | -0.90638900 | Thermal correction to Gibbs Free Energy= | 0.216350 |
| C | 5.42023000 | -1.24176700 | -0.02427500 | Sum of electronic and zero-point Energies= | -1156.512901 |
| C | 3.09694200 | -1.69774500 | -0.61858200 | Sum of electronic and thermal Energies= | -1156.495568 |
| C | 4.36293600 | -2.18828300 | -0.18152600 | Sum of electronic and thermal Enthalpies= | -1156.494624 |
| C | 6.40319400 | 0.73846800 | -0.14166600 | Sum of electronic and thermal Free Energies= | -1156.557882 |
| C | 1.60601700 | -0.18607400 | -1.24514300 | | |
| C | 6.79705500 | -1.44219300 | 0.14616500 | | |
| C | 1.86649200 | -2.35442800 | -0.77260200 | | |
| C | 7.41237200 | -0.19229400 | 0.08740600 | | |
| C | 0.93416400 | -1.40221600 | -1.18709700 | | |
| B | 3.87616200 | 0.78334200 | -0.57100500 | | |
| H | 8.46546100 | 0.02318000 | 0.18043700 | | |
| H | -0.11004500 | -1.56232900 | -1.40623800 | | |
| H | 1.68273300 | -3.40021000 | -0.58433400 | | |
| H | 1.22633700 | 0.79595900 | -1.48478500 | | |
| H | 6.47272100 | 1.80712400 | -0.27791000 | | |
| H | 7.27922900 | -2.39702800 | 0.28451400 | | |
| C | 4.56741000 | -3.59026500 | 0.02142800 | | |
| C | 5.29160000 | -4.14969800 | 1.14472600 | | |
| C | 4.09037300 | -4.49959400 | -0.94935900 | | |
| C | 5.62095700 | -3.40372200 | 2.30035100 | | |
| C | 5.57563100 | -5.53641500 | 1.19448100 | | |
| C | 4.36339700 | -5.84147100 | -0.92938200 | | |
| H | 3.55539200 | -4.09758300 | -1.80250100 | | |
| C | 6.25800700 | -4.00556800 | 3.35369100 | | |
| H | 5.36610300 | -2.35295000 | 2.35397100 | | |
| C | 5.14295600 | -6.45678000 | 0.10668600 | | |
| H | 4.02880700 | -6.47910200 | -1.74064500 | | |
| C | 6.55642100 | -5.37347400 | 3.26481500 | | |
| H | 6.51813200 | -3.44562500 | 4.24380700 | | |
| H | 7.07558000 | -5.87396400 | 4.07842400 | | |
| O | 5.43116000 | -7.66125900 | 0.11530000 | | |
| N | 6.21356000 | -6.11628900 | 2.23444800 | | |
| **Name** | | | | **8QBDY-O-anion-S1** | |
| Cartesian Coordinates | | | | Energy (Hartree) | |
| F | 3.81977500 | 1.76804200 | 0.28722000 | Zero-point correction= | 0.259507 (Hartree/Particle) |
| F | 3.74347700 | 1.32344800 | -1.95010900 | Thermal correction to Energy= | 0.278229 |
| N | 5.35098700 | 0.10591400 | -0.59685600 | Thermal correction to Enthalpy= | 0.279173 |
| N | 2.92746800 | -0.37543100 | -0.41847600 | Thermal correction to Gibbs Free Energy= | 0.210802 |
| C | 5.61637600 | -1.24181600 | -0.47668600 | Sum of electronic and zero-point Energies= | -1156.453529 |
| C | 3.21426200 | -1.71876000 | -0.29851300 | Sum of electronic and thermal Energies= | -1156.434807 |
| C | 4.55730700 | -2.18018700 | -0.34666400 | Sum of electronic and thermal Enthalpies= | -1156.433863 |
| C | 6.54442200 | 0.76426500 | -0.68018700 | Sum of electronic and thermal Free Energies= | -1156.502234 |
| C | 1.57474200 | -0.22260800 | -0.31129200 | | |
| C | 7.00093300 | -1.42530100 | -0.48412800 | | |

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|---|---|---|---|
| C | 2.01778700 | -2.41459900 | -0.11204800 |
| C | 7.58132800 | -0.14222000 | -0.61436400 |
| C | 0.98109300 | -1.45278700 | -0.12255100 |
| B | 3.95380900 | 0.73703400 | -0.67452200 |
| H | 8.63392200 | 0.09513800 | -0.65222500 |
| H | -0.07640300 | -1.63421500 | -0.00208500 |
| H | 1.92620200 | -3.48244500 | 0.01969000 |
| H | 1.12730300 | 0.75751400 | -0.37653000 |
| H | 6.57155600 | 1.83861500 | -0.78079300 |
| H | 7.50949100 | -2.37403200 | -0.39867200 |
| C | 4.85049000 | -3.59801200 | -0.20625800 |
| C | 5.06152900 | -4.17874600 | 1.09665300 |
| C | 4.93812800 | -4.43556400 | -1.34995100 |
| C | 4.98827000 | -3.40947700 | 2.27076200 |
| C | 5.35147700 | -5.55110300 | 1.23410000 |
| C | 5.21671600 | -5.76185100 | -1.26125300 |
| H | 4.77493100 | -3.97920900 | -2.31970100 |
| C | 5.19930600 | -4.02206100 | 3.48648300 |
| H | 4.76807200 | -2.35098000 | 2.20458200 |
| C | 5.44440900 | -6.41933000 | 0.01826300 |
| H | 5.28123800 | -6.38582200 | -2.14420100 |
| C | 5.47941700 | -5.38980000 | 3.50762200 |
| H | 5.15124100 | -3.46325600 | 4.41238700 |
| H | 5.64953200 | -5.89687800 | 4.45244100 |
| O | 5.69792600 | -7.61418200 | 0.09584700 |
| N | 5.55514600 | -6.13970000 | 2.41553900 |

| **Name** | | | **8QBDY-O-cation-S0** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy (Hartree) |
| F | 3.61671200 | 1.67601900 | 0.44137300 |
| F | 3.86361300 | 1.49697100 | -1.81798700 |
| N | 5.27610400 | 0.12857300 | -0.40709100 |
| N | 2.85907500 | -0.35811100 | -0.62875800 |
| C | 5.50731900 | -1.23530000 | -0.26138700 |
| C | 3.14584300 | -1.70907200 | -0.45833900 |
| C | 4.45427900 | -2.15093800 | -0.27731900 |
| C | 6.45774600 | 0.75303400 | -0.38049900 |
| C | 1.53646200 | -0.23123700 | -0.76603300 |
| C | 6.89940000 | -1.42680900 | -0.14518000 |
| C | 1.92529300 | -2.41691100 | -0.49425300 |
| C | 7.49190200 | -0.17817400 | -0.21668700 |
| C | 0.91965200 | -1.48812000 | -0.69113900 |
| B | 3.89538700 | 0.78204200 | -0.60821700 |
| H | 8.54411800 | 0.05393300 | -0.16461400 |
| H | -0.14009700 | -1.67344600 | -0.77053500 |
| H | 1.81964900 | -3.48498100 | -0.38391700 |
| H | 1.08219600 | 0.73904900 | -0.90670500 |
| H | 6.52252600 | 1.82658900 | -0.48344300 |
| H | 7.39157700 | -2.38003300 | -0.02730000 |
| C | 4.72573800 | -3.60342200 | -0.13076500 |
| C | 5.17854200 | -4.15352700 | 1.10235200 |
| C | 4.54702900 | -4.43916200 | -1.20457700 |

Zero-point correction= 0.288310 (Hartree/Particle)
Thermal correction to Energy= 0.307247
Thermal correction to Enthalpy= 0.308191
Thermal correction to Gibbs Free Energy= 0.239736
Sum of electronic and zero-point Energies= -1157.410348
Sum of electronic and thermal Energies= -1157.391411
Sum of electronic and thermal Enthalpies= -1157.390466
Sum of electronic and thermal Free Energies= -1157.458922

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|---|---|---|---|---|
| C | 5.34135900 | -3.41513300 | 2.29820600 | |
| C | 5.45330000 | -5.53320100 | 1.15719600 | |
| C | 4.82795800 | -5.81528000 | -1.13497400 | |
| H | 4.19835600 | -4.03159000 | -2.14496900 | |
| C | 5.77605400 | -4.01872800 | 3.44980700 | |
| H | 5.11509600 | -2.35675000 | 2.30674800 | |
| C | 5.28390200 | -6.36679600 | 0.02994500 | |
| H | 4.68624800 | -6.44015700 | -2.00930400 | |
| C | 6.05298800 | -5.38251200 | 3.44103400 | |
| H | 5.90436300 | -3.46020700 | 4.36583300 | |
| H | 6.40080000 | -5.92602000 | 4.30894900 | |
| O | 5.59119500 | -7.66687100 | 0.21514600 | |
| N | 5.88423000 | -6.07989100 | 2.33127400 | |
| H | 5.44539700 | -8.17957700 | -0.59407700 | |
| H | 6.08072700 | -7.07985200 | 2.34547700 | |
| **Name** | | | | **8QBDY-O-cation-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.60948700 | 1.54873900 | 0.63446300 | Zero-point correction= 0.285802 (Hartree/Particle) |
| F | 3.84420100 | 1.61313200 | -1.63872400 | Thermal correction to Energy= 0.305014 |
| N | 5.27593200 | 0.11875000 | -0.38295100 | Thermal correction to Enthalpy= 0.305958 |
| N | 2.85674600 | -0.36201700 | -0.64101800 | Thermal correction to Gibbs Free Energy= 0.237474 |
| C | 5.50084000 | -1.24409400 | -0.25322900 | Sum of electronic and zero-point Energies= -1157.315849 |
| C | 3.13789700 | -1.71253600 | -0.48141600 | Sum of electronic and thermal Energies= -1157.296638 |
| C | 4.44365400 | -2.15434500 | -0.28830000 | Sum of electronic and thermal Enthalpies= -1157.295694 |
| C | 6.46088100 | 0.73337200 | -0.36370900 | Sum of electronic and thermal Free Energies= -1157.364177 |
| C | 1.54039400 | -0.23628000 | -0.81590500 | |
| C | 6.89406200 | -1.45130900 | -0.15538200 | |
| C | 1.92016200 | -2.42601900 | -0.56143400 | |
| C | 7.49373300 | -0.20635300 | -0.22145700 | |
| C | 0.92048000 | -1.49629000 | -0.77793800 | |
| B | 3.88470200 | 0.79491200 | -0.50999100 | |
| H | 8.54770300 | 0.01777200 | -0.18281200 | |
| H | -0.13525600 | -1.68161100 | -0.89473200 | |
| H | 1.81536400 | -3.49610900 | -0.46930300 | |
| H | 1.09018600 | 0.73573000 | -0.95351800 | |
| H | 6.52955300 | 1.80733100 | -0.45377400 | |
| H | 7.38050900 | -2.41042500 | -0.06082700 | |
| C | 4.71402500 | -3.60402200 | -0.14113300 | |
| C | 5.18622900 | -4.13845700 | 1.09112300 | |
| C | 4.51939000 | -4.45354700 | -1.20296500 | |
| C | 5.36893200 | -3.38439300 | 2.27526700 | |
| C | 5.45648600 | -5.51849500 | 1.15863000 | |
| C | 4.79657400 | -5.83052300 | -1.12119100 | |
| H | 4.15785600 | -4.05466000 | -2.14263400 | |
| C | 5.81693200 | -3.97772100 | 3.42903700 | |
| H | 5.14989200 | -2.32388700 | 2.27036800 | |
| C | 5.26896400 | -6.37345300 | 0.04566000 | |
| H | 4.63943500 | -6.46137800 | -1.98770700 | |
| C | 6.08751300 | -5.34447800 | 3.43313600 | |
| H | 5.96067400 | -3.40950500 | 4.33617100 | |
| H | 6.44316700 | -5.87693200 | 4.30355300 | |

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|---|---|---|---|---|
| O | 5.57568000 | -7.66111000 | 0.25956200 | |
| N | 5.90171600 | -6.05413200 | 2.33246800 | |
| H | 5.41783400 | -8.19825700 | -0.52186800 | |
| H | 6.08950600 | -7.05299700 | 2.33974800 | |
| **Name** | | | | **8QBDY-S-enol-S0** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.62031400 | 1.58472500 | 0.61409500 | Zero-point correction= 0.268875 (Hartree/Particle) |
| F | 3.86536800 | 1.62522200 | -1.65818200 | Thermal correction to Energy= 0.288211 |
| N | 5.28052400 | 0.13185400 | -0.38228500 | Thermal correction to Enthalpy= 0.289155 |
| N | 2.86112100 | -0.33421500 | -0.64607000 | Thermal correction to Gibbs Free Energy= 0.219387 |
| C | 5.49691300 | -1.23198300 | -0.24532600 | Sum of electronic and zero-point Energies= -1479.956550 |
| C | 3.13319000 | -1.68579000 | -0.48021100 | Sum of electronic and thermal Energies= -1479.937215 |
| C | 4.43606000 | -2.14015000 | -0.27952000 | Sum of electronic and thermal Enthalpies= -1479.936271 |
| C | 6.46947000 | 0.74026300 | -0.36301800 | Sum of electronic and thermal Free Energies= -1480.006038 |
| C | 1.54495200 | -0.19954900 | -0.82341100 | |
| C | 6.88722400 | -1.44608100 | -0.14265300 | |
| C | 1.91165700 | -2.39007100 | -0.55854500 | |
| C | 7.49555600 | -0.20445700 | -0.21326400 | |
| C | 0.91712500 | -1.45397100 | -0.78055000 | |
| B | 3.89583700 | 0.81501800 | -0.52135700 | |
| H | 8.55083200 | 0.01344100 | -0.17183100 | |
| H | -0.13977000 | -1.63311000 | -0.89736000 | |
| H | 1.80139300 | -3.45905500 | -0.46123600 | |
| H | 1.10227700 | 0.77523600 | -0.96584900 | |
| H | 6.54418000 | 1.81332300 | -0.45902800 | |
| H | 7.36429500 | -2.40855700 | -0.03688200 | |
| C | 4.69444800 | -3.59152400 | -0.13373800 | |
| C | 5.18051700 | -4.13654300 | 1.09130600 | |
| C | 4.47167600 | -4.42685000 | -1.20022900 | |
| C | 5.37279600 | -3.36736400 | 2.26671800 | |
| C | 5.45370100 | -5.52611200 | 1.17845700 | |
| C | 4.74402700 | -5.80381500 | -1.12063500 | |
| H | 4.09884300 | -4.01873600 | -2.13216100 | |
| C | 5.82975100 | -3.97010600 | 3.40337200 | |
| H | 5.15425600 | -2.30650900 | 2.25998200 | |
| C | 5.23233000 | -6.35967300 | 0.03558000 | |
| H | 4.56708600 | -6.42371000 | -1.99152800 | |
| C | 6.09682700 | -5.35464100 | 3.37595400 | |
| H | 5.98493100 | -3.40811400 | 4.31512800 | |
| H | 6.46804000 | -5.85309900 | 4.26662900 | |
| H | 5.97491100 | -8.06187300 | 1.38762800 | |
| N | 5.91417300 | -6.10356000 | 2.31735200 | |
| S | 5.57389600 | -8.09208300 | 0.10179200 | |
| **Name** | | | | **8QBDY-S-enol-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.58291700 | 1.45589900 | 0.80757400 | Zero-point correction= 0.266302 (Hartree/Particle) |
| F | 3.84494900 | 1.76891500 | -1.43920500 | Thermal correction to Energy= 0.285912 |
| N | 5.25029200 | 0.13196500 | -0.34442700 | Thermal correction to Enthalpy= 0.286856 |
| N | 2.86013200 | -0.30934500 | -0.68206800 | Thermal correction to Gibbs Free Energy= 0.216923 |
| C | 5.46376200 | -1.24113400 | -0.20721100 | Sum of electronic and zero-point Energies= -1479.861083 |

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|---|---|---|---|---|
| C | 3.10004900 | -1.67539000 | -0.50486900 | Sum of electronic and thermal Energies= -1479.841473 |
| C | 4.39274900 | -2.16459000 | -0.22076000 | Sum of electronic and thermal Enthalpies= -1479.840529 |
| C | 6.44376900 | 0.73945900 | -0.34214500 | Sum of electronic and thermal Free Energies= -1479.910462 |
| C | 1.56111200 | -0.15013500 | -0.96870900 | |
| C | 6.87011100 | -1.45925800 | -0.12164300 | |
| C | 1.86736300 | -2.36221100 | -0.69269000 | |
| C | 7.47392000 | -0.22089200 | -0.20299300 | |
| C | 0.91447800 | -1.40629600 | -0.98791400 | |
| B | 3.87198500 | 0.82331300 | -0.41110400 | |
| H | 8.52985700 | -0.00018500 | -0.17567400 | |
| H | -0.13339200 | -1.56385500 | -1.19205000 | |
| H | 1.73495900 | -3.42981300 | -0.61748500 | |
| H | 1.14349200 | 0.83269800 | -1.13147900 | |
| H | 6.52276500 | 1.81264500 | -0.43721600 | |
| H | 7.34222200 | -2.42447700 | -0.02604500 | |
| C | 4.65014800 | -3.61066400 | -0.08702300 | |
| C | 5.19039300 | -4.15536400 | 1.11758200 | |
| C | 4.38811700 | -4.46101400 | -1.13544000 | |
| C | 5.43594400 | -3.37547100 | 2.27489400 | |
| C | 5.47980900 | -5.54212600 | 1.20259600 | |
| C | 4.65476100 | -5.83946900 | -1.05358100 | |
| H | 3.98425300 | -4.06154700 | -2.05861800 | |
| C | 5.96200400 | -3.96244700 | 3.39073000 | |
| H | 5.19759800 | -2.31855900 | 2.27130700 | |
| C | 5.19954000 | -6.38677900 | 0.08116400 | |
| H | 4.43676300 | -6.46715600 | -1.90977500 | |
| C | 6.24044200 | -5.34413200 | 3.36016900 | |
| H | 6.15947400 | -3.39125900 | 4.28856800 | |
| H | 6.66448700 | -5.83135200 | 4.23339700 | |
| H | 6.01961500 | -8.07690800 | 1.40561500 | |
| N | 6.00575400 | -6.10536200 | 2.31978800 | |
| S | 5.54413800 | -8.11992400 | 0.14586400 | |
| **Name** | | | | **8QBDY-S-keto-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.49867100 | 1.45246400 | 0.70087100 | Zero-point correction= 0.270687 (Hartree/Particle) |
| F | 3.98425300 | 1.71687900 | -1.51695100 | Thermal correction to Energy= 0.289843 |
| N | 5.25176400 | 0.08527900 | -0.26035200 | Thermal correction to Enthalpy= 0.290787 |
| N | 2.88427400 | -0.32620800 | -0.81355500 | Thermal correction to Gibbs Free Energy= 0.221856 |
| C | 5.43552500 | -1.27125300 | -0.07432700 | Sum of electronic and zero-point Energies= -1479.871479 |
| C | 3.08067200 | -1.67966500 | -0.60354400 | Sum of electronic and thermal Energies= -1479.852324 |
| C | 4.34699500 | -2.17902700 | -0.20711800 | Sum of electronic and thermal Enthalpies= -1479.851380 |
| C | 6.45735800 | 0.68522300 | -0.22504300 | Sum of electronic and thermal Free Energies= -1479.920311 |
| C | 1.59229300 | -0.13330100 | -1.13715200 | |
| C | 6.81433400 | -1.50405300 | 0.06523400 | |
| C | 1.84599500 | -2.32893100 | -0.79601000 | |
| C | 7.45226500 | -0.26825400 | -0.02127200 | |
| C | 0.91678900 | -1.35180800 | -1.14528700 | |
| B | 3.89747400 | 0.78687000 | -0.47301700 | |
| H | 8.51167000 | -0.07483000 | 0.04281100 | |
| H | -0.12693800 | -1.49644700 | -1.37628000 | |
| H | 1.66200300 | -3.38618200 | -0.68605400 | |

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|---|---|---|---|
| H | 1.21661100 | 0.85965300 | -1.33370100 |
| H | 6.54464500 | 1.75361200 | -0.35151000 |
| H | 7.28118600 | -2.46691000 | 0.20554000 |
| C | 4.53927500 | -3.59830600 | -0.02851000 |
| C | 5.19089000 | -4.13682900 | 1.14680700 |
| C | 4.11523400 | -4.49757500 | -1.03826300 |
| C | 5.42077500 | -3.40090500 | 2.31339900 |
| C | 5.53684300 | -5.50993200 | 1.14685500 |
| C | 4.43950500 | -5.82477800 | -0.99961000 |
| H | 3.60511800 | -4.10094100 | -1.90614000 |
| C | 6.08368800 | -3.97555400 | 3.40185800 |
| H | 5.09845500 | -2.37019600 | 2.36852800 |
| C | 5.18895900 | -6.38924500 | 0.07682600 |
| H | 4.15952600 | -6.47717000 | -1.81686800 |
| C | 6.48622200 | -5.28224100 | 3.33090700 |
| H | 6.28150800 | -3.40355700 | 4.29694800 |
| H | 7.01685800 | -5.79615300 | 4.11853300 |
| N | 6.19968000 | -6.00686600 | 2.22699500 |
| S | 5.61612200 | -8.02830000 | 0.10380800 |
| H | 6.45979100 | -6.98855200 | 2.17360400 |

| **Name** | | | **8QBDY-S-anion-S0** |
|---|---|---|---|
| Cartesian Coordinates | | | Energy (Hartree) |
| F | 3.53096300 | 1.55354300 | 0.61101100 |
| F | 3.89830600 | 1.62978500 | -1.64363700 |
| N | 5.24883500 | 0.12164900 | -0.31802000 |
| N | 2.85410100 | -0.35087900 | -0.71466600 |
| C | 5.46289200 | -1.23956500 | -0.15730900 |
| C | 3.11222000 | -1.69891600 | -0.50691900 |
| C | 4.40550700 | -2.15974500 | -0.22808600 |
| C | 6.43745000 | 0.73423900 | -0.28772100 |
| C | 1.54614900 | -0.21267000 | -0.95480200 |
| C | 6.85011100 | -1.44844000 | -0.03149400 |
| C | 1.89195700 | -2.39655600 | -0.62159600 |
| C | 7.45989000 | -0.20551900 | -0.10686700 |
| C | 0.91184700 | -1.46078300 | -0.91372900 |
| B | 3.87274900 | 0.79881700 | -0.51958200 |
| H | 8.51465200 | 0.01264900 | -0.05207800 |
| H | -0.13964100 | -1.63943600 | -1.07350000 |
| H | 1.76893500 | -3.46118500 | -0.49805400 |
| H | 1.11661100 | 0.76219800 | -1.13243200 |
| H | 6.51071500 | 1.80542900 | -0.40317500 |
| H | 7.32669800 | -2.40888700 | 0.09097700 |
| C | 4.65330300 | -3.60129400 | -0.06805800 |
| C | 5.23078800 | -4.15404500 | 1.11634200 |
| C | 4.34411200 | -4.45673000 | -1.10556700 |
| C | 5.46775200 | -3.37919500 | 2.28031700 |
| C | 5.52170300 | -5.54788800 | 1.18621400 |
| C | 4.63847500 | -5.82062200 | -1.04566000 |
| H | 3.90146100 | -4.05537500 | -2.01076300 |
| C | 5.99612800 | -3.96362100 | 3.39475300 |
| H | 5.22308000 | -2.32403300 | 2.28349000 |

Zero-point correction= 0.259319 (Hartree/Particle)
Thermal correction to Energy= 0.278129
Thermal correction to Enthalpy= 0.279073
Thermal correction to Gibbs Free Energy= 0.210429
Sum of electronic and zero-point Energies= -1479.500176
Sum of electronic and thermal Energies= -1479.481366
Sum of electronic and thermal Enthalpies= -1479.480422
Sum of electronic and thermal Free Energies= -1479.549066

| | | | | |
|---|---|---|---|---|
| C | 5.23934000 | -6.41643500 | 0.05843400 | |
| H | 4.40358500 | -6.43973400 | -1.90336300 | |
| C | 6.28600200 | -5.34165800 | 3.34994200 | |
| H | 6.18479500 | -3.39395900 | 4.29614400 | |
| H | 6.71637200 | -5.83100000 | 4.22070200 | |
| N | 6.05577900 | -6.09946200 | 2.30720200 | |
| S | 5.61286900 | -8.12216300 | 0.05435000 | |
| **Name** | | | | **8QBDY-S-anion-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.52626500 | 1.51929300 | 0.64196400 | Zero-point correction= 0.257924 (Hartree/Particle) |
| F | 3.93548600 | 1.63763400 | -1.60117400 | Thermal correction to Energy= 0.276920 |
| N | 5.24262900 | 0.07848000 | -0.28785600 | Thermal correction to Enthalpy= 0.277864 |
| N | 2.85567000 | -0.35529600 | -0.74024700 | Thermal correction to Gibbs Free Energy= 0.208857 |
| C | 5.44766000 | -1.27195900 | -0.09614900 | Sum of electronic and zero-point Energies= -1479.425318 |
| C | 3.06997300 | -1.70577600 | -0.55219600 | Sum of electronic and thermal Energies= -1479.406322 |
| C | 4.36129400 | -2.19426100 | -0.19011400 | Sum of electronic and thermal Enthalpies= -1479.405378 |
| C | 6.44756600 | 0.70699300 | -0.23105700 | Sum of electronic and thermal Free Energies= -1479.474385 |
| C | 1.54315800 | -0.16882100 | -1.04554900 | |
| C | 6.82469200 | -1.48164600 | 0.07419100 | |
| C | 1.84945000 | -2.36834300 | -0.73962500 | |
| C | 7.44684400 | -0.22389000 | -0.00829000 | |
| C | 0.89125200 | -1.38793300 | -1.05692000 | |
| B | 3.88315000 | 0.75808100 | -0.49836200 | |
| H | 8.50191700 | -0.01295100 | 0.07991900 | |
| H | -0.15414500 | -1.54688700 | -1.27442500 | |
| H | 1.68625500 | -3.43142200 | -0.65177100 | |
| H | 1.15953500 | 0.82223200 | -1.23489100 | |
| H | 6.51413800 | 1.77766300 | -0.35105800 | |
| H | 7.30282500 | -2.43633100 | 0.23064800 | |
| C | 4.58918400 | -3.61486800 | -0.03541900 | |
| C | 5.22616200 | -4.16714800 | 1.13739700 | |
| C | 4.21016400 | -4.51597400 | -1.05604100 | |
| C | 5.46523600 | -3.38528700 | 2.28302400 | |
| C | 5.59381800 | -5.53720800 | 1.19175600 | |
| C | 4.51801800 | -5.84770500 | -0.99891300 | |
| H | 3.70284800 | -4.12399300 | -1.92922400 | |
| C | 6.09965200 | -3.94137200 | 3.36787700 | |
| H | 5.14475600 | -2.35184100 | 2.30085900 | |
| C | 5.25102600 | -6.42806900 | 0.07943100 | |
| H | 4.23407800 | -6.49788900 | -1.81737200 | |
| C | 6.48459300 | -5.28395500 | 3.29144500 | |
| H | 6.29512200 | -3.36556700 | 4.26331600 | |
| H | 7.00764100 | -5.74926600 | 4.12218700 | |
| N | 6.23119100 | -6.05913900 | 2.25311000 | |
| S | 5.66738700 | -8.05706500 | 0.03232700 | |
| **Name** | | | | **8QBDY-S-cation-S0** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.72841900 | 1.61255500 | 0.59874000 | Zero-point correction= 0.282723 (Hartree/Particle) |
| F | 3.84809600 | 1.59251600 | -1.68401600 | Thermal correction to Energy= 0.302391 |
| N | 5.31098500 | 0.11076300 | -0.44898100 | Thermal correction to Enthalpy= 0.303336 |

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|---|---|---|---|---|
| N | 2.86944700 | -0.32307400 | -0.56933900 | Thermal correction to Gibbs Free Energy= 0.232137 |
| C | 5.51507900 | -1.25612900 | -0.32696100 | Sum of electronic and zero-point Energies= -1480.383526 |
| C | 3.13454900 | -1.67934900 | -0.43231300 | Sum of electronic and thermal Energies= -1480.363857 |
| C | 4.43975200 | -2.14142300 | -0.31193900 | Sum of electronic and thermal Enthalpies= -1480.362913 |
| C | 6.50736900 | 0.70174300 | -0.46705100 | Sum of electronic and thermal Free Energies= -1480.434112 |
| C | 1.54803100 | -0.17436300 | -0.66735300 | |
| C | 6.90665500 | -1.49097700 | -0.27174100 | |
| C | 1.90215400 | -2.37239900 | -0.44647000 | |
| C | 7.52683200 | -0.25810400 | -0.35773300 | |
| C | 0.90884900 | -1.42433800 | -0.59842000 | |
| B | 3.92828900 | 0.81430600 | -0.52971000 | |
| H | 8.58537200 | -0.05334600 | -0.35054300 | |
| H | -0.15504500 | -1.59012900 | -0.65415000 | |
| H | 1.78470600 | -3.44149600 | -0.35618000 | |
| H | 1.10721900 | 0.80535100 | -0.77812100 | |
| H | 6.59432800 | 1.77439300 | -0.55703000 | |
| H | 7.37642600 | -2.45942800 | -0.18760500 | |
| C | 4.69169200 | -3.59857200 | -0.17815400 | |
| C | 5.09889300 | -4.14863400 | 1.07122800 | |
| C | 4.53609300 | -4.42252600 | -1.26099800 | |
| C | 5.23663500 | -3.38559200 | 2.25351500 | |
| C | 5.35194600 | -5.53570000 | 1.14099700 | |
| C | 4.79643100 | -5.80477800 | -1.16652400 | |
| H | 4.22031700 | -4.00936500 | -2.21054200 | |
| C | 5.62097900 | -3.97477000 | 3.43228900 | |
| H | 5.03377700 | -2.32202600 | 2.22759300 | |
| C | 5.21657000 | -6.37392800 | 0.00706000 | |
| H | 4.66773300 | -6.42693600 | -2.04281800 | |
| C | 5.86892500 | -5.34359600 | 3.45089200 | |
| H | 5.73039400 | -3.40375300 | 4.34227700 | |
| H | 6.17081700 | -5.87970700 | 4.33944700 | |
| N | 5.73143000 | -6.05708900 | 2.34429500 | |
| H | 6.81451000 | -8.09070600 | -0.17654100 | |
| H | 5.89941200 | -7.06243000 | 2.36580100 | |
| S | 5.50797500 | -8.13256000 | 0.14237600 | |
| **Name** | | | | **8QBDY-S-cation-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.59410000 | 1.38602700 | 0.88803900 | Zero-point correction= 0.280600 (Hartree/Particle) |
| F | 3.87447700 | 1.80662600 | -1.34021000 | Thermal correction to Energy= 0.300378 |
| N | 5.25505200 | 0.10486100 | -0.31830500 | Thermal correction to Enthalpy= 0.301322 |
| N | 2.86290700 | -0.29380500 | -0.69126700 | Thermal correction to Gibbs Free Energy= 0.231323 |
| C | 5.44761500 | -1.27341200 | -0.20684400 | Sum of electronic and zero-point Energies= -1480.289532 |
| C | 3.07662600 | -1.66713900 | -0.53822500 | Sum of electronic and thermal Energies= -1480.269754 |
| C | 4.35857300 | -2.17536800 | -0.23263200 | Sum of electronic and thermal Enthalpies= -1480.268810 |
| C | 6.45625800 | 0.69213800 | -0.32098900 | Sum of electronic and thermal Free Energies= -1480.338809 |
| C | 1.57518800 | -0.10756200 | -1.00077300 | |
| C | 6.84946600 | -1.51684900 | -0.14227400 | |
| C | 1.83720400 | -2.33026400 | -0.76351400 | |
| C | 7.47278600 | -0.28781500 | -0.20810400 | |
| C | 0.90738600 | -1.35403500 | -1.05843700 | |
| B | 3.88451600 | 0.81726900 | -0.35837500 | |

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|---|---|---|---|---|
| H | 8.53256200 | -0.08599700 | -0.19186700 | |
| H | -0.13830600 | -1.49023000 | -1.28682400 | |
| H | 1.68052900 | -3.39586200 | -0.71150600 | |
| H | 1.17669800 | 0.88497300 | -1.15224200 | |
| H | 6.55191900 | 1.76491800 | -0.40354100 | |
| H | 7.31189000 | -2.48951400 | -0.07816000 | |
| C | 4.58694600 | -3.62144900 | -0.08718000 | |
| C | 5.14932000 | -4.15827100 | 1.11414500 | |
| C | 4.27535000 | -4.48673600 | -1.10997800 | |
| C | 5.41875800 | -3.37932000 | 2.26107100 | |
| C | 5.41174000 | -5.54522800 | 1.18156700 | |
| C | 4.52807100 | -5.86735300 | -1.01164300 | |
| H | 3.85183400 | -4.09911600 | -2.02809000 | |
| C | 5.96298200 | -3.94086200 | 3.39071000 | |
| H | 5.18484900 | -2.32205900 | 2.25105400 | |
| C | 5.11303700 | -6.41224800 | 0.10330200 | |
| H | 4.27518500 | -6.51029400 | -1.84512600 | |
| C | 6.23311900 | -5.30408000 | 3.39846400 | |
| H | 6.17469700 | -3.35229300 | 4.27097300 | |
| H | 6.65868200 | -5.82056000 | 4.24705500 | |
| N | 5.95389200 | -6.03963800 | 2.33300600 | |
| H | 6.66852900 | -8.14396900 | -0.25872000 | |
| H | 6.12905800 | -7.04345600 | 2.35162200 | |
| S | 5.41854800 | -8.16762400 | 0.23909500 | |
| **Name** | | | | **8QBDY-Se-enol-S0** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.59105000 | 1.75855400 | 0.59508000 | Zero-point correction= 0.267265 (Hartree/Particle) |
| F | 3.82462300 | 1.78855200 | -1.67853700 | Thermal correction to Energy= 0.287042 |
| N | 5.24601900 | 0.30080000 | -0.40286100 | Thermal correction to Enthalpy= 0.287986 |
| N | 2.82489600 | -0.16594700 | -0.65257300 | Thermal correction to Gibbs Free Energy= 0.216484 |
| C | 5.46308300 | -1.06287400 | -0.26528100 | Sum of electronic and zero-point Energies= -3483.332021 |
| C | 3.09843500 | -1.51737800 | -0.48789500 | Sum of electronic and thermal Energies= -3483.312245 |
| C | 4.40227300 | -1.97075600 | -0.29377500 | Sum of electronic and thermal Enthalpies= -3483.311301 |
| C | 6.43490500 | 0.90931600 | -0.38647600 | Sum of electronic and thermal Free Energies= -3483.382802 |
| C | 1.50779900 | -0.03211500 | -0.82299600 | |
| C | 6.85361300 | -1.27679400 | -0.16497700 | |
| C | 1.87697300 | -2.22249800 | -0.55993800 | |
| C | 7.46152800 | -0.03517300 | -0.23806600 | |
| C | 0.88082400 | -1.28697100 | -0.77653400 | |
| B | 3.86061900 | 0.98366000 | -0.53812500 | |
| H | 8.51681600 | 0.18304000 | -0.19875500 | |
| H | -0.17658600 | -1.46660800 | -0.88774700 | |
| H | 1.76812500 | -3.29163900 | -0.46248900 | |
| H | 1.06379500 | 0.94231400 | -0.96372600 | |
| H | 6.50934100 | 1.98233800 | -0.48316600 | |
| H | 7.33080800 | -2.23916900 | -0.05866500 | |
| C | 4.66222000 | -3.42240700 | -0.14776000 | |
| C | 5.14002300 | -3.96663800 | 1.08079600 | |
| C | 4.44885500 | -4.25550400 | -1.21691700 | |
| C | 5.32066900 | -3.19177000 | 2.25433700 | |
| C | 5.41686100 | -5.35694900 | 1.17187400 | |

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|---|---|---|---|---|
| C | 4.72417100 | -5.63244600 | -1.13317400 | |
| H | 4.08200600 | -3.84786500 | -2.15142300 | |
| C | 5.77061700 | -3.78820200 | 3.39659600 | |
| H | 5.09859000 | -2.13167800 | 2.24130100 | |
| C | 5.20479100 | -6.18693000 | 0.02618500 | |
| H | 4.55359200 | -6.24954000 | -2.00769600 | |
| C | 6.04225100 | -5.17201300 | 3.37451000 | |
| H | 5.91705400 | -3.22273500 | 4.30766700 | |
| H | 6.40855200 | -5.66583100 | 4.27001200 | |
| H | 5.99353400 | -8.01472500 | 1.47815600 | |
| N | 5.87102800 | -5.92658400 | 2.31833600 | |
| Se | 5.57141200 | -8.06066700 | 0.07659900 | |
| **Name** | | | | **8QBDY-Se-enol-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.54931900 | 1.62295300 | 0.79651200 | Zero-point correction= 0.264575 (Hartree/Particle) |
| F | 3.80606600 | 1.93830400 | -1.45059400 | Thermal correction to Energy= 0.284642 |
| N | 5.21452800 | 0.30081500 | -0.36054100 | Thermal correction to Enthalpy= 0.285586 |
| N | 2.82370300 | -0.14103500 | -0.69319400 | Thermal correction to Gibbs Free Energy= 0.213851 |
| C | 5.42842300 | -1.07217600 | -0.22294300 | Sum of electronic and zero-point Energies= -3483.236719 |
| C | 3.06434600 | -1.50708500 | -0.51680800 | Sum of electronic and thermal Energies= -3483.216652 |
| C | 4.35750000 | -1.99553300 | -0.23425000 | Sum of electronic and thermal Enthalpies= -3483.215708 |
| C | 6.40794200 | 0.90837500 | -0.36045700 | Sum of electronic and thermal Free Energies= -3483.287443 |
| C | 1.52428600 | 0.01771700 | -0.97795600 | |
| C | 6.83481600 | -1.29021900 | -0.13929100 | |
| C | 1.83170500 | -2.19442500 | -0.70323000 | |
| C | 7.43839200 | -0.05184300 | -0.22233300 | |
| C | 0.87807800 | -1.23879000 | -0.99671300 | |
| B | 3.83583400 | 0.99182100 | -0.42348300 | |
| H | 8.49434900 | 0.16897600 | -0.19678600 | |
| H | -0.16999900 | -1.39664400 | -1.19954500 | |
| H | 1.69996200 | -3.26214900 | -0.62849200 | |
| H | 1.10604300 | 1.00040900 | -1.13999800 | |
| H | 6.48672500 | 1.98152100 | -0.45615900 | |
| H | 7.30705400 | -2.25538800 | -0.04371100 | |
| C | 4.61536000 | -3.44168900 | -0.09915500 | |
| C | 5.15210500 | -3.98503600 | 1.10778300 | |
| C | 4.35695400 | -4.29102500 | -1.14848100 | |
| C | 5.39043200 | -3.19920500 | 2.26265100 | |
| C | 5.44423400 | -5.37268000 | 1.19673100 | |
| C | 4.62577200 | -5.66947600 | -1.06261400 | |
| H | 3.95570100 | -3.89257000 | -2.07322400 | |
| C | 5.91365000 | -3.77942000 | 3.38281700 | |
| H | 5.14849700 | -2.14315000 | 2.25338600 | |
| C | 5.16738700 | -6.21473300 | 0.07399800 | |
| H | 4.40970900 | -6.29504400 | -1.92124900 | |
| C | 6.19629800 | -5.16037700 | 3.35711300 | |
| H | 6.10576300 | -3.20436700 | 4.27936700 | |
| H | 6.61902700 | -5.64261500 | 4.23396000 | |
| H | 6.04330300 | -8.02894500 | 1.49513200 | |
| N | 5.96842500 | -5.92766900 | 2.32001700 | |
| Se | 5.53347600 | -8.08943500 | 0.12363400 | |

| **Name** | | | | **8QBDY-Se-keto-S1** |
|---|---|---|---|---|
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.45788200 | 1.65559400 | 0.64450000 | Zero-point correction= 0.270042 (Hartree/Particle) |
| F | 3.94324600 | 1.86519700 | -1.57928300 | Thermal correction to Energy= 0.289503 |
| N | 5.21297400 | 0.26755700 | -0.28220100 | Thermal correction to Enthalpy= 0.290448 |
| N | 2.84476200 | -0.16041800 | -0.82503800 | Thermal correction to Gibbs Free Energy= 0.219776 |
| C | 5.40264400 | -1.08957900 | -0.09447600 | Sum of electronic and zero-point Energies= -3483.253446 |
| C | 3.05322100 | -1.51176600 | -0.60530000 | Sum of electronic and thermal Energies= -3483.233984 |
| C | 4.32302800 | -2.00179200 | -0.22221200 | Sum of electronic and thermal Enthalpies= -3483.233040 |
| C | 6.41384700 | 0.87036700 | -0.24576400 | Sum of electronic and thermal Free Energies= -3483.303712 |
| C | 1.55054300 | 0.01920000 | -1.13599800 | |
| C | 6.78295700 | -1.31568500 | 0.04814600 | |
| C | 1.82060100 | -2.17142700 | -0.77967900 | |
| C | 7.41461600 | -0.07933500 | -0.03818200 | |
| C | 0.88235200 | -1.20558700 | -1.12750300 | |
| B | 3.85676400 | 0.96360500 | -0.51194300 | |
| H | 8.47271000 | 0.12004500 | 0.02742200 | |
| H | -0.16305300 | -1.35819300 | -1.34489000 | |
| H | 1.64772200 | -3.22927900 | -0.65804000 | |
| H | 1.16374200 | 1.00751000 | -1.33475700 | |
| H | 6.49860400 | 1.93861600 | -0.37589000 | |
| H | 7.25160600 | -2.27713500 | 0.19159100 | |
| C | 4.52483500 | -3.42539900 | -0.04534700 | |
| C | 5.16101700 | -3.96316100 | 1.13325500 | |
| C | 4.11457200 | -4.31110000 | -1.06674500 | |
| C | 5.39855700 | -3.22609600 | 2.29969600 | |
| C | 5.48479400 | -5.34720400 | 1.13938100 | |
| C | 4.42045800 | -5.64586200 | -1.02480000 | |
| H | 3.62462900 | -3.90600400 | -1.94258200 | |
| C | 6.04256700 | -3.80915600 | 3.39674800 | |
| H | 5.09640600 | -2.18928300 | 2.34947200 | |
| C | 5.13497700 | -6.20822800 | 0.06776400 | |
| H | 4.14631200 | -6.29140300 | -1.84930500 | |
| C | 6.42036800 | -5.12147700 | 3.33856500 | |
| H | 6.24442200 | -3.23494300 | 4.28978300 | |
| H | 6.93346600 | -5.64187500 | 4.13321600 | |
| N | 6.13134400 | -5.84929900 | 2.23144000 | |
| Se | 5.55635400 | -8.00550300 | 0.09767800 | |
| H | 6.37699100 | -6.83426600 | 2.19005300 | |
| **Name** | | | | **8QBDY-Se-anion-S0** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 4.12464000 | 1.64177200 | 0.59894000 | Zero-point correction= 0.258778 (Hartree/Particle) |
| F | 3.46378900 | 1.55980700 | -1.58800000 | Thermal correction to Energy= 0.277875 |
| N | 5.31668500 | 0.15952600 | -0.89190300 | Thermal correction to Enthalpy= 0.278819 |
| N | 3.00460200 | -0.35668400 | -0.18239900 | Thermal correction to Gibbs Free Energy= 0.209019 |
| C | 5.64846400 | -1.17339200 | -0.68970200 | Sum of electronic and zero-point Energies= -3482.879499 |
| C | 3.37695800 | -1.68453400 | -0.03080900 | Sum of electronic and thermal Energies= -3482.860403 |
| C | 4.69539400 | -2.10343900 | -0.25887100 | Sum of electronic and thermal Enthalpies= -3482.859458 |
| C | 6.41456300 | 0.80013400 | -1.30496500 | Sum of electronic and thermal Free Energies= -3482.929259 |
| C | 1.68540200 | -0.27151700 | 0.01778600 | |

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|---|---|---|---|---|
| C | 7.01752600 | -1.33040400 | -0.99169000 | |
| C | 2.21871100 | -2.42873300 | 0.26901000 | |
| C | 7.49305800 | -0.09059800 | -1.38775400 | |
| C | 1.15794100 | -1.53734300 | 0.30461100 | |
| B | 3.96211000 | 0.81140500 | -0.51840700 | |
| H | 8.49538700 | 0.15997300 | -1.69688900 | |
| H | 0.12081900 | -1.75855200 | 0.50082100 | |
| H | 2.18759700 | -3.49578300 | 0.42752200 | |
| H | 1.17465100 | 0.67699800 | -0.05689600 | |
| H | 6.39157000 | 1.85983000 | -1.51228600 | |
| H | 7.56944900 | -2.25460200 | -0.92008700 | |
| C | 5.07017100 | -3.52013200 | -0.09976800 | |
| C | 4.94215800 | -4.20665200 | 1.14603400 | |
| C | 5.54099100 | -4.21862500 | -1.18990800 | |
| C | 4.57507500 | -3.54484100 | 2.34561900 | |
| C | 5.25402600 | -5.59581600 | 1.22927300 | |
| C | 5.84351000 | -5.58287000 | -1.11010300 | |
| H | 5.64578000 | -3.71171800 | -2.14297300 | |
| C | 4.48617900 | -4.24661800 | 3.51241600 | |
| H | 4.37071800 | -2.48118600 | 2.33346500 | |
| C | 5.70850200 | -6.31421100 | 0.06013300 | |
| H | 6.18732300 | -6.08757800 | -2.00521000 | |
| C | 4.77151100 | -5.62653200 | 3.48275700 | |
| H | 4.20990600 | -3.76511200 | 4.44208600 | |
| H | 4.69556900 | -6.21232500 | 4.39598200 | |
| N | 5.14341100 | -6.27003600 | 2.40534700 | |
| Se | 6.12563600 | -8.16702200 | 0.07300300 | |

| **Name** | | | | **8QBDY-Se-anion-S1** |
|---|---|---|---|---|
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 4.21253700 | 1.59876900 | 0.64374000 | Zero-point correction= 0.257090 (Hartree/Particle) |
| F | 3.40522300 | 1.57045000 | -1.49296500 | Thermal correction to Energy= 0.276334 |
| N | 5.29858100 | 0.15062000 | -0.96629000 | Thermal correction to Enthalpy= 0.277278 |
| N | 3.04974400 | -0.38923100 | -0.11672700 | Thermal correction to Gibbs Free Energy= 0.207407 |
| C | 5.68443100 | -1.16131600 | -0.77691200 | Sum of electronic and zero-point Energies= -3482.804800 |
| C | 3.43461100 | -1.70124200 | 0.06356700 | Sum of electronic and thermal Energies= -3482.785556 |
| C | 4.77631400 | -2.11464200 | -0.21754300 | Sum of electronic and thermal Enthalpies= -3482.784612 |
| C | 6.35426100 | 0.83978800 | -1.47509700 | Sum of electronic and thermal Free Energies= -3482.854483 |
| C | 1.71298600 | -0.29696300 | 0.11272600 | |
| C | 7.02410500 | -1.27728900 | -1.17314700 | |
| C | 2.29298500 | -2.44196500 | 0.40446800 | |
| C | 7.43600300 | -0.00909400 | -1.62046000 | |
| C | 1.21201700 | -1.54518500 | 0.43858100 | |
| B | 3.98156200 | 0.77158400 | -0.48362800 | |
| H | 8.40660400 | 0.25917800 | -2.00951200 | |
| H | 0.18254100 | -1.77600100 | 0.66732400 | |
| H | 2.26193600 | -3.50411300 | 0.59179000 | |
| H | 1.20606600 | 0.65217500 | 0.02819400 | |
| H | 6.26584000 | 1.89241800 | -1.69726300 | |
| H | 7.62100600 | -2.17518700 | -1.13498300 | |
| C | 5.17191500 | -3.49154200 | -0.05305000 | |
| C | 4.93780800 | -4.22123100 | 1.17522900 | |

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|---|---|---|---|---|
| C | 5.78796500 | -4.19228800 | -1.11419200 | |
| C | 4.54632100 | -3.56832500 | 2.35845000 | |
| C | 5.16124200 | -5.62256200 | 1.24563400 | |
| C | 6.04399400 | -5.53660200 | -1.04261900 | |
| H | 5.99997300 | -3.66108900 | -2.03365900 | |
| C | 4.31219800 | -4.29925800 | 3.49827300 | |
| H | 4.43355400 | -2.49211000 | 2.36190900 | |
| C | 5.71440100 | -6.32326300 | 0.09375800 | |
| H | 6.47892000 | -6.03910700 | -1.89809400 | |
| C | 4.48052600 | -5.68682000 | 3.43835000 | |
| H | 4.01174900 | -3.82258400 | 4.42244100 | |
| H | 4.27861000 | -6.29867000 | 4.31327300 | |
| N | 4.90331600 | -6.32606100 | 2.36437200 | |
| Se | 6.00793800 | -8.12865200 | 0.05024800 | |
| **Name** | | | | **8QBDY-Se-cation-S0** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.73946000 | 1.61764200 | 0.61322100 | Zero-point correction= 0.281148 (Hartree/Particle) |
| F | 3.85038600 | 1.60711100 | -1.67005800 | Thermal correction to Energy= 0.301161 |
| N | 5.31260000 | 0.11476300 | -0.44694100 | Thermal correction to Enthalpy= 0.302105 |
| N | 2.86917000 | -0.30982600 | -0.55995300 | Thermal correction to Gibbs Free Energy= 0.229124 |
| C | 5.51212000 | -1.25316800 | -0.32920400 | Sum of electronic and zero-point Energies= -3483.760971 |
| C | 3.12970200 | -1.66735200 | -0.42647100 | Sum of electronic and thermal Energies= -3483.740957 |
| C | 4.43360000 | -2.13460000 | -0.31186000 | Sum of electronic and thermal Enthalpies= -3483.740013 |
| C | 6.51108300 | 0.70142000 | -0.46823400 | Sum of electronic and thermal Free Energies= -3483.812994 |
| C | 1.54803700 | -0.15610100 | -0.65424000 | |
| C | 6.90300400 | -1.49326400 | -0.28011500 | |
| C | 1.89475800 | -2.35585000 | -0.43879800 | |
| C | 7.52741000 | -0.26245800 | -0.36554300 | |
| C | 0.90450200 | -1.40386400 | -0.58614400 | |
| B | 3.93219700 | 0.82358500 | -0.51947000 | |
| H | 8.58672700 | -0.06165800 | -0.36212900 | |
| H | -0.16012400 | -1.56569200 | -0.63949500 | |
| H | 1.77369200 | -3.42470400 | -0.35052700 | |
| H | 1.11052100 | 0.82544300 | -0.76181600 | |
| H | 6.60156200 | 1.77398200 | -0.55573500 | |
| H | 7.36951800 | -2.46366200 | -0.20037200 | |
| C | 4.68048400 | -3.59303400 | -0.18260100 | |
| C | 5.09285500 | -4.14780300 | 1.06322600 | |
| C | 4.51653900 | -4.41326900 | -1.26658100 | |
| C | 5.23968500 | -3.38602500 | 2.24521400 | |
| C | 5.34049800 | -5.53681700 | 1.12908600 | |
| C | 4.77762800 | -5.79645900 | -1.17771000 | |
| H | 4.19809300 | -3.99669400 | -2.21379500 | |
| C | 5.62696500 | -3.97699900 | 3.42195100 | |
| H | 5.04124400 | -2.32159500 | 2.22066200 | |
| C | 5.19737100 | -6.37051600 | -0.00654000 | |
| H | 4.64893500 | -6.41108700 | -2.05938100 | |
| C | 5.86719700 | -5.34711100 | 3.43848600 | |
| H | 5.74336100 | -3.40692100 | 4.33166400 | |
| H | 6.16881000 | -5.88567900 | 4.32566500 | |
| N | 5.72160000 | -6.05914800 | 2.33217800 | |

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|---|---|---|---|---|
| H | 6.95999200 | -8.15210300 | -0.07008000 | |
| H | 5.88230700 | -7.06661100 | 2.35461600 | |
| Se | 5.50855500 | -8.26947200 | 0.11310000 | |
| **Name** | | | | **8QBDY-Se-cation-S1** |
| Cartesian Coordinates | | | | Energy (Hartree) |
| F | 3.59468400 | 1.38401000 | 0.90644600 | Zero-point correction= 0.279548 (Hartree/Particle) |
| F | 3.87588500 | 1.82195500 | -1.31842100 | Thermal correction to Energy= 0.299619 |
| N | 5.25464100 | 0.11086100 | -0.30968700 | Thermal correction to Enthalpy= 0.300563 |
| N | 2.86271400 | -0.28269900 | -0.68627000 | Thermal correction to Gibbs Free Energy= 0.229252 |
| C | 5.44549200 | -1.26824200 | -0.20575700 | Sum of electronic and zero-point Energies= -3483.666426 |
| C | 3.07390000 | -1.65699800 | -0.53842300 | Sum of electronic and thermal Energies= -3483.646355 |
| C | 4.35503900 | -2.16863800 | -0.23381600 | Sum of electronic and thermal Enthalpies= -3483.645411 |
| C | 6.45647800 | 0.69681300 | -0.30947400 | Sum of electronic and thermal Free Energies= -3483.716722 |
| C | 1.57587600 | -0.09278500 | -0.99717900 | |
| C | 6.84718400 | -1.51356100 | -0.14353000 | |
| C | 1.83344100 | -2.31681100 | -0.76822900 | |
| C | 7.47189000 | -0.28489400 | -0.20248500 | |
| C | 0.90591800 | -1.33773200 | -1.06086700 | |
| B | 3.88492000 | 0.82493500 | -0.34441800 | |
| H | 8.53189600 | -0.08438800 | -0.18523700 | |
| H | -0.13958200 | -1.47125400 | -1.29170000 | |
| H | 1.67423900 | -3.38221200 | -0.72080000 | |
| H | 1.17951200 | 0.90112200 | -1.14515700 | |
| H | 6.55321300 | 1.76996200 | -0.38575700 | |
| H | 7.30859700 | -2.48705500 | -0.08506200 | |
| C | 4.57903900 | -3.61562400 | -0.09083500 | |
| C | 5.14763600 | -4.15594700 | 1.10631100 | |
| C | 4.25565800 | -4.47888200 | -1.11136500 | |
| C | 5.43207600 | -3.37637100 | 2.24927700 | |
| C | 5.39992000 | -5.54559700 | 1.17358300 | |
| C | 4.49921200 | -5.86179500 | -1.01358000 | |
| H | 3.83052500 | -4.08884900 | -2.02775100 | |
| C | 5.98385300 | -3.93810000 | 3.37491500 | |
| H | 5.20375500 | -2.31791900 | 2.23922000 | |
| C | 5.08200100 | -6.41094500 | 0.10022300 | |
| H | 4.23763600 | -6.49944400 | -1.84854000 | |
| C | 6.24531700 | -5.30294600 | 3.38273800 | |
| H | 6.20727300 | -3.34888500 | 4.25184000 | |
| H | 6.67556100 | -5.82049400 | 4.22834100 | |
| N | 5.95057200 | -6.03899200 | 2.32214900 | |
| H | 6.78392400 | -8.23250600 | -0.20260600 | |
| H | 6.11754500 | -7.04518900 | 2.34345400 | |
| Se | 5.38460400 | -8.30949900 | 0.23372400 | |