**Supplementary Text**

Computational Methods

All electronic structure calculations were performed with density functional theory (DFT) using the B3LYP-D3BJ functional with empirical dispersion (*1-6*) and the 6-31G\*\* basis set (*7, 8*) for all atoms. All geometries were optimized in solution (CH2Cl2) using the conductor-like polarizable continuum model (C-PCM) (*9, 10*)with the Bondi atomic radii (*11*), including the nonelectrostatic contributions of dispersion (*12, 13*), repulsion (*12, 13*), and cavitation energies (*14*). This electronic structure method has previously been shown to perform well for similar calculations on substituted benzimidazole-phenol constructs (*15, 16*). All DFT calculations were performed using the Gaussian 16 electronic structure program (*17*).

Thermochemical data were calculated at *T =* 298.15 K, and all calculated free energies include zero-point energy, entropic contributions, and solvation effects. The solution free energies were calculated using the standard Gibbs relation . The relative redox potentials were computed from the corresponding reaction free energies () using an experimentally known reference potential within a thermodynamic cycle, as outlined elsewhere (*15, 16, 18*). In the current work, the reference potential was set to agree with the experimental value of  for the E3PT compound **3**. This computational protocol has been shown previously to yield food agreement between the calculations and experiment, even when the calculations were performed prior to the experimental measurement of the redox potentials (*15, 16*). The structures and energies for all the systems studies are provided in Tables S##.

In order to aid the assignment of band changes in the IRSEC spectra, we computed infrared spectra for the compounds **2**, **3**, and **4**, which clearly show the formation of the final E2PT, E3PT, and E4PT product, respectively. For the optimized DFT structures discussed above, frequency calculations were performed for both the reduced (neutral) and oxidized (+1) species. All frequency calculations were computed at the same level of theory as described above. As is common practice (*19*), to make direct comparison with experimental IRSEC spectra, all computed frequencies were empirically scaled by a factor of 0.9631, corresponding to an alignment of the computed and experimental C=NH+ protonated azomethine stretch for compound **4**. Simulated spectra are depicted in Figure S##.

To simulate line broadening, the peaks were dressed with an artificial Lorentzian function for a full-width-half-max (FWHM) of 12 cm-1 . Selected vibrations are given in Table S##. Band assignments were performed by visually inspecting displacements along the computed normal mode of each vibration. Consistent with experiment, oxidation of compounds **2**, **3**, and **4** result in a strong peak that grows in around 1651–1659 cm-1 from the azomethine C=NH+ stretch, shifted from the weaker reduced azomethine C=N stretch from 1638–1643 cm-1.

**Fig. S#.**

|  |  |
| --- | --- |
|  |  |
| **Fig. S#.** Computed IRSEC spectra for compound **2**. Each peak was scaled empirically by a factor of 0.9631 and dressed with a Lorentzian function for a FWHM of 12 cm-1 . To simulate the increasing applied potential, spectra corresponding to the reduced, neutral (black) and oxidized, positively charged (blue) **2** were computed, and the intermediate values (gray) correspond to superpositions of the reduced and oxidized states. | |

**Fig. S#.**

|  |  |
| --- | --- |
|  |  |
| **Fig. S#.** Computed IRSEC spectra for compound **3**. Each peak was scaled empirically by a factor of 0.9631 and dressed with a Lorentzian function for a FWHM of 12 cm-1 . To simulate the increasing applied potential, spectra corresponding to the reduced, neutral (black) and oxidized, positively charged (green) **3** were computed, and the intermediate values (gray) correspond to superpositions of the reduced and oxidized states. | |

**Fig. S#.**

|  |  |
| --- | --- |
|  |  |
| **Fig. S#.** Computed IRSEC spectra for compound **4**. Each peak was scaled empirically by a factor of 0.9631 and dressed with a Lorentzian function for a FWHM of 12 cm-1 . To simulate the increasing applied potential, spectra corresponding to the reduced, neutral (black) and oxidized, positively charged (red) **4** were computed, and the intermediate values (gray) correspond to superpositions of the reduced and oxidized states. | |

**Table S#.** Redox potentials calculated for selected intermediates in thermodynamic cycle

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Expt.  (V vs SCE) | Calc.  (V vs SCE) | | | | |
| Compound | E0PT | E1PT | E2PT | E3PT | E4PT |
| **(1)** | 1.04 | 1.38a | 0.99a | − | − | − |
| **(2)** | 0.82 | 1.57 | 1.17 | 0.87 | − | − |
| **(3)** | 0.76 | 1.54 | 1.16 | 1.00 | 0.76b | − |
| **(4)** | 0.70 | 1.52 | 1.18 | 0.99 | 0.89 | 0.67 |
| aReference reaction used to compute was unsubstituted BIP; data from Ref. (*20*).  bThis couple was used as the reference reaction for all other calculated potentials, so the experimental and calculated values agree by construction. | | | | | | |

**Table S#.** Selected peaks and assignments in simulated IRSEC spectrum of **2**.

|  |  |  |  |
| --- | --- | --- | --- |
| 2 | | 2+⦁ | |
| (cm-1) | assignmenta | (cm-1) | assignmenta |
| 1504 | phenol-Bz C-C str | 1508 | phenol-Bz C-C str |
| 1611,1593 | Bz C=C str | 1569 | Bz C=C str |
| 1643 | imine C=N str | 1651 | imine C=NH+ str |
| 3466 | Bz N-H str | 3412 | Bz N-H str |

aApproximate mode description.

**Table S#.** Selected peaks and assignments in simulated IRSEC spectrum of **3**.

|  |  |  |  |
| --- | --- | --- | --- |
| 3 | | 3+⦁ | |
| (cm-1) | assignmenta | (cm-1) | assignmenta |
| 1501 | phenol-Bz C-C str | 1524 | Bz-Bz C-C str |
| 1599-1591 | Bz C=C str | 1563 | Bz C=C str |
| 1638 | imine C=N str | 1653 | imine C=NH+ str |
| 3463,3446 | Bz N-H str | 3426,3339 | Bz N-H str |

aApproximate mode description.

**Table S#.** Selected peaks and assignments in simulated IRSEC spectrum of **4**.

|  |  |  |  |
| --- | --- | --- | --- |
| 4 | | 4+⦁ | |
| (cm-1) | assignmenta | (cm-1) | assignmenta |
| 1526 | Bz-Bz C-C str | 1515 | Bz-Bz C-C str |
| 1616-1593 | Bz C=C str | 1572-1564 | Bz C=C str |
| 1643 | imine C=N str | 1659 | imine C=NH+ str |
| 3464,3447,3446 | Bz N-H str | 3418,3352,3332 | Bz N-H str |

aApproximate mode description.

**Table S#.** Cartesian coordinates for **2**: neutral. (-1328.99836749 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.483053 | 2.715584 | 0.416145 |
| C | -1.881052 | 2.898359 | 0.327601 |
| C | -2.412894 | 4.190122 | 0.243421 |
| C | -1.520456 | 5.261988 | 0.256277 |
| C | -0.133595 | 5.064531 | 0.350314 |
| C | 0.427051 | 3.782688 | 0.429804 |
| C | -1.518543 | 0.752015 | 0.424651 |
| H | -3.482079 | 4.346339 | 0.169021 |
| H | -1.905266 | 6.273153 | 0.194132 |
| H | 0.529539 | 5.922761 | 0.360617 |
| N | -2.496427 | 1.656282 | 0.336302 |
| C | -3.063668 | -1.189037 | 0.352314 |
| C | -1.739219 | -0.685003 | 0.447265 |
| C | -0.658724 | -1.573623 | 0.540497 |
| C | -0.848757 | -2.950289 | 0.541355 |
| C | -2.167874 | -3.417641 | 0.446447 |
| C | -3.286126 | -2.585001 | 0.353326 |
| H | 0.347044 | -1.175374 | 0.612680 |
| H | -2.332312 | -4.483825 | 0.445491 |
| C | 0.361420 | -3.887798 | 0.614442 |
| C | -4.705200 | -3.167413 | 0.253385 |
| O | -4.117255 | -0.346876 | 0.257497 |
| H | -3.767809 | 0.591511 | 0.268641 |
| N | -0.287014 | 1.356600 | 0.476439 |
| H | 0.638260 | 0.947632 | 0.528152 |
| C | 1.869640 | 3.577070 | 0.516071 |
| H | 2.471751 | 4.490981 | 0.533986 |
| N | 2.383342 | 2.403646 | 0.562666 |
| C | 3.846217 | 2.273148 | 0.605015 |
| C | 4.417796 | 2.330347 | -0.823282 |
| C | 4.574369 | 3.275291 | 1.514632 |
| H | 4.045818 | 1.268606 | 0.997125 |
| C | 5.930590 | 2.085737 | -0.826620 |
| H | 4.198843 | 3.321293 | -1.239881 |
| H | 3.906197 | 1.596844 | -1.453374 |
| C | 6.083737 | 3.008000 | 1.520530 |
| H | 4.402404 | 4.296059 | 1.156042 |
| H | 4.163006 | 3.214757 | 2.526856 |
| C | 6.660178 | 3.063293 | 0.101127 |
| H | 6.316771 | 2.164127 | -1.847368 |
| H | 6.127826 | 1.059566 | -0.492795 |
| H | 6.585310 | 3.735122 | 2.166713 |
| H | 6.276761 | 2.017185 | 1.950502 |
| H | 7.732058 | 2.843665 | 0.116826 |
| H | 6.551014 | 4.082402 | -0.290657 |
| C | 1.245777 | -3.654521 | -0.627285 |
| H | 1.575562 | -2.614306 | -0.683508 |
| H | 2.133816 | -4.292376 | -0.588643 |
| H | 0.697384 | -3.887082 | -1.544179 |
| C | 1.182786 | -3.575549 | 1.880731 |
| H | 0.588653 | -3.743887 | 2.782861 |
| H | 2.064321 | -4.221634 | 1.926387 |
| H | 1.524899 | -2.537627 | 1.887374 |
| C | -0.049460 | -5.366088 | 0.652100 |
| H | -0.664682 | -5.591665 | 1.527396 |
| H | -0.608161 | -5.652070 | -0.243331 |
| H | 0.845240 | -5.991639 | 0.701283 |
| C | -5.359002 | -2.732161 | -1.075251 |
| H | -6.372934 | -3.138229 | -1.139958 |
| H | -5.413698 | -1.647265 | -1.155355 |
| H | -4.786354 | -3.113816 | -1.925275 |
| C | -5.557474 | -2.682549 | 1.445687 |
| H | -5.658132 | -1.598206 | 1.446625 |
| H | -6.556546 | -3.125767 | 1.394151 |
| H | -5.097957 | -2.986879 | 2.390277 |
| C | -4.694231 | -4.704659 | 0.283816 |
| H | -4.126052 | -5.123400 | -0.551056 |
| H | -4.268835 | -5.089758 | 1.214382 |
| H | -5.721459 | -5.069139 | 0.207540 |

**Table S#.** Cartesian coordinates for **2**+⦁: E0PT. (-1328.80078256 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.439440 | 2.706702 | 0.233437 |
| C | -1.853311 | 2.850428 | 0.181340 |
| C | -2.429226 | 4.130552 | 0.090664 |
| C | -1.563901 | 5.212027 | 0.063520 |
| C | -0.157618 | 5.052289 | 0.121858 |
| C | 0.445060 | 3.799185 | 0.207637 |
| C | -1.402749 | 0.722167 | 0.305223 |
| H | -3.503059 | 4.256798 | 0.044728 |
| H | -1.968018 | 6.214719 | -0.002494 |
| H | 0.472399 | 5.934041 | 0.100720 |
| N | -2.415280 | 1.603316 | 0.228748 |
| C | -2.999650 | -1.174786 | 0.386006 |
| C | -1.621065 | -0.695104 | 0.370601 |
| C | -0.574464 | -1.613381 | 0.410639 |
| C | -0.831237 | -2.980675 | 0.474553 |
| C | -2.191578 | -3.420842 | 0.513391 |
| C | -3.278998 | -2.583328 | 0.479802 |
| H | 0.445112 | -1.255711 | 0.389146 |
| H | -2.365061 | -4.484469 | 0.574653 |
| C | 0.269738 | -4.027582 | 0.492357 |
| C | -4.717358 | -3.103367 | 0.531321 |
| O | -3.988374 | -0.329443 | 0.309942 |
| H | -3.605028 | 0.640678 | 0.257613 |
| N | -0.193794 | 1.365944 | 0.309553 |
| H | 0.759381 | 1.012910 | 0.363181 |
| C | 1.893310 | 3.609600 | 0.268696 |
| H | 2.499635 | 4.519893 | 0.229757 |
| N | 2.395102 | 2.434920 | 0.362530 |
| C | 3.858521 | 2.306049 | 0.420645 |
| C | 4.523200 | 2.728347 | -0.900440 |
| C | 4.480820 | 3.069454 | 1.601497 |
| H | 4.060451 | 1.239359 | 0.569807 |
| C | 6.037375 | 2.498321 | -0.842440 |
| H | 4.315097 | 3.791488 | -1.070852 |
| H | 4.076671 | 2.173459 | -1.730843 |
| C | 5.994034 | 2.833810 | 1.663334 |
| H | 4.288400 | 4.141430 | 1.475245 |
| H | 3.996318 | 2.762428 | 2.532841 |
| C | 6.669576 | 3.231840 | 0.345642 |
| H | 6.501609 | 2.815720 | -1.780936 |
| H | 6.229190 | 1.422408 | -0.744130 |
| H | 6.422655 | 3.395072 | 2.499215 |
| H | 6.185828 | 1.772057 | 1.862442 |
| H | 7.743456 | 3.026819 | 0.391654 |
| H | 6.557747 | 4.313665 | 0.199753 |
| C | -5.445873 | -2.513320 | 1.759564 |
| H | -5.512598 | -1.427384 | 1.707410 |
| H | -6.459874 | -2.919027 | 1.801482 |
| H | -4.930297 | -2.789100 | 2.682986 |
| C | -4.745119 | -4.634511 | 0.658226 |
| H | -5.784161 | -4.965060 | 0.709220 |
| H | -4.278356 | -5.125191 | -0.199970 |
| H | -4.238938 | -4.972103 | 1.566425 |
| C | -5.460758 | -2.714377 | -0.765995 |
| H | -5.548313 | -1.633984 | -0.873552 |
| H | -4.938023 | -3.110790 | -1.640021 |
| H | -6.466519 | -3.141702 | -0.745004 |
| C | 0.115348 | -4.901007 | 1.758254 |
| H | -0.853380 | -5.403221 | 1.792669 |
| H | 0.893241 | -5.668761 | 1.758513 |
| H | 0.224080 | -4.298236 | 2.662557 |
| C | 1.671192 | -3.405321 | 0.488863 |
| H | 1.842969 | -2.805151 | -0.407908 |
| H | 1.833030 | -2.775727 | 1.367253 |
| H | 2.417216 | -4.202656 | 0.504637 |
| C | 0.113216 | -4.917393 | -0.763085 |
| H | 0.882649 | -5.693537 | -0.748728 |
| H | -0.862473 | -5.406452 | -0.794656 |
| H | 0.233535 | -4.328006 | -1.674794 |

**Table S#.** Cartesian coordinates for **2**+⦁: E0PT. (-1328.81564424 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.500700 | 2.795099 | 0.366564 |
| C | -1.888756 | 2.988755 | 0.285152 |
| C | -2.439117 | 4.269532 | 0.195180 |
| C | -1.539354 | 5.331386 | 0.197421 |
| C | -0.147530 | 5.133655 | 0.282622 |
| C | 0.414372 | 3.857939 | 0.366325 |
| C | -1.472879 | 0.789421 | 0.397006 |
| H | -3.507434 | 4.423448 | 0.125656 |
| H | -1.920620 | 6.342852 | 0.132039 |
| H | 0.511075 | 5.994513 | 0.282171 |
| N | -2.443276 | 1.720964 | 0.307419 |
| C | -3.051167 | -1.165079 | 0.324995 |
| C | -1.681522 | -0.639533 | 0.436730 |
| C | -0.608879 | -1.496606 | 0.563803 |
| C | -0.787015 | -2.897044 | 0.585282 |
| C | -2.095986 | -3.411943 | 0.477239 |
| C | -3.223380 | -2.622391 | 0.349004 |
| H | 0.395795 | -1.102185 | 0.650899 |
| H | -2.218517 | -4.483276 | 0.495940 |
| C | 0.439552 | -3.791576 | 0.699391 |
| C | -4.620524 | -3.224009 | 0.230773 |
| O | -4.026144 | -0.380290 | 0.211266 |
| N | -0.287163 | 1.435613 | 0.433712 |
| H | 0.662886 | 1.069181 | 0.482507 |
| C | 1.855667 | 3.620564 | 0.438970 |
| H | 2.487593 | 4.512926 | 0.429056 |
| N | 2.319926 | 2.428818 | 0.504615 |
| C | 3.776936 | 2.240335 | 0.536736 |
| C | 4.373273 | 2.434557 | -0.868008 |
| C | 4.511964 | 3.116880 | 1.562939 |
| H | 3.936810 | 1.194257 | 0.820326 |
| C | 5.875025 | 2.129741 | -0.872772 |
| H | 4.202597 | 3.474257 | -1.173386 |
| H | 3.843548 | 1.797243 | -1.582001 |
| C | 6.011139 | 2.797698 | 1.565411 |
| H | 4.372407 | 4.175044 | 1.314526 |
| H | 4.078484 | 2.957532 | 2.554789 |
| C | 6.620745 | 2.970221 | 0.169900 |
| H | 6.285843 | 2.309867 | -1.870635 |
| H | 6.025716 | 1.064803 | -0.656505 |
| H | 6.525113 | 3.438601 | 2.287819 |
| H | 6.157286 | 1.763038 | 1.900122 |
| H | 7.681306 | 2.701871 | 0.183810 |
| H | 6.564094 | 4.027534 | -0.117509 |
| H | -3.417409 | 1.425694 | 0.257575 |
| C | -5.508812 | -2.709140 | 1.386591 |
| H | -5.627835 | -1.628402 | 1.339394 |
| H | -6.494993 | -3.175805 | 1.317385 |
| H | -5.072553 | -2.972996 | 2.353618 |
| C | -4.585105 | -4.758692 | 0.305618 |
| H | -3.994593 | -5.192688 | -0.505392 |
| H | -4.175341 | -5.106811 | 1.257247 |
| H | -5.604931 | -5.138941 | 0.219065 |
| C | 0.080920 | -5.282855 | 0.729016 |
| H | -0.539622 | -5.533050 | 1.593350 |
| H | -0.446737 | -5.587369 | -0.178160 |
| H | 0.999174 | -5.869919 | 0.794722 |
| C | 1.347725 | -3.520089 | -0.521647 |
| H | 0.833683 | -3.773873 | -1.451824 |
| H | 1.649485 | -2.471465 | -0.569562 |
| H | 2.250453 | -4.131637 | -0.448319 |
| C | 1.207268 | -3.438260 | 1.991994 |
| H | 0.587763 | -3.612041 | 2.874598 |
| H | 2.095175 | -4.070806 | 2.065117 |
| H | 1.534375 | -2.396151 | 1.998954 |
| C | -5.243062 | -2.825314 | -1.126819 |
| H | -6.240036 | -3.266669 | -1.206510 |
| H | -5.332081 | -1.744307 | -1.222704 |
| H | -4.637640 | -3.202658 | -1.954963 |

**Table S#.** Cartesian coordinates for **2**+⦁: E0PT. (-1328.82800246 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.528073 | 2.742572 | 0.404197 |
| C | -1.921436 | 2.980419 | 0.301064 |
| C | -2.451704 | 4.265809 | 0.212852 |
| C | -1.550554 | 5.334546 | 0.236214 |
| C | -0.170901 | 5.128033 | 0.341490 |
| C | 0.373135 | 3.833989 | 0.422135 |
| C | -1.476384 | 0.809681 | 0.407582 |
| H | -3.518023 | 4.431858 | 0.127295 |
| H | -1.930374 | 6.346308 | 0.172118 |
| H | 0.499623 | 5.979267 | 0.359395 |
| N | -2.483178 | 1.726588 | 0.306580 |
| C | -3.060964 | -1.168598 | 0.322868 |
| C | -1.700320 | -0.624250 | 0.437828 |
| C | -0.618761 | -1.472146 | 0.564038 |
| C | -0.778274 | -2.871255 | 0.591400 |
| C | -2.082512 | -3.404573 | 0.481720 |
| C | -3.216356 | -2.628047 | 0.346212 |
| H | 0.371068 | -1.041120 | 0.641954 |
| H | -2.192376 | -4.477493 | 0.503258 |
| C | 0.459199 | -3.752098 | 0.713784 |
| C | -4.606812 | -3.245875 | 0.216236 |
| O | -4.050358 | -0.398428 | 0.206418 |
| N | -0.270650 | 1.400503 | 0.468577 |
| C | 1.787972 | 3.650514 | 0.503480 |
| H | 2.430179 | 4.524088 | 0.516824 |
| N | 2.355102 | 2.483039 | 0.555389 |
| C | 3.811698 | 2.240422 | 0.578233 |
| C | 4.374110 | 2.283257 | -0.851756 |
| C | 4.545498 | 3.216531 | 1.502221 |
| H | 3.920675 | 1.227482 | 0.972873 |
| C | 5.881885 | 2.008778 | -0.845664 |
| H | 4.175034 | 3.277269 | -1.268103 |
| H | 3.849587 | 1.555510 | -1.476661 |
| C | 6.049534 | 2.919561 | 1.503417 |
| H | 4.393648 | 4.242088 | 1.149431 |
| H | 4.129611 | 3.150194 | 2.510928 |
| C | 6.626406 | 2.971977 | 0.084535 |
| H | 6.267702 | 2.081106 | -1.866169 |
| H | 6.056732 | 0.978853 | -0.512923 |
| H | 6.556979 | 3.637847 | 2.153217 |
| H | 6.224463 | 1.925172 | 1.931036 |
| H | 7.692933 | 2.730728 | 0.101749 |
| H | 6.537202 | 3.994116 | -0.303449 |
| H | -3.454655 | 1.434506 | 0.245286 |
| H | 1.725533 | 1.671887 | 0.519365 |
| C | -5.220585 | -2.855122 | -1.147165 |
| H | -6.215850 | -3.299278 | -1.235630 |
| H | -5.310687 | -1.774484 | -1.246725 |
| H | -4.606579 | -3.232660 | -1.969068 |
| C | -5.513324 | -2.742357 | 1.361939 |
| H | -5.640604 | -1.662598 | 1.314981 |
| H | -6.494929 | -3.217532 | 1.282137 |
| H | -5.085021 | -3.003350 | 2.333502 |
| C | -4.556574 | -4.779951 | 0.292061 |
| H | -3.953177 | -5.208439 | -0.512409 |
| H | -4.152113 | -5.123254 | 1.247789 |
| H | -5.571438 | -5.171520 | 0.195653 |
| C | 0.118948 | -5.247457 | 0.757546 |
| H | -0.501333 | -5.496081 | 1.622661 |
| H | -0.404050 | -5.567051 | -0.147173 |
| H | 1.043267 | -5.824453 | 0.831086 |
| C | 1.222104 | -3.377016 | 2.002363 |
| H | 2.122267 | -3.991682 | 2.082176 |
| H | 1.527087 | -2.328136 | 1.998990 |
| H | 0.606277 | -3.554211 | 2.887099 |
| C | 1.365468 | -3.482177 | -0.508343 |
| H | 0.854895 | -3.749925 | -1.436629 |
| H | 1.651813 | -2.429646 | -0.565562 |
| H | 2.276450 | -4.081239 | -0.430712 |

**Table S#.** Cartesian coordinates for **3**: neutral. (-1707.73604777 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.579646 | 1.136284 | -0.019745 |
| C | 0.355893 | 1.840489 | -0.092226 |
| C | 0.362978 | 3.230381 | -0.262889 |
| C | 1.597756 | 3.869434 | -0.363470 |
| C | 2.804621 | 3.153702 | -0.289169 |
| C | 2.830903 | 1.763921 | -0.117108 |
| C | -0.137715 | -0.252300 | 0.152837 |
| H | -0.566227 | 3.784842 | -0.318110 |
| H | 1.632829 | 4.944331 | -0.496917 |
| H | 3.746349 | 3.685758 | -0.369261 |
| C | -2.294973 | -1.447086 | 0.243218 |
| C | -3.099072 | -2.606364 | 0.320701 |
| C | -2.500455 | -3.862028 | 0.462987 |
| C | -1.107351 | -3.913422 | 0.519312 |
| C | -0.317965 | -2.756965 | 0.426261 |
| C | -0.893110 | -1.486640 | 0.282551 |
| C | -4.442588 | -0.903056 | 0.118962 |
| H | -3.101625 | -4.760623 | 0.526456 |
| H | -0.615908 | -4.872186 | 0.634263 |
| H | 0.760516 | -2.852417 | 0.470382 |
| N | -0.698828 | 0.948693 | 0.021320 |
| C | -6.907407 | -0.758504 | -0.129589 |
| C | -5.652859 | -0.106102 | -0.004073 |
| C | -5.591059 | 1.295062 | 0.000445 |
| C | -6.737564 | 2.072803 | -0.112340 |
| C | -7.960695 | 1.398395 | -0.249255 |
| C | -8.087971 | 0.006995 | -0.264163 |
| H | -4.626123 | 1.777567 | 0.105101 |
| H | -8.860185 | 1.987260 | -0.342553 |
| C | -6.632765 | 3.602781 | -0.094821 |
| C | -9.460204 | -0.665236 | -0.425656 |
| O | -6.985743 | -2.108799 | -0.127919 |
| H | -6.064722 | -2.472012 | 0.014244 |
| N | -3.168783 | -0.393205 | 0.121262 |
| N | -4.431224 | -2.233015 | 0.236694 |
| H | -2.847068 | 0.564431 | 0.031955 |
| N | 1.235487 | -0.182725 | 0.137535 |
| H | 1.928737 | -0.918827 | 0.199437 |
| C | 4.081740 | 1.017629 | -0.038901 |
| H | 4.994280 | 1.618192 | -0.124222 |
| N | 4.104334 | -0.255385 | 0.116217 |
| C | 5.424452 | -0.904756 | 0.179755 |
| C | 6.223189 | -0.728433 | -1.122776 |
| C | 6.249245 | -0.433770 | 1.389520 |
| H | 5.232464 | -1.976407 | 0.307943 |
| C | 7.572009 | -1.451524 | -1.048620 |
| H | 6.391038 | 0.342368 | -1.290540 |
| H | 5.631004 | -1.096572 | -1.965785 |
| C | 7.597186 | -1.159373 | 1.459603 |
| H | 6.421442 | 0.645534 | 1.301154 |
| H | 5.674858 | -0.593491 | 2.306775 |
| C | 8.390516 | -0.984866 | 0.160142 |
| H | 8.129706 | -1.289658 | -1.976028 |
| H | 7.398311 | -2.532068 | -0.968534 |
| H | 8.172723 | -0.790951 | 2.314312 |
| H | 7.422579 | -2.228855 | 1.633580 |
| H | 9.334991 | -1.535121 | 0.214542 |
| H | 8.645678 | 0.075026 | 0.033517 |
| C | -5.823565 | 4.067776 | -1.322262 |
| H | -5.708832 | 5.155979 | -1.312118 |
| H | -4.825860 | 3.621147 | -1.327972 |
| H | -6.328601 | 3.784734 | -2.249842 |
| C | -5.907264 | 4.056108 | 1.187732 |
| H | -4.898761 | 3.639775 | 1.244164 |
| H | -5.821367 | 5.146489 | 1.207647 |
| H | -6.455869 | 3.738729 | 2.078624 |
| C | -8.012688 | 4.273603 | -0.131216 |
| H | -8.559145 | 4.020360 | -1.043486 |
| H | -8.621763 | 3.975402 | 0.726470 |
| H | -7.892483 | 5.359255 | -0.100500 |
| C | -9.472073 | -1.512027 | -1.715444 |
| H | -8.697785 | -2.278585 | -1.692806 |
| H | -10.443817 | -2.001634 | -1.830641 |
| H | -9.306983 | -0.876791 | -2.590095 |
| C | -9.764863 | -1.560093 | 0.795199 |
| H | -10.744141 | -2.031779 | 0.669086 |
| H | -9.015180 | -2.340198 | 0.915013 |
| H | -9.793595 | -0.960055 | 1.708980 |
| C | -10.594370 | 0.366618 | -0.531112 |
| H | -10.658891 | 0.990042 | 0.364579 |
| H | -10.472351 | 1.023477 | -1.396497 |
| H | -11.544965 | -0.160808 | -0.644661 |

**Table S#.** Cartesian coordinates for **3**+⦁: E0PT. (-1707.53809208 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.610101 | 1.119883 | -0.016592 |
| C | 0.387656 | 1.823096 | -0.110287 |
| C | 0.394710 | 3.214202 | -0.279632 |
| C | 1.629510 | 3.853350 | -0.353541 |
| C | 2.836706 | 3.137914 | -0.255890 |
| C | 2.862618 | 1.749108 | -0.088019 |
| C | -0.103131 | -0.271397 | 0.119371 |
| H | -0.533868 | 3.767138 | -0.354503 |
| H | 1.667300 | 4.928378 | -0.484298 |
| H | 3.778460 | 3.672297 | -0.314961 |
| C | -2.275850 | -1.433338 | 0.174278 |
| C | -3.111216 | -2.583342 | 0.225820 |
| C | -2.541321 | -3.860289 | 0.354030 |
| C | -1.158460 | -3.930605 | 0.424495 |
| C | -0.336480 | -2.780903 | 0.359909 |
| C | -0.871185 | -1.500346 | 0.226931 |
| C | -4.394122 | -0.832702 | 0.047233 |
| H | -3.161207 | -4.746075 | 0.396066 |
| H | -0.681793 | -4.897402 | 0.528314 |
| H | 0.737996 | -2.907235 | 0.417622 |
| N | -0.665704 | 0.928925 | -0.017998 |
| C | -6.863890 | -0.743781 | -0.156652 |
| C | -5.588834 | -0.044256 | -0.056591 |
| C | -5.562568 | 1.346985 | -0.066492 |
| C | -6.744588 | 2.077089 | -0.172470 |
| C | -7.980363 | 1.366129 | -0.289263 |
| C | -8.091217 | -0.003048 | -0.292257 |
| H | -4.611982 | 1.855483 | 0.014406 |
| H | -8.880074 | 1.956966 | -0.374776 |
| C | -6.779707 | 3.595639 | -0.158115 |
| C | -9.435184 | -0.719512 | -0.436069 |
| O | -6.895862 | -2.046517 | -0.124920 |
| H | -5.923588 | -2.409292 | -0.004699 |
| N | -3.111042 | -0.358834 | 0.066848 |
| N | -4.416139 | -2.172553 | 0.138836 |
| H | -2.744952 | 0.589115 | -0.006368 |
| N | 1.266954 | -0.201072 | 0.128893 |
| H | 1.964434 | -0.933313 | 0.203255 |
| C | 4.111998 | 1.001782 | 0.009376 |
| H | 5.026329 | 1.601080 | -0.059890 |
| N | 4.127943 | -0.271481 | 0.160363 |
| C | 5.445441 | -0.925356 | 0.238983 |
| C | 6.255362 | -0.751213 | -1.057132 |
| C | 6.260564 | -0.455195 | 1.455688 |
| H | 5.248440 | -1.996106 | 0.365956 |
| C | 7.602365 | -1.475987 | -0.971520 |
| H | 6.426131 | 0.319317 | -1.223561 |
| H | 5.669185 | -1.118262 | -1.904836 |
| C | 7.607012 | -1.182458 | 1.536398 |
| H | 6.435451 | 0.623749 | 1.368878 |
| H | 5.678669 | -0.613913 | 2.368429 |
| C | 8.411143 | -1.008744 | 0.243479 |
| H | 8.167328 | -1.315508 | -1.894690 |
| H | 7.426916 | -2.556250 | -0.891905 |
| H | 8.175962 | -0.814608 | 2.395630 |
| H | 7.430042 | -2.251724 | 1.709004 |
| H | 9.354823 | -1.559294 | 0.306033 |
| H | 8.667791 | 0.050935 | 0.118290 |
| C | -7.470514 | 4.095689 | -1.447673 |
| H | -8.490284 | 3.717250 | -1.539750 |
| H | -7.517707 | 5.186948 | -1.425971 |
| H | -6.909152 | 3.789816 | -2.333539 |
| C | -7.599160 | 4.051843 | 1.072452 |
| H | -7.684396 | 5.141438 | 1.062828 |
| H | -8.607614 | 3.632469 | 1.067684 |
| H | -7.104036 | 3.752218 | 1.999033 |
| C | -5.377687 | 4.212210 | -0.079000 |
| H | -4.858618 | 3.917732 | 0.836575 |
| H | -4.765204 | 3.920627 | -0.935755 |
| H | -5.464905 | 5.300479 | -0.079885 |
| C | -9.423869 | -1.582651 | -1.716963 |
| H | -8.645552 | -2.344805 | -1.685668 |
| H | -10.390793 | -2.081529 | -1.821153 |
| H | -9.266635 | -0.958115 | -2.599853 |
| C | -10.588784 | 0.287923 | -0.549637 |
| H | -10.660965 | 0.921666 | 0.337767 |
| H | -10.482898 | 0.931564 | -1.426532 |
| H | -11.526753 | -0.261773 | -0.649550 |
| C | -9.702914 | -1.606796 | 0.800333 |
| H | -10.679377 | -2.085145 | 0.688893 |
| H | -8.949350 | -2.384195 | 0.913878 |
| H | -9.722634 | -1.001766 | 1.710050 |

**Table S#.** Cartesian coordinates for **3**+⦁: E0PT. (-1707.55346068 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.544444 | 1.095848 | -0.051665 |
| C | 0.306818 | 1.773909 | -0.129153 |
| C | 0.283341 | 3.163491 | -0.309520 |
| C | 1.504058 | 3.825007 | -0.414714 |
| C | 2.727063 | 3.133936 | -0.335477 |
| C | 2.783196 | 1.748067 | -0.153649 |
| C | -0.136172 | -0.327905 | 0.129720 |
| H | -0.656922 | 3.698350 | -0.369246 |
| H | 1.517485 | 4.899365 | -0.555490 |
| H | 3.657122 | 3.685289 | -0.419961 |
| C | -2.278139 | -1.534629 | 0.220001 |
| C | -3.070012 | -2.691845 | 0.296456 |
| C | -2.494973 | -3.955313 | 0.440265 |
| C | -1.104240 | -3.998364 | 0.498552 |
| C | -0.309799 | -2.840712 | 0.406288 |
| C | -0.876061 | -1.571531 | 0.261253 |
| C | -4.412252 | -0.909159 | 0.085186 |
| H | -3.098734 | -4.850629 | 0.503063 |
| H | -0.612829 | -4.956133 | 0.615141 |
| H | 0.767604 | -2.940784 | 0.451601 |
| N | -0.726106 | 0.859064 | -0.008890 |
| C | -6.909029 | -0.772199 | -0.154003 |
| C | -5.606002 | -0.103524 | -0.025275 |
| C | -5.520727 | 1.272420 | -0.000232 |
| C | -6.673547 | 2.081028 | -0.101259 |
| C | -7.927450 | 1.449850 | -0.244850 |
| C | -8.098564 | 0.078571 | -0.273781 |
| H | -4.556271 | 1.751700 | 0.112747 |
| H | -8.799574 | 2.078725 | -0.328449 |
| C | -6.524791 | 3.594508 | -0.016874 |
| C | -9.475988 | -0.559735 | -0.419910 |
| O | -6.981423 | -2.027034 | -0.159084 |
| N | -3.138042 | -0.464939 | 0.095951 |
| N | -4.379568 | -2.251662 | 0.204315 |
| H | -2.770430 | 0.483759 | 0.010548 |
| N | 1.231225 | -0.230038 | 0.114239 |
| H | 1.944620 | -0.947666 | 0.182051 |
| C | 4.047556 | 1.024336 | -0.068581 |
| H | 4.949837 | 1.638520 | -0.158411 |
| N | 4.087581 | -0.246382 | 0.097765 |
| C | 5.415473 | -0.878413 | 0.168648 |
| C | 6.217129 | -0.698209 | -1.131580 |
| C | 6.229553 | -0.391763 | 1.379498 |
| H | 5.235956 | -1.951702 | 0.300747 |
| C | 7.570612 | -1.411486 | -1.049254 |
| H | 6.378877 | 0.373159 | -1.301227 |
| H | 5.630530 | -1.072105 | -1.975971 |
| C | 7.582746 | -1.106709 | 1.458285 |
| H | 6.392408 | 0.688626 | 1.285396 |
| H | 5.652759 | -0.551300 | 2.295287 |
| C | 8.380126 | -0.933134 | 0.161113 |
| H | 8.130810 | -1.249016 | -1.974941 |
| H | 7.404253 | -2.492910 | -0.965717 |
| H | 8.152511 | -0.730039 | 2.313102 |
| H | 7.414700 | -2.176397 | 1.637091 |
| H | 9.328228 | -1.476161 | 0.222484 |
| H | 8.628185 | 0.127906 | 0.030297 |
| H | -5.252851 | -2.776503 | 0.177687 |
| C | -7.858748 | 4.325319 | -0.216881 |
| H | -7.692620 | 5.402336 | -0.147339 |
| H | -8.290298 | 4.112548 | -1.198198 |
| H | -8.589063 | 4.050968 | 0.548364 |
| C | -5.529280 | 4.073943 | -1.094980 |
| H | -4.542725 | 3.622441 | -0.968839 |
| H | -5.894081 | 3.835512 | -2.096744 |
| H | -5.412991 | 5.157927 | -1.018992 |
| C | -5.967030 | 3.945125 | 1.381647 |
| H | -6.652995 | 3.619136 | 2.166971 |
| H | -4.997045 | 3.474413 | 1.557188 |
| H | -5.839563 | 5.027547 | 1.462989 |
| C | -9.515274 | -1.398385 | -1.717217 |
| H | -8.772271 | -2.194523 | -1.693536 |
| H | -10.506821 | -1.845005 | -1.828421 |
| H | -9.325704 | -0.767566 | -2.589450 |
| C | -10.588152 | 0.496896 | -0.495892 |
| H | -10.613857 | 1.121144 | 0.400776 |
| H | -10.478054 | 1.148368 | -1.366656 |
| H | -11.550965 | -0.011790 | -0.580254 |
| C | -9.768528 | -1.463580 | 0.800807 |
| H | -10.765138 | -1.899004 | 0.690154 |
| H | -9.039638 | -2.267402 | 0.883948 |
| H | -9.755842 | -0.877188 | 1.723194 |

**Table S#.** Cartesian coordinates for **3**+⦁: E0PT. (-1707.55886850 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.534153 | 1.142325 | -0.140101 |
| C | 0.315025 | 1.827814 | -0.253790 |
| C | 0.273384 | 3.207213 | -0.458280 |
| C | 1.500366 | 3.861097 | -0.548959 |
| C | 2.720728 | 3.171848 | -0.431608 |
| C | 2.773444 | 1.789941 | -0.226388 |
| C | -0.108695 | -0.350362 | 0.055363 |
| H | -0.665880 | 3.737222 | -0.545725 |
| H | 1.516647 | 4.932365 | -0.707580 |
| H | 3.651427 | 3.722650 | -0.502527 |
| C | -2.278102 | -1.507903 | 0.168358 |
| C | -3.037888 | -2.700357 | 0.275050 |
| C | -2.441462 | -3.949887 | 0.433622 |
| C | -1.046816 | -3.985527 | 0.481724 |
| C | -0.270702 | -2.823557 | 0.364502 |
| C | -0.865947 | -1.566600 | 0.204374 |
| C | -4.348952 | -0.922040 | 0.052803 |
| H | -3.031374 | -4.853871 | 0.517318 |
| H | -0.546391 | -4.937090 | 0.610165 |
| H | 0.808607 | -2.905738 | 0.401647 |
| N | -0.671792 | 0.862816 | -0.120683 |
| C | -6.873592 | -0.783310 | -0.132787 |
| C | -5.561363 | -0.128729 | -0.042350 |
| C | -5.467298 | 1.248997 | -0.035209 |
| C | -6.611719 | 2.065600 | -0.106061 |
| C | -7.877779 | 1.444123 | -0.211075 |
| C | -8.059004 | 0.075981 | -0.227844 |
| H | -4.485265 | 1.698439 | 0.040518 |
| H | -8.747942 | 2.078414 | -0.273797 |
| C | -6.449960 | 3.581379 | -0.067926 |
| C | -9.447241 | -0.551184 | -0.337219 |
| O | -6.962599 | -2.039847 | -0.127289 |
| N | -3.106236 | -0.421567 | 0.035106 |
| N | -4.344608 | -2.281821 | 0.191841 |
| N | 1.230480 | -0.192235 | 0.047300 |
| H | 1.969166 | -0.885637 | 0.148488 |
| C | 4.030018 | 1.054855 | -0.097681 |
| H | 4.940919 | 1.656206 | -0.174951 |
| N | 4.041872 | -0.212230 | 0.091524 |
| C | 5.353622 | -0.871238 | 0.208090 |
| C | 6.194503 | -0.717626 | -1.070957 |
| C | 6.137886 | -0.383612 | 1.438361 |
| H | 5.147609 | -1.938469 | 0.345929 |
| C | 7.534885 | -1.447354 | -0.941694 |
| H | 6.376808 | 0.348979 | -1.247371 |
| H | 5.625603 | -1.091894 | -1.927140 |
| C | 7.479028 | -1.114445 | 1.560975 |
| H | 6.316955 | 0.693713 | 1.338195 |
| H | 5.531666 | -0.526349 | 2.337963 |
| C | 8.315027 | -0.962841 | 0.285339 |
| H | 8.122485 | -1.304704 | -1.853693 |
| H | 7.352474 | -2.525321 | -0.848692 |
| H | 8.029561 | -0.737298 | 2.427894 |
| H | 7.293501 | -2.180318 | 1.743739 |
| H | 9.255061 | -1.514921 | 0.379881 |
| H | 8.578245 | 0.093929 | 0.149809 |
| H | -5.211756 | -2.810984 | 0.188414 |
| H | -1.691093 | 0.960487 | -0.139304 |
| C | -9.526998 | -1.400333 | -1.625307 |
| H | -8.793265 | -2.205122 | -1.608902 |
| H | -10.526368 | -1.835258 | -1.712967 |
| H | -9.346323 | -0.780989 | -2.507913 |
| C | -5.622697 | 4.022820 | -1.295365 |
| H | -5.484875 | 5.107199 | -1.271184 |
| H | -4.635681 | 3.554017 | -1.302590 |
| H | -6.134566 | 3.760829 | -2.224559 |
| C | -10.551804 | 0.514721 | -0.396939 |
| H | -10.553540 | 1.146172 | 0.495235 |
| H | -10.455307 | 1.159329 | -1.274649 |
| H | -11.521079 | 0.014454 | -0.455811 |
| C | -9.722305 | -1.442671 | 0.896001 |
| H | -8.999767 | -2.253510 | 0.967530 |
| H | -9.681222 | -0.850622 | 1.814109 |
| H | -10.726122 | -1.868667 | 0.814377 |
| C | -7.798508 | 4.312813 | -0.087578 |
| H | -8.356786 | 4.101101 | -1.002757 |
| H | -8.417169 | 4.031174 | 0.768416 |
| H | -7.625670 | 5.389851 | -0.039270 |
| C | -5.695433 | 3.974899 | 1.220613 |
| H | -6.248859 | 3.660539 | 2.108845 |
| H | -4.700883 | 3.525304 | 1.259073 |
| H | -5.577395 | 5.061103 | 1.256579 |

**Table S#.** Cartesian coordinates for **3**+⦁: E0PT. (-1707.56917917 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.515357 | 1.140998 | -0.113375 |
| C | 0.308673 | 1.872680 | -0.241594 |
| C | 0.292942 | 3.245087 | -0.467487 |
| C | 1.527908 | 3.897325 | -0.571223 |
| C | 2.732150 | 3.201040 | -0.446946 |
| C | 2.756622 | 1.811201 | -0.220445 |
| C | -0.081832 | -0.285406 | 0.094216 |
| H | -0.637967 | 3.789279 | -0.565962 |
| H | 1.549083 | 4.965497 | -0.747010 |
| H | 3.672401 | 3.733311 | -0.529121 |
| C | -2.272992 | -1.460771 | 0.234428 |
| C | -3.016043 | -2.665142 | 0.341462 |
| C | -2.404517 | -3.909929 | 0.489163 |
| C | -1.010435 | -3.925905 | 0.520427 |
| C | -0.252675 | -2.750184 | 0.397408 |
| C | -0.859411 | -1.499147 | 0.251958 |
| C | -4.356214 | -0.906714 | 0.132121 |
| H | -2.983627 | -4.820872 | 0.573741 |
| H | -0.495114 | -4.871656 | 0.636236 |
| H | 0.828555 | -2.803754 | 0.409898 |
| N | -0.681957 | 0.927611 | -0.097725 |
| C | -6.879499 | -0.810955 | -0.103068 |
| C | -5.582276 | -0.134692 | 0.031679 |
| C | -5.516293 | 1.245149 | 0.068201 |
| C | -6.671872 | 2.040615 | -0.031255 |
| C | -7.922482 | 1.398102 | -0.190796 |
| C | -8.076947 | 0.027657 | -0.230796 |
| H | -4.546112 | 1.709954 | 0.189757 |
| H | -8.799787 | 2.019769 | -0.277898 |
| C | -6.544524 | 3.556888 | 0.074777 |
| C | -9.447257 | -0.625856 | -0.397001 |
| O | -6.946999 | -2.069191 | -0.108687 |
| N | -3.123378 | -0.386420 | 0.111698 |
| N | -4.329869 | -2.267896 | 0.268065 |
| N | 1.255571 | -0.189484 | 0.093918 |
| C | 4.001304 | 1.121071 | -0.106654 |
| H | 4.924805 | 1.684958 | -0.189515 |
| N | 4.096070 | -0.160800 | 0.087095 |
| C | 5.375658 | -0.891611 | 0.197985 |
| C | 6.187284 | -0.761060 | -1.097890 |
| C | 6.174028 | -0.410074 | 1.417200 |
| H | 5.095126 | -1.936276 | 0.343303 |
| C | 7.522237 | -1.502980 | -0.979322 |
| H | 6.377508 | 0.302025 | -1.285565 |
| H | 5.599050 | -1.140875 | -1.937030 |
| C | 7.509154 | -1.155238 | 1.519466 |
| H | 6.362323 | 0.664684 | 1.309027 |
| H | 5.577949 | -0.547807 | 2.322882 |
| C | 8.326027 | -1.016644 | 0.231031 |
| H | 8.093280 | -1.369857 | -1.902371 |
| H | 7.330377 | -2.578034 | -0.877054 |
| H | 8.071669 | -0.776056 | 2.376925 |
| H | 7.315477 | -2.217573 | 1.711498 |
| H | 9.260827 | -1.578396 | 0.313730 |
| H | 8.597413 | 0.036372 | 0.085366 |
| H | -5.185939 | -2.813474 | 0.251305 |
| H | -1.696305 | 1.033360 | -0.116055 |
| H | 3.211821 | -0.677874 | 0.158998 |
| C | -5.535374 | 4.065575 | -0.975956 |
| H | -5.429324 | 5.149627 | -0.882881 |
| H | -4.548559 | 3.618252 | -0.837955 |
| H | -5.878587 | 3.839113 | -1.988264 |
| C | -7.882798 | 4.276424 | -0.139841 |
| H | -8.297517 | 4.068366 | -1.129436 |
| H | -8.622464 | 3.987476 | 0.610946 |
| H | -7.729313 | 5.354780 | -0.057932 |
| C | -6.020210 | 3.896363 | 1.488051 |
| H | -6.719918 | 3.553592 | 2.253992 |
| H | -5.051818 | 3.428352 | 1.677373 |
| H | -5.902500 | 4.978643 | 1.587970 |
| C | -9.461036 | -1.466752 | -1.692736 |
| H | -8.703895 | -2.249278 | -1.660534 |
| H | -10.443110 | -1.931823 | -1.814976 |
| H | -9.273961 | -0.833483 | -2.563984 |
| C | -10.570062 | 0.418313 | -0.492375 |
| H | -10.622793 | 1.037990 | 0.406449 |
| H | -10.446665 | 1.076250 | -1.356561 |
| H | -11.525737 | -0.099631 | -0.602165 |
| C | -9.750987 | -1.530077 | 0.819721 |
| H | -10.736804 | -1.985715 | 0.691573 |
| H | -9.008135 | -2.318874 | 0.921224 |
| H | -9.767487 | -0.939849 | 1.739808 |

**Table S#.** Cartesian coordinates for **4**: neutral. (-2086.47631873 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.683327 | 0.325129 | 0.811766 |
| C | 0.582343 | 1.159606 | 0.505270 |
| C | 0.775533 | 2.535448 | 0.339355 |
| C | 2.069272 | 3.032118 | 0.490090 |
| C | 3.152290 | 2.195237 | 0.803194 |
| C | 2.988532 | 0.813856 | 0.974442 |
| C | -0.186535 | -0.855556 | 0.686338 |
| H | -0.057017 | 3.186700 | 0.101869 |
| H | 2.249693 | 4.093237 | 0.364727 |
| H | 4.139127 | 2.630505 | 0.907216 |
| C | -2.468807 | -1.778997 | 0.506168 |
| C | -3.415223 | -2.828563 | 0.522128 |
| C | -2.997956 | -4.141362 | 0.760497 |
| C | -1.637214 | -4.359268 | 0.976751 |
| C | -0.704964 | -3.310570 | 0.958020 |
| C | -1.098137 | -1.985947 | 0.720947 |
| C | -4.502132 | -0.987399 | 0.098589 |
| H | -3.710108 | -4.957675 | 0.775135 |
| H | -1.283837 | -5.365841 | 1.165591 |
| H | 0.341020 | -3.533209 | 1.130754 |
| N | -0.570215 | 0.394583 | 0.434976 |
| C | -6.892730 | -0.564799 | -0.389805 |
| C | -5.578920 | -0.064602 | -0.216938 |
| C | -5.324332 | 1.311817 | -0.358184 |
| C | -6.337128 | 2.200654 | -0.680255 |
| C | -7.629164 | 1.670528 | -0.860189 |
| C | -7.946790 | 0.321820 | -0.723827 |
| H | -4.314192 | 1.670665 | -0.210703 |
| H | -8.422811 | 2.358155 | -1.118603 |
| C | -6.110220 | 3.706959 | -0.844610 |
| C | -9.382229 | -0.189613 | -0.918761 |
| O | -7.156857 | -1.881604 | -0.245165 |
| H | -6.298874 | -2.346660 | -0.016857 |
| N | -3.183561 | -0.634955 | 0.240930 |
| N | -4.671173 | -2.301499 | 0.267302 |
| H | -2.736459 | 0.271427 | 0.158559 |
| N | 1.165506 | -0.942572 | 0.916756 |
| H | 1.740700 | -1.753124 | 1.114379 |
| C | 4.068004 | -0.093754 | 1.325495 |
| N | 3.944015 | -1.418926 | 1.386735 |
| N | 5.337590 | 0.320413 | 1.650251 |
| C | 7.406371 | -0.942680 | 2.356888 |
| C | 7.838848 | -2.257037 | 2.569694 |
| C | 6.983715 | -3.357336 | 2.380812 |
| C | 5.656641 | -3.194035 | 1.985114 |
| C | 5.192199 | -1.890195 | 1.768611 |
| C | 6.072809 | -0.798761 | 1.945649 |
| H | 8.861684 | -2.424663 | 2.889967 |
| H | 7.366898 | -4.355767 | 2.556059 |
| H | 4.999059 | -4.044933 | 1.853804 |
| H | 5.732696 | 1.251679 | 1.718959 |
| C | 8.275016 | 0.214643 | 2.563479 |
| H | 9.289521 | -0.008571 | 2.903732 |
| N | 7.853451 | 1.406853 | 2.356821 |
| C | 8.742029 | 2.551722 | 2.548430 |
| C | 10.125151 | 2.279307 | 3.149871 |
| C | 8.875616 | 3.289196 | 1.204503 |
| H | 8.207078 | 3.226666 | 3.231751 |
| C | 10.906889 | 3.587153 | 3.322531 |
| H | 10.686314 | 1.609068 | 2.486752 |
| H | 10.023442 | 1.767269 | 4.112232 |
| C | 9.672602 | 4.588490 | 1.357902 |
| H | 9.381658 | 2.621469 | 0.496552 |
| H | 7.878400 | 3.488955 | 0.801332 |
| C | 11.044309 | 4.335861 | 1.992897 |
| H | 11.893380 | 3.376782 | 3.747200 |
| H | 10.383939 | 4.227028 | 4.044251 |
| H | 9.787381 | 5.072783 | 0.383281 |
| H | 9.105232 | 5.281170 | 1.991949 |
| H | 11.571351 | 5.283091 | 2.144517 |
| H | 11.655217 | 3.736936 | 1.305825 |
| C | -9.425032 | -1.215329 | -2.071101 |
| H | -8.759357 | -2.055827 | -1.879648 |
| H | -10.444406 | -1.595180 | -2.189532 |
| H | -9.130420 | -0.742532 | -3.012408 |
| C | -6.464197 | 4.117945 | -2.288548 |
| H | -7.500838 | 3.869218 | -2.529012 |
| H | -6.335354 | 5.196677 | -2.418323 |
| H | -5.816500 | 3.607916 | -3.006693 |
| C | -9.887829 | -0.841923 | 0.385551 |
| H | -10.909069 | -1.208007 | 0.243896 |
| H | -9.257404 | -1.678752 | 0.683053 |
| H | -9.899134 | -0.109627 | 1.197958 |
| C | -10.348894 | 0.950764 | -1.275031 |
| H | -10.392201 | 1.707305 | -0.486569 |
| H | -10.067065 | 1.445575 | -2.208291 |
| H | -11.354060 | 0.541610 | -1.402317 |
| C | -7.018723 | 4.475176 | 0.136833 |
| H | -6.875627 | 5.552971 | 0.015981 |
| H | -8.075104 | 4.256310 | -0.036501 |
| H | -6.782726 | 4.211949 | 1.171294 |
| C | -4.654137 | 4.102836 | -0.562847 |
| H | -4.361292 | 3.848584 | 0.459706 |
| H | -3.961195 | 3.608968 | -1.249138 |
| H | -4.537081 | 5.182212 | -0.687496 |

**Table S#.** Cartesian coordinates for **4**+⦁: E0PT. (-2086.27776155 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.686007 | 0.361764 | 0.917055 |
| C | 0.587259 | 1.199034 | 0.612043 |
| C | 0.781258 | 2.577313 | 0.459913 |
| C | 2.073885 | 3.070049 | 0.620924 |
| C | 3.156511 | 2.228360 | 0.928872 |
| C | 2.992176 | 0.846886 | 1.086213 |
| C | -0.175816 | -0.819539 | 0.760356 |
| H | -0.048969 | 3.231254 | 0.222734 |
| H | 2.256553 | 4.131793 | 0.505466 |
| H | 4.144159 | 2.661027 | 1.036227 |
| C | -2.457463 | -1.726367 | 0.511476 |
| C | -3.422329 | -2.771591 | 0.513707 |
| C | -3.031633 | -4.093691 | 0.780862 |
| C | -1.686896 | -4.314528 | 1.034131 |
| C | -0.734355 | -3.268717 | 1.029245 |
| C | -1.092581 | -1.946301 | 0.771582 |
| C | -4.454516 | -0.910681 | 0.048987 |
| H | -3.755302 | -4.898672 | 0.786894 |
| H | -1.343566 | -5.319447 | 1.245453 |
| H | 0.301583 | -3.509219 | 1.234449 |
| N | -0.562630 | 0.432344 | 0.522127 |
| C | -6.865163 | -0.574484 | -0.430357 |
| C | -5.526322 | -0.015226 | -0.283247 |
| C | -5.326245 | 1.348937 | -0.466756 |
| C | -6.392165 | 2.185937 | -0.792470 |
| C | -7.695144 | 1.612193 | -0.928495 |
| C | -7.976947 | 0.278642 | -0.760882 |
| H | -4.329455 | 1.752444 | -0.360179 |
| H | -8.504791 | 2.280429 | -1.180295 |
| C | -6.230046 | 3.680577 | -1.012574 |
| C | -9.389126 | -0.290113 | -0.910883 |
| O | -7.061045 | -1.851551 | -0.263356 |
| H | -6.149231 | -2.309657 | -0.030923 |
| N | -3.137661 | -0.578505 | 0.217569 |
| N | -4.646336 | -2.227914 | 0.225349 |
| H | -2.662620 | 0.320861 | 0.161308 |
| N | 1.170722 | -0.908587 | 1.001906 |
| H | 1.748706 | -1.719982 | 1.192281 |
| C | 4.070961 | -0.070391 | 1.412813 |
| N | 3.935711 | -1.395031 | 1.455332 |
| N | 5.351149 | 0.327495 | 1.712416 |
| C | 7.428833 | -0.969099 | 2.330569 |
| C | 7.853077 | -2.290988 | 2.508251 |
| C | 6.979725 | -3.379393 | 2.334320 |
| C | 5.644065 | -3.196506 | 1.979771 |
| C | 5.188533 | -1.884330 | 1.795467 |
| C | 6.084172 | -0.804011 | 1.965940 |
| H | 8.884109 | -2.473742 | 2.791689 |
| H | 7.357050 | -4.383970 | 2.484442 |
| H | 4.973665 | -4.038513 | 1.856276 |
| H | 5.750776 | 1.255507 | 1.797534 |
| C | 8.320415 | 0.171532 | 2.531401 |
| H | 9.352001 | -0.078248 | 2.792875 |
| N | 7.901059 | 1.376420 | 2.414537 |
| C | 8.814559 | 2.500511 | 2.623062 |
| C | 10.267968 | 2.166125 | 2.976745 |
| C | 8.752164 | 3.410805 | 1.385044 |
| H | 8.388489 | 3.072323 | 3.460435 |
| C | 11.090846 | 3.442544 | 3.185458 |
| H | 10.708468 | 1.577679 | 2.162488 |
| H | 10.304669 | 1.543792 | 3.876337 |
| C | 9.578409 | 4.685121 | 1.586077 |
| H | 9.138058 | 2.849257 | 0.525241 |
| H | 7.706634 | 3.651870 | 1.169926 |
| C | 11.028828 | 4.359772 | 1.959519 |
| H | 12.128590 | 3.180360 | 3.413937 |
| H | 10.703031 | 3.982537 | 4.058361 |
| H | 9.546556 | 5.298528 | 0.680359 |
| H | 9.126970 | 5.281368 | 2.388822 |
| H | 11.586158 | 5.282382 | 2.149875 |
| H | 11.515951 | 3.860104 | 1.112788 |
| C | -6.685369 | 4.022195 | -2.450814 |
| H | -7.722990 | 3.735241 | -2.632275 |
| H | -6.600659 | 5.101277 | -2.601974 |
| H | -6.053716 | 3.519530 | -3.186585 |
| C | -7.124903 | 4.433955 | -0.000992 |
| H | -7.019185 | 5.509076 | -0.165150 |
| H | -8.179858 | 4.176727 | -0.115206 |
| H | -6.823093 | 4.211327 | 1.024918 |
| C | -4.780006 | 4.146408 | -0.831349 |
| H | -4.418788 | 3.956864 | 0.182534 |
| H | -4.106444 | 3.654360 | -1.537307 |
| H | -4.723383 | 5.221842 | -1.010553 |
| C | -9.415464 | -1.329564 | -2.052973 |
| H | -8.729265 | -2.154076 | -1.866168 |
| H | -10.427027 | -1.733096 | -2.145576 |
| H | -9.148057 | -0.860107 | -3.003169 |
| C | -10.395511 | 0.817707 | -1.255115 |
| H | -10.440315 | 1.579446 | -0.472201 |
| H | -10.149592 | 1.308101 | -2.200405 |
| H | -11.389654 | 0.376978 | -1.352606 |
| C | -9.834112 | -0.943758 | 0.416199 |
| H | -9.189509 | -1.775767 | 0.697028 |
| H | -9.828947 | -0.208310 | 1.225054 |
| H | -10.853691 | -1.320360 | 0.303823 |

**Table S#.** Cartesian coordinates for **4**+⦁: E0PT. (-2086.29343325 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.614824 | 0.282626 | 1.100875 |
| C | 0.502040 | 1.104017 | 0.804249 |
| C | 0.671437 | 2.487186 | 0.666569 |
| C | 1.955459 | 3.000159 | 0.831828 |
| C | 3.053265 | 2.173613 | 1.128226 |
| C | 2.912826 | 0.788286 | 1.271886 |
| C | -0.223260 | -0.930650 | 0.924476 |
| H | -0.170602 | 3.128585 | 0.436249 |
| H | 2.119829 | 4.065994 | 0.727692 |
| H | 4.033667 | 2.622098 | 1.239201 |
| C | -2.479831 | -1.867570 | 0.625047 |
| C | -3.412588 | -2.917874 | 0.594331 |
| C | -3.031368 | -4.236384 | 0.846418 |
| C | -1.684848 | -4.445862 | 1.130147 |
| C | -0.747994 | -3.395768 | 1.159293 |
| C | -1.120970 | -2.072625 | 0.910249 |
| C | -4.469599 | -0.999371 | 0.122409 |
| H | -3.746461 | -5.047836 | 0.824551 |
| H | -1.340592 | -5.451811 | 1.334329 |
| H | 0.286389 | -3.623296 | 1.384751 |
| N | -0.632660 | 0.317216 | 0.701599 |
| C | -6.872154 | -0.579852 | -0.465540 |
| C | -5.515645 | -0.068543 | -0.222763 |
| C | -5.236839 | 1.283151 | -0.323863 |
| C | -6.236085 | 2.204174 | -0.679801 |
| C | -7.543716 | 1.716751 | -0.939377 |
| C | -7.902614 | 0.391281 | -0.853928 |
| H | -4.234609 | 1.638648 | -0.127991 |
| H | -8.295692 | 2.439271 | -1.221849 |
| C | -5.964079 | 3.697790 | -0.796748 |
| C | -9.317264 | -0.089540 | -1.161010 |
| O | -7.121439 | -1.805400 | -0.345642 |
| N | -3.166989 | -0.710003 | 0.331273 |
| N | -4.624596 | -2.329458 | 0.280457 |
| H | -2.679924 | 0.186611 | 0.297035 |
| N | 1.123098 | -0.998071 | 1.169297 |
| H | 1.715934 | -1.800816 | 1.352701 |
| C | 4.009930 | -0.113375 | 1.578565 |
| N | 3.892142 | -1.439001 | 1.642855 |
| N | 5.294176 | 0.303183 | 1.828158 |
| C | 7.412624 | -0.958359 | 2.371441 |
| C | 7.861457 | -2.272180 | 2.547474 |
| C | 6.994121 | -3.373106 | 2.428972 |
| C | 5.642450 | -3.212382 | 2.127878 |
| C | 5.162495 | -1.908755 | 1.944164 |
| C | 6.051022 | -0.815836 | 2.064200 |
| H | 8.907546 | -2.438243 | 2.781249 |
| H | 7.390758 | -4.370747 | 2.576425 |
| H | 4.979526 | -4.064931 | 2.041335 |
| H | 5.690205 | 1.235710 | 1.873959 |
| C | 8.297251 | 0.198499 | 2.500169 |
| H | 9.343495 | -0.026870 | 2.723249 |
| N | 7.852997 | 1.391600 | 2.358774 |
| C | 8.749457 | 2.540515 | 2.477267 |
| C | 10.228508 | 2.256384 | 2.763596 |
| C | 8.599157 | 3.399014 | 1.210101 |
| H | 8.353241 | 3.134374 | 3.313587 |
| C | 11.021118 | 3.564099 | 2.883605 |
| H | 10.643516 | 1.651737 | 1.947132 |
| H | 10.331616 | 1.669555 | 3.682192 |
| C | 9.393751 | 4.703460 | 1.321609 |
| H | 8.961541 | 2.815726 | 0.354697 |
| H | 7.537433 | 3.600011 | 1.036856 |
| C | 10.870119 | 4.430280 | 1.628518 |
| H | 12.076736 | 3.342681 | 3.068782 |
| H | 10.658528 | 4.124411 | 3.754300 |
| H | 9.295558 | 5.279792 | 0.396362 |
| H | 8.965865 | 5.316158 | 2.125052 |
| H | 11.414524 | 5.372151 | 1.749678 |
| H | 11.322372 | 3.906950 | 0.776701 |
| H | -5.548068 | -2.741782 | 0.151909 |
| C | -9.269712 | -1.091594 | -2.338215 |
| H | -8.694496 | -1.977828 | -2.074189 |
| H | -10.287939 | -1.396381 | -2.594923 |
| H | -8.819302 | -0.627062 | -3.219384 |
| C | -10.238215 | 1.073084 | -1.559592 |
| H | -11.233422 | 0.676176 | -1.769253 |
| H | -10.333179 | 1.810990 | -0.758097 |
| H | -9.884751 | 1.585383 | -2.458162 |
| C | -9.922243 | -0.770651 | 0.087455 |
| H | -9.338156 | -1.639292 | 0.386842 |
| H | -9.964617 | -0.069444 | 0.924964 |
| H | -10.942679 | -1.092127 | -0.137640 |
| C | -6.268425 | 4.142905 | -2.245032 |
| H | -7.302724 | 3.931265 | -2.524577 |
| H | -6.107342 | 5.220123 | -2.334253 |
| H | -5.609220 | 3.636356 | -2.953794 |
| C | -6.896269 | 4.453622 | 0.176822 |
| H | -6.728926 | 5.528816 | 0.074773 |
| H | -7.949442 | 4.255241 | -0.032204 |
| H | -6.690564 | 4.168713 | 1.211187 |
| C | -4.510266 | 4.058138 | -0.461138 |
| H | -4.252688 | 3.777283 | 0.563397 |
| H | -3.805042 | 3.574602 | -1.142043 |
| H | -4.378624 | 5.137880 | -0.556710 |

**Table S#.** Cartesian coordinates for **4**+⦁: E0PT. (-2086.29902013 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.590076 | 0.353309 | 1.105904 |
| C | 0.492351 | 1.177945 | 0.812503 |
| C | 0.633962 | 2.557454 | 0.672190 |
| C | 1.919519 | 3.068944 | 0.838583 |
| C | 3.019434 | 2.246619 | 1.133778 |
| C | 2.885387 | 0.861050 | 1.276796 |
| C | -0.213832 | -0.944387 | 0.938511 |
| H | -0.211686 | 3.191796 | 0.441712 |
| H | 2.079306 | 4.134964 | 0.735069 |
| H | 3.997295 | 2.698653 | 1.245443 |
| C | -2.484304 | -1.841410 | 0.623100 |
| C | -3.387661 | -2.934367 | 0.591313 |
| C | -2.979665 | -4.244318 | 0.835453 |
| C | -1.628403 | -4.443541 | 1.120011 |
| C | -0.711583 | -3.382115 | 1.155355 |
| C | -1.118147 | -2.065080 | 0.912626 |
| C | -4.417542 | -1.020855 | 0.136819 |
| H | -3.678857 | -5.070455 | 0.808031 |
| H | -1.271294 | -5.446508 | 1.316902 |
| H | 0.327271 | -3.590642 | 1.378654 |
| N | -0.600436 | 0.329673 | 0.722078 |
| C | -6.842799 | -0.603090 | -0.456427 |
| C | -5.483757 | -0.102899 | -0.211715 |
| C | -5.201471 | 1.250854 | -0.316407 |
| C | -6.192369 | 2.175159 | -0.667828 |
| C | -7.506448 | 1.696029 | -0.926320 |
| C | -7.869415 | 0.373394 | -0.842298 |
| H | -4.190074 | 1.578375 | -0.122265 |
| H | -8.254886 | 2.423672 | -1.206294 |
| C | -5.915115 | 3.669325 | -0.781606 |
| C | -9.288102 | -0.101067 | -1.149020 |
| O | -7.104696 | -1.829519 | -0.342165 |
| N | -3.139247 | -0.669561 | 0.341904 |
| N | -4.599892 | -2.368266 | 0.281083 |
| N | 1.113270 | -0.943128 | 1.173115 |
| C | 3.976165 | -0.048739 | 1.581876 |
| N | 3.831799 | -1.371101 | 1.657056 |
| N | 5.268419 | 0.344844 | 1.816342 |
| C | 7.365048 | -0.954931 | 2.352861 |
| C | 7.787992 | -2.275529 | 2.535078 |
| C | 6.897020 | -3.360529 | 2.434395 |
| C | 5.547415 | -3.176832 | 2.143046 |
| C | 5.093317 | -1.864573 | 1.951695 |
| C | 6.003737 | -0.788399 | 2.054525 |
| H | 8.831818 | -2.461089 | 2.763678 |
| H | 7.275921 | -4.364063 | 2.587369 |
| H | 4.866719 | -4.016370 | 2.069412 |
| C | 8.271161 | 0.186719 | 2.472751 |
| H | 9.313420 | -0.055712 | 2.696045 |
| N | 7.845137 | 1.386151 | 2.329888 |
| C | 8.756791 | 2.522264 | 2.456255 |
| C | 10.230957 | 2.216560 | 2.744199 |
| C | 8.620235 | 3.394279 | 1.197032 |
| H | 8.366469 | 3.114047 | 3.296901 |
| C | 11.037725 | 3.513639 | 2.881653 |
| H | 10.641782 | 1.615897 | 1.922677 |
| H | 10.323367 | 1.618808 | 3.656847 |
| C | 9.429924 | 4.688145 | 1.324462 |
| H | 8.978007 | 2.815412 | 0.336744 |
| H | 7.561478 | 3.610189 | 1.023471 |
| C | 10.901751 | 4.395594 | 1.635753 |
| H | 12.089900 | 3.278187 | 3.068716 |
| H | 10.677712 | 4.068161 | 3.757125 |
| H | 9.343141 | 5.274637 | 0.404349 |
| H | 9.005162 | 5.297880 | 2.131818 |
| H | 11.454890 | 5.330499 | 1.770534 |
| H | 11.352947 | 3.877322 | 0.780308 |
| H | -1.580292 | 0.545535 | 0.516636 |
| H | -5.515798 | -2.787873 | 0.147649 |
| H | 1.737346 | -1.726651 | 1.360575 |
| H | 5.689365 | 1.267912 | 1.850279 |
| C | -9.248969 | -1.098880 | -2.329460 |
| H | -8.672350 | -1.985926 | -2.071166 |
| H | -10.268345 | -1.402843 | -2.583722 |
| H | -8.802008 | -0.631607 | -3.211162 |
| C | -10.205549 | 1.066200 | -1.542560 |
| H | -11.203314 | 0.674855 | -1.751737 |
| H | -10.295234 | 1.802486 | -0.738870 |
| H | -9.851195 | 1.580211 | -2.439877 |
| C | -9.895604 | -0.782897 | 0.097174 |
| H | -9.311168 | -1.651693 | 0.395491 |
| H | -9.936945 | -0.082734 | 0.935857 |
| H | -10.916738 | -1.103794 | -0.126782 |
| C | -6.222936 | 4.124135 | -2.225421 |
| H | -7.258799 | 3.916115 | -2.502290 |
| H | -6.059635 | 5.201475 | -2.312244 |
| H | -5.568269 | 3.618522 | -2.939327 |
| C | -6.837215 | 4.426649 | 0.199678 |
| H | -6.667023 | 5.502185 | 0.103232 |
| H | -7.892424 | 4.233066 | -0.004193 |
| H | -6.627858 | 4.135409 | 1.231720 |
| C | -4.457741 | 4.020198 | -0.451412 |
| H | -4.197621 | 3.730977 | 0.570119 |
| H | -3.759671 | 3.532939 | -1.137082 |
| H | -4.318358 | 5.099707 | -0.542347 |

**Table S#.** Cartesian coordinates for **4**+⦁: E0PT. (-2086.30288096 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.596536 | 0.409325 | 1.107915 |
| C | 0.512513 | 1.270575 | 0.806546 |
| C | 0.669602 | 2.646846 | 0.674798 |
| C | 1.956833 | 3.159702 | 0.854289 |
| C | 3.046402 | 2.333488 | 1.154540 |
| C | 2.891325 | 0.945378 | 1.286021 |
| C | -0.144983 | -0.846332 | 0.931189 |
| H | -0.168067 | 3.291836 | 0.440843 |
| H | 2.119135 | 4.226003 | 0.757651 |
| H | 4.023834 | 2.781700 | 1.282101 |
| C | -2.431903 | -1.780219 | 0.602381 |
| C | -3.311364 | -2.894303 | 0.562873 |
| C | -2.877321 | -4.198679 | 0.798545 |
| C | -1.523295 | -4.366410 | 1.082825 |
| C | -0.632158 | -3.280615 | 1.125626 |
| C | -1.060799 | -1.971543 | 0.892163 |
| C | -4.386471 | -1.002861 | 0.117645 |
| H | -3.558906 | -5.039178 | 0.764048 |
| H | -1.141423 | -5.362195 | 1.273167 |
| H | 0.414116 | -3.451793 | 1.344681 |
| N | -0.575294 | 0.432823 | 0.705440 |
| C | -6.821986 | -0.639363 | -0.472993 |
| C | -5.474724 | -0.109438 | -0.225118 |
| C | -5.225301 | 1.253087 | -0.322134 |
| C | -6.236108 | 2.154369 | -0.668622 |
| C | -7.539063 | 1.645395 | -0.932307 |
| C | -7.870342 | 0.314625 | -0.855918 |
| H | -4.222023 | 1.602144 | -0.123663 |
| H | -8.303788 | 2.357006 | -1.209823 |
| C | -5.994130 | 3.655679 | -0.774989 |
| C | -9.277937 | -0.191981 | -1.165245 |
| O | -7.056781 | -1.872289 | -0.363379 |
| N | -3.118646 | -0.622202 | 0.325139 |
| N | -4.536867 | -2.356437 | 0.255044 |
| N | 1.167087 | -0.897630 | 1.179074 |
| C | 3.981818 | 0.054196 | 1.591617 |
| N | 3.842619 | -1.285280 | 1.689921 |
| N | 5.276655 | 0.354080 | 1.819952 |
| C | 7.337154 | -0.998425 | 2.363971 |
| C | 7.731822 | -2.325548 | 2.557660 |
| C | 6.817846 | -3.391551 | 2.473737 |
| C | 5.469542 | -3.188983 | 2.186274 |
| C | 5.066008 | -1.868357 | 1.986021 |
| C | 5.980648 | -0.808118 | 2.068399 |
| H | 8.771348 | -2.531728 | 2.785534 |
| H | 7.174932 | -4.400847 | 2.636374 |
| H | 4.768680 | -4.011011 | 2.124231 |
| C | 8.258910 | 0.134520 | 2.472607 |
| H | 9.298519 | -0.115339 | 2.695666 |
| N | 7.836485 | 1.333446 | 2.323783 |
| C | 8.747704 | 2.470194 | 2.445384 |
| C | 10.221561 | 2.162277 | 2.729495 |
| C | 8.606114 | 3.341797 | 1.186590 |
| H | 8.357426 | 3.059954 | 3.287040 |
| C | 11.028445 | 3.459469 | 2.866185 |
| H | 10.629885 | 1.562489 | 1.906105 |
| H | 10.315756 | 1.564212 | 3.641694 |
| C | 9.416257 | 4.635447 | 1.314321 |
| H | 8.962252 | 2.764016 | 0.325111 |
| H | 7.546875 | 3.558148 | 1.016542 |
| C | 10.888883 | 4.342637 | 1.621552 |
| H | 12.080895 | 3.223375 | 3.050081 |
| H | 10.670743 | 4.012603 | 3.743387 |
| H | 9.326874 | 5.222590 | 0.395031 |
| H | 8.993102 | 5.243913 | 2.123369 |
| H | 11.441785 | 5.277572 | 1.756286 |
| H | 11.338204 | 3.825646 | 0.764406 |
| H | 2.923611 | -1.718731 | 1.555333 |
| H | -1.549383 | 0.648876 | 0.495146 |
| H | -5.441314 | -2.797775 | 0.118639 |
| H | 5.756071 | 1.253414 | 1.842896 |
| C | -9.215986 | -1.191455 | -2.343220 |
| H | -8.618047 | -2.063361 | -2.082391 |
| H | -10.227799 | -1.520817 | -2.596310 |
| H | -8.781105 | -0.715536 | -3.226401 |
| C | -10.220014 | 0.953842 | -1.563618 |
| H | -10.328394 | 1.689872 | -0.762048 |
| H | -9.873452 | 1.473421 | -2.460916 |
| H | -11.208743 | 0.541198 | -1.775387 |
| C | -9.871232 | -0.884159 | 0.081859 |
| H | -9.263672 | -1.735191 | 0.385830 |
| H | -9.933123 | -0.181336 | 0.917147 |
| H | -10.882559 | -1.234505 | -0.142751 |
| C | -6.306379 | 4.109621 | -2.217967 |
| H | -7.337216 | 3.882245 | -2.498543 |
| H | -6.163684 | 5.190228 | -2.301258 |
| H | -5.640253 | 3.619413 | -2.931969 |
| C | -6.937740 | 4.387973 | 0.204387 |
| H | -6.789072 | 5.467474 | 0.115965 |
| H | -7.987368 | 4.173826 | -0.007955 |
| H | -6.729379 | 4.094687 | 1.236027 |
| C | -4.546379 | 4.038264 | -0.437361 |
| H | -4.285162 | 3.754294 | 0.585361 |
| H | -3.834639 | 3.565731 | -1.119318 |
| H | -4.428915 | 5.120398 | -0.527469 |

**Table S#.** Cartesian coordinates for **4**+⦁: E0PT. (-2086.31247864 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | 1.604844 | 0.342192 | 1.143316 |
| C | 0.532362 | 1.214834 | 0.830867 |
| C | 0.703427 | 2.590103 | 0.690696 |
| C | 1.995276 | 3.087488 | 0.871799 |
| C | 3.072571 | 2.246059 | 1.181922 |
| C | 2.904490 | 0.862822 | 1.323041 |
| C | -0.153020 | -0.893168 | 0.964898 |
| H | -0.127128 | 3.241678 | 0.449200 |
| H | 2.171002 | 4.151587 | 0.769096 |
| H | 4.063571 | 2.661969 | 1.313863 |
| C | -2.452560 | -1.800755 | 0.626472 |
| C | -3.346813 | -2.903666 | 0.591933 |
| C | -2.932565 | -4.211710 | 0.843294 |
| C | -1.582927 | -4.393911 | 1.137545 |
| C | -0.677271 | -3.319364 | 1.175072 |
| C | -1.085682 | -2.006655 | 0.927679 |
| C | -4.394612 | -1.002596 | 0.123099 |
| H | -3.625716 | -5.042896 | 0.812812 |
| H | -1.215250 | -5.392741 | 1.339843 |
| H | 0.365280 | -3.502932 | 1.401743 |
| N | -0.566337 | 0.391091 | 0.729067 |
| C | -6.822926 | -0.611006 | -0.478253 |
| C | -5.468898 | -0.097712 | -0.232200 |
| C | -5.199856 | 1.260589 | -0.341423 |
| C | -6.197082 | 2.172494 | -0.697280 |
| C | -7.507509 | 1.679690 | -0.955856 |
| C | -7.857801 | 0.354730 | -0.867917 |
| H | -4.191491 | 1.596592 | -0.145931 |
| H | -8.262195 | 2.399393 | -1.239901 |
| C | -5.934537 | 3.669095 | -0.819181 |
| C | -9.272198 | -0.134051 | -1.175052 |
| O | -7.074293 | -1.840216 | -0.361922 |
| N | -3.123466 | -0.636554 | 0.334467 |
| N | -4.563330 | -2.353152 | 0.271485 |
| N | 1.154485 | -0.961280 | 1.220378 |
| C | 4.016652 | -0.010783 | 1.640127 |
| N | 3.858344 | -1.364953 | 1.743326 |
| N | 5.284920 | 0.363604 | 1.858379 |
| C | 7.330595 | -0.998773 | 2.407874 |
| C | 7.769664 | -2.320286 | 2.614394 |
| C | 6.885358 | -3.399416 | 2.540184 |
| C | 5.527168 | -3.216551 | 2.251387 |
| C | 5.086270 | -1.913868 | 2.042226 |
| C | 5.962174 | -0.802679 | 2.109382 |
| H | 8.815440 | -2.495229 | 2.838255 |
| H | 7.259304 | -4.401487 | 2.708227 |
| H | 4.848180 | -4.058293 | 2.196119 |
| C | 8.244206 | 0.098278 | 2.507746 |
| H | 9.284985 | -0.098539 | 2.737241 |
| N | 7.877901 | 1.333460 | 2.346072 |
| C | 8.722076 | 2.534033 | 2.434866 |
| C | 10.191668 | 2.225119 | 2.705817 |
| C | 8.543776 | 3.364325 | 1.156961 |
| H | 8.320742 | 3.110005 | 3.276647 |
| C | 10.986705 | 3.533889 | 2.809170 |
| H | 10.590503 | 1.617522 | 1.884335 |
| H | 10.296919 | 1.647068 | 3.628650 |
| C | 9.339986 | 4.669398 | 1.260983 |
| H | 8.900378 | 2.773708 | 0.306185 |
| H | 7.480873 | 3.568555 | 0.996060 |
| C | 10.819358 | 4.394506 | 1.552111 |
| H | 12.041962 | 3.303938 | 2.978772 |
| H | 10.638626 | 4.094908 | 3.684367 |
| H | 9.229810 | 5.238573 | 0.333939 |
| H | 8.918458 | 5.283668 | 2.065724 |
| H | 11.363823 | 5.336438 | 1.665915 |
| H | 11.261917 | 3.869178 | 0.697063 |
| H | 6.882607 | 1.479253 | 2.125144 |
| H | 2.951443 | -1.814538 | 1.613233 |
| H | -1.535219 | 0.619805 | 0.512439 |
| H | -5.472586 | -2.784224 | 0.135154 |
| C | -9.222821 | -1.135623 | -2.351643 |
| H | -8.637116 | -2.015340 | -2.088960 |
| H | -10.238684 | -1.451451 | -2.605930 |
| H | -8.779722 | -0.667146 | -3.234709 |
| C | -6.243692 | 4.112844 | -2.266081 |
| H | -7.277642 | 3.895225 | -2.542983 |
| H | -6.088388 | 5.190868 | -2.360042 |
| H | -5.584515 | 3.607600 | -2.976145 |
| C | -10.199857 | 1.023152 | -1.574367 |
| H | -10.297025 | 1.762136 | -0.773983 |
| H | -9.848782 | 1.536759 | -2.473296 |
| H | -11.194084 | 0.622529 | -1.783322 |
| C | -9.875250 | -0.817127 | 0.072390 |
| H | -9.280519 | -1.677040 | 0.376339 |
| H | -9.926793 | -0.113510 | 0.907691 |
| H | -10.891942 | -1.151921 | -0.151907 |
| C | -6.865428 | 4.424080 | 0.155179 |
| H | -6.704131 | 5.500610 | 0.053790 |
| H | -7.918478 | 4.220657 | -0.050627 |
| H | -6.656813 | 4.140181 | 1.189476 |
| C | -4.481145 | 4.035590 | -0.488424 |
| H | -4.221109 | 3.757044 | 0.536099 |
| H | -3.777356 | 3.547957 | -1.167917 |
| H | -4.350227 | 5.115435 | -0.588230 |

**Table S#.** Cartesian coordinates for **1**: neutral. (-1169.54988210 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.471013 | 2.719230 | 0.404467 |
| C | -1.870202 | 2.906417 | 0.296027 |
| C | -2.393723 | 4.196481 | 0.184858 |
| C | -1.495704 | 5.264154 | 0.184021 |
| C | -0.111614 | 5.065418 | 0.297463 |
| C | 0.440692 | 3.783150 | 0.418279 |
| C | -1.520203 | 0.761602 | 0.415033 |
| H | -3.461023 | 4.356807 | 0.094799 |
| H | -1.873611 | 6.275398 | 0.091861 |
| H | 0.535348 | 5.934541 | 0.275421 |
| N | -2.493061 | 1.668373 | 0.309223 |
| C | -3.064558 | -1.180883 | 0.359005 |
| C | -1.740478 | -0.674759 | 0.437918 |
| C | -0.656527 | -1.560914 | 0.512119 |
| C | -0.842709 | -2.937533 | 0.512881 |
| C | -2.162572 | -3.407603 | 0.441611 |
| C | -3.284265 | -2.577537 | 0.367178 |
| H | 0.349407 | -1.160354 | 0.564120 |
| H | -2.324358 | -4.474191 | 0.443043 |
| C | 0.372067 | -3.870485 | 0.562377 |
| C | -4.703466 | -3.164133 | 0.294389 |
| O | -4.120509 | -0.340363 | 0.274156 |
| H | -3.773508 | 0.597669 | 0.268360 |
| N | -0.287037 | 1.359615 | 0.480757 |
| H | 0.631217 | 0.939665 | 0.537028 |
| C | 1.888924 | 3.472959 | 0.551452 |
| C | 1.236211 | -3.630258 | -0.692437 |
| H | 1.560530 | -2.588531 | -0.751958 |
| H | 2.128127 | -4.263454 | -0.667599 |
| H | 0.676152 | -3.864086 | -1.601848 |
| C | 1.212889 | -3.557266 | 1.815795 |
| H | 0.634486 | -3.729862 | 2.727402 |
| H | 2.098218 | -4.199146 | 1.845727 |
| H | 1.550258 | -2.517789 | 1.818098 |
| C | -0.032944 | -5.350114 | 0.602283 |
| H | -0.630636 | -5.581040 | 1.488274 |
| H | -0.607251 | -5.635205 | -0.283545 |
| H | 0.864667 | -5.972723 | 0.632625 |
| C | -5.382271 | -2.736305 | -1.023974 |
| H | -6.394280 | -3.149723 | -1.070858 |
| H | -5.446118 | -1.652031 | -1.105040 |
| H | -4.821026 | -3.115547 | -1.882644 |
| C | -5.536110 | -2.677154 | 1.499787 |
| H | -5.637656 | -1.592723 | 1.500692 |
| H | -6.535677 | -3.120853 | 1.465186 |
| H | -5.061653 | -2.980695 | 2.437132 |
| C | -4.687461 | -4.701279 | 0.330629 |
| H | -4.135209 | -5.121203 | -0.514251 |
| H | -4.241050 | -5.081316 | 1.253410 |
| H | -5.714901 | -5.069031 | 0.276888 |
| O | 2.289504 | 2.296552 | 0.528805 |
| N | 2.746838 | 4.509291 | 0.681735 |
| H | 2.432542 | 5.446434 | 0.872382 |
| H | 3.716352 | 4.293268 | 0.856797 |

**Table S#.** Cartesian coordinates for **1**+⦁: E0PT. (-1169.35039383 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.460429 | 2.735524 | 0.446323 |
| C | -1.869382 | 2.860977 | 0.319118 |
| C | -2.459229 | 4.128065 | 0.212125 |
| C | -1.611824 | 5.226396 | 0.239777 |
| C | -0.212951 | 5.087825 | 0.366657 |
| C | 0.403475 | 3.841091 | 0.470839 |
| C | -1.402163 | 0.736962 | 0.439368 |
| H | -3.531181 | 4.239010 | 0.111285 |
| H | -2.027979 | 6.223212 | 0.162848 |
| H | 0.385151 | 5.990745 | 0.386241 |
| N | -2.418292 | 1.600557 | 0.320075 |
| C | -2.981818 | -1.178361 | 0.350491 |
| C | -1.610148 | -0.691346 | 0.456400 |
| C | -0.575082 | -1.600797 | 0.544414 |
| C | -0.825097 | -2.986204 | 0.536308 |
| C | -2.167945 | -3.436468 | 0.442228 |
| C | -3.256643 | -2.596661 | 0.352899 |
| H | 0.445286 | -1.247657 | 0.614561 |
| H | -2.340147 | -4.499892 | 0.440207 |
| C | 0.344584 | -3.953435 | 0.600540 |
| C | -4.687489 | -3.124153 | 0.253743 |
| O | -3.964111 | -0.334742 | 0.243709 |
| H | -3.574839 | 0.649737 | 0.249351 |
| N | -0.206714 | 1.390931 | 0.521192 |
| H | 0.737656 | 1.034509 | 0.618380 |
| C | 1.868559 | 3.589189 | 0.592765 |
| C | 1.231363 | -3.712792 | -0.644456 |
| H | 1.598602 | -2.685387 | -0.680988 |
| H | 2.093341 | -4.383355 | -0.604857 |
| H | 0.677092 | -3.916211 | -1.563499 |
| C | 1.171921 | -3.665528 | 1.874069 |
| H | 0.573104 | -3.825687 | 2.773318 |
| H | 2.026535 | -4.345768 | 1.903068 |
| H | 1.553789 | -2.642931 | 1.888956 |
| C | -0.099791 | -5.421726 | 0.620714 |
| H | -0.717561 | -5.645628 | 1.494086 |
| H | -0.657753 | -5.688837 | -0.280284 |
| H | 0.785206 | -6.059173 | 0.665662 |
| C | -5.318263 | -2.681336 | -1.086270 |
| H | -6.327499 | -3.094501 | -1.155508 |
| H | -5.385280 | -1.597440 | -1.168956 |
| H | -4.736228 | -3.061420 | -1.929323 |
| C | -5.525635 | -2.591310 | 1.438599 |
| H | -5.615198 | -1.506346 | 1.416330 |
| H | -6.528499 | -3.022147 | 1.386748 |
| H | -5.075468 | -2.885194 | 2.389897 |
| C | -4.714164 | -4.660198 | 0.305642 |
| H | -4.159200 | -5.104099 | -0.524841 |
| H | -4.298834 | -5.039954 | 1.242534 |
| H | -5.750160 | -4.996818 | 0.235438 |
| O | 2.292593 | 2.425831 | 0.702111 |
| N | 2.693045 | 4.653346 | 0.587151 |
| H | 2.374103 | 5.593269 | 0.419829 |
| H | 3.687634 | 4.487257 | 0.620327 |

**Table S#.** Cartesian coordinates for **1**+⦁: E0PT. (-1169.36621356 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.484912 | 2.742772 | 0.431986 |
| C | -1.873615 | 2.958505 | 0.377560 |
| C | -2.407400 | 4.244916 | 0.313207 |
| C | -1.494219 | 5.295135 | 0.310520 |
| C | -0.105210 | 5.077738 | 0.365757 |
| C | 0.440471 | 3.794168 | 0.426227 |
| C | -1.494794 | 0.753089 | 0.449032 |
| H | -3.474761 | 4.413493 | 0.265328 |
| H | -1.861289 | 6.312502 | 0.262797 |
| H | 0.545778 | 5.943262 | 0.358718 |
| N | -2.450222 | 1.700633 | 0.391313 |
| C | -3.104629 | -1.173812 | 0.357770 |
| C | -1.725783 | -0.672873 | 0.464089 |
| C | -0.665956 | -1.549334 | 0.558846 |
| C | -0.865644 | -2.947302 | 0.549275 |
| C | -2.183024 | -3.438874 | 0.440318 |
| C | -3.299036 | -2.628504 | 0.344932 |
| H | 0.345933 | -1.173525 | 0.643605 |
| H | -2.322353 | -4.508179 | 0.430390 |
| C | 0.348050 | -3.861854 | 0.631814 |
| C | -4.706659 | -3.204895 | 0.227827 |
| O | -4.068744 | -0.371888 | 0.277269 |
| N | -0.297941 | 1.377500 | 0.476550 |
| H | 0.637868 | 0.982793 | 0.501224 |
| C | 1.892365 | 3.449439 | 0.467721 |
| C | 1.249708 | -3.576758 | -0.591131 |
| H | 1.571246 | -2.533177 | -0.615556 |
| H | 2.141524 | -4.206507 | -0.540391 |
| H | 0.723394 | -3.798850 | -1.522615 |
| C | 1.133478 | -3.548135 | 1.924328 |
| H | 0.522163 | -3.738580 | 2.809199 |
| H | 2.015964 | -4.190695 | 1.971533 |
| H | 1.471129 | -2.509821 | 1.954257 |
| C | -0.033123 | -5.347717 | 0.634362 |
| H | -0.652697 | -5.604809 | 1.497423 |
| H | -0.569567 | -5.627956 | -0.275591 |
| H | 0.876564 | -5.949484 | 0.684424 |
| C | -5.342845 | -2.753034 | -1.106920 |
| H | -6.347552 | -3.176435 | -1.185453 |
| H | -5.415974 | -1.668339 | -1.167626 |
| H | -4.755234 | -3.114080 | -1.955050 |
| C | -5.567222 | -2.714196 | 1.414945 |
| H | -5.677713 | -1.631497 | 1.398964 |
| H | -6.558433 | -3.171339 | 1.354851 |
| H | -5.112694 | -3.005752 | 2.365393 |
| C | -4.693771 | -4.741435 | 0.250824 |
| H | -4.121201 | -5.155633 | -0.583038 |
| H | -4.276886 | -5.129740 | 1.183614 |
| H | -5.720329 | -5.103372 | 0.165284 |
| O | 2.245992 | 2.257998 | 0.501391 |
| N | 2.775117 | 4.462561 | 0.467213 |
| H | 2.500896 | 5.430215 | 0.421799 |
| H | 3.759522 | 4.243189 | 0.480774 |
| H | -3.430014 | 1.422387 | 0.352680 |

**Table S#.** Cartesian coordinates for **1**+⦁: E0PT. (-1169.35567448 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.527014 | 2.714588 | 0.427516 |
| C | -1.909055 | 2.974525 | 0.291997 |
| C | -2.394626 | 4.274071 | 0.180270 |
| C | -1.453489 | 5.308416 | 0.206050 |
| C | -0.079948 | 5.067957 | 0.344054 |
| C | 0.414124 | 3.761689 | 0.462404 |
| C | -1.505324 | 0.789626 | 0.416936 |
| H | -3.452029 | 4.478784 | 0.071821 |
| H | -1.796353 | 6.331300 | 0.117990 |
| H | 0.594180 | 5.915516 | 0.355087 |
| N | -2.490361 | 1.726673 | 0.292805 |
| C | -3.119246 | -1.161314 | 0.336256 |
| C | -1.748567 | -0.640870 | 0.433854 |
| C | -0.677667 | -1.505850 | 0.521103 |
| C | -0.858727 | -2.903849 | 0.524037 |
| C | -2.173186 | -3.414399 | 0.443508 |
| C | -3.298416 | -2.618375 | 0.354005 |
| H | 0.322045 | -1.094590 | 0.580987 |
| H | -2.298893 | -4.485612 | 0.451438 |
| C | 0.366826 | -3.805547 | 0.590679 |
| C | -4.702515 | -3.213817 | 0.274013 |
| O | -4.096245 | -0.373870 | 0.237528 |
| N | -0.296396 | 1.366735 | 0.503430 |
| C | 1.814594 | 3.395675 | 0.621095 |
| C | 1.248233 | -3.515747 | -0.645225 |
| H | 1.553213 | -2.467599 | -0.679165 |
| H | 2.149838 | -4.132485 | -0.604236 |
| H | 0.713217 | -3.749581 | -1.568936 |
| C | 1.168231 | -3.477392 | 1.869023 |
| H | 0.576762 | -3.679859 | 2.764990 |
| H | 2.065985 | -4.099936 | 1.902576 |
| H | 1.481018 | -2.431276 | 1.891175 |
| C | 0.004137 | -5.296029 | 0.602903 |
| H | -0.598207 | -5.558767 | 1.476421 |
| H | -0.544674 | -5.584532 | -0.297177 |
| H | 0.921353 | -5.887654 | 0.638954 |
| C | -5.368251 | -2.804110 | -1.059228 |
| H | -6.367788 | -3.244277 | -1.112485 |
| H | -5.458700 | -1.722329 | -1.142961 |
| H | -4.788652 | -3.174730 | -1.908879 |
| C | -5.549864 | -2.706825 | 1.463678 |
| H | -5.660407 | -1.624206 | 1.434827 |
| H | -6.542340 | -3.163781 | 1.422880 |
| H | -5.084500 | -2.986786 | 2.412439 |
| C | -4.670899 | -4.749397 | 0.334707 |
| H | -4.109725 | -5.177305 | -0.500123 |
| H | -4.227618 | -5.107421 | 1.267530 |
| H | -5.694261 | -5.126489 | 0.280422 |
| O | 2.152359 | 2.137227 | 0.689980 |
| N | 2.789425 | 4.270832 | 0.708043 |
| H | 2.622135 | 5.265214 | 0.684808 |
| H | 3.741021 | 3.946652 | 0.815779 |
| H | -3.465489 | 1.449139 | 0.218568 |
| H | 1.324753 | 1.545401 | 0.629920 |

**Table S#.** Cartesian coordinates for BIP. (-1000.81868882 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.471802 | 2.722723 | 0.443310 |
| C | -1.871767 | 2.899459 | 0.317472 |
| C | -2.408152 | 4.186799 | 0.204121 |
| C | -1.522447 | 5.260833 | 0.218935 |
| C | -0.132853 | 5.068795 | 0.345862 |
| C | 0.419239 | 3.794568 | 0.462094 |
| C | -1.517936 | 0.754492 | 0.440144 |
| H | -3.476711 | 4.333862 | 0.104043 |
| H | -1.909695 | 6.269666 | 0.132042 |
| H | 0.522568 | 5.932132 | 0.353976 |
| N | -2.490260 | 1.658528 | 0.321200 |
| C | -3.063165 | -1.187424 | 0.361181 |
| C | -1.738927 | -0.683865 | 0.458471 |
| C | -0.659758 | -1.574795 | 0.544670 |
| C | -0.849361 | -2.951304 | 0.540640 |
| C | -2.168657 | -3.417812 | 0.448074 |
| C | -3.286212 | -2.583583 | 0.359384 |
| H | 0.348704 | -1.182283 | 0.609838 |
| H | -2.333657 | -4.483886 | 0.443163 |
| C | 0.362442 | -3.887409 | 0.606004 |
| C | -4.705491 | -3.165536 | 0.259631 |
| O | -4.116051 | -0.344182 | 0.266260 |
| H | -3.764876 | 0.593734 | 0.265146 |
| N | -0.287388 | 1.354581 | 0.522300 |
| H | 0.597063 | 0.878639 | 0.609942 |
| C | 1.245627 | -3.645420 | -0.635110 |
| H | 1.574078 | -2.604514 | -0.686049 |
| H | 2.134937 | -4.281753 | -0.600644 |
| H | 0.697174 | -3.873580 | -1.553070 |
| C | 1.184672 | -3.582215 | 1.873652 |
| H | 0.592147 | -3.758562 | 2.775299 |
| H | 2.068169 | -4.226022 | 1.913691 |
| H | 1.524114 | -2.543558 | 1.887937 |
| C | -0.046683 | -5.366238 | 0.635030 |
| H | -0.660111 | -5.597953 | 1.509992 |
| H | -0.606655 | -5.647117 | -0.261186 |
| H | 0.848751 | -5.991159 | 0.678804 |
| C | -5.360351 | -2.728215 | -1.067792 |
| H | -6.374132 | -3.134647 | -1.132489 |
| H | -5.415470 | -1.643224 | -1.146011 |
| H | -4.788099 | -3.108300 | -1.918807 |
| C | -5.556228 | -2.682320 | 1.453634 |
| H | -5.656814 | -1.597940 | 1.456262 |
| H | -6.555381 | -3.125408 | 1.402799 |
| H | -5.095490 | -2.988033 | 2.397197 |
| C | -4.694862 | -4.702893 | 0.287551 |
| H | -4.128631 | -5.120375 | -0.549276 |
| H | -4.267527 | -5.089882 | 1.216460 |
| H | -5.722320 | -5.066982 | 0.212788 |
| H | 1.487330 | 3.644658 | 0.561168 |

**Table S#.** Cartesian coordinates for BIP+⦁: E0PT. (-1000.61974403 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.476280 | 2.748976 | 0.453646 |
| C | -1.889081 | 2.864294 | 0.303522 |
| C | -2.491128 | 4.128114 | 0.187570 |
| C | -1.657085 | 5.231819 | 0.226438 |
| C | -0.253106 | 5.101642 | 0.377442 |
| C | 0.362790 | 3.863798 | 0.495843 |
| C | -1.419161 | 0.741992 | 0.429069 |
| H | -3.563092 | 4.224299 | 0.071725 |
| H | -2.081216 | 6.224891 | 0.139839 |
| H | 0.355168 | 5.997667 | 0.401104 |
| N | -2.434039 | 1.606165 | 0.295295 |
| C | -2.992800 | -1.177100 | 0.341194 |
| C | -1.622599 | -0.683611 | 0.445112 |
| C | -0.581827 | -1.592793 | 0.533476 |
| C | -0.825432 | -2.973480 | 0.532616 |
| C | -2.169266 | -3.428525 | 0.445948 |
| C | -3.261320 | -2.593943 | 0.354705 |
| H | 0.439125 | -1.240279 | 0.596788 |
| H | -2.337787 | -4.492651 | 0.451894 |
| C | 0.348979 | -3.937522 | 0.597883 |
| C | -4.691387 | -3.129229 | 0.265311 |
| O | -3.981241 | -0.338149 | 0.227430 |
| H | -3.600275 | 0.641859 | 0.225932 |
| N | -0.224128 | 1.398929 | 0.530467 |
| H | 0.684995 | 0.975108 | 0.643368 |
| C | 1.231491 | -3.702213 | -0.650575 |
| H | 1.596208 | -2.673912 | -0.693565 |
| H | 2.095444 | -4.370335 | -0.611345 |
| H | 0.675050 | -3.910992 | -1.567145 |
| C | 1.179883 | -3.641011 | 1.866815 |
| H | 0.584410 | -3.796770 | 2.769170 |
| H | 2.036583 | -4.318601 | 1.898112 |
| H | 1.559133 | -2.616989 | 1.874488 |
| C | -0.091521 | -5.406937 | 0.627239 |
| H | -0.705299 | -5.628007 | 1.504145 |
| H | -0.652774 | -5.679742 | -0.270059 |
| H | 0.794959 | -6.042455 | 0.671604 |
| C | -5.329757 | -2.704140 | -1.076357 |
| H | -6.336963 | -3.123657 | -1.138503 |
| H | -5.403743 | -1.621515 | -1.169908 |
| H | -4.748464 | -3.088958 | -1.917817 |
| C | -5.528432 | -2.590090 | 1.447755 |
| H | -5.619299 | -1.505321 | 1.419250 |
| H | -6.531172 | -3.021927 | 1.400923 |
| H | -5.076413 | -2.877862 | 2.400101 |
| C | -4.710093 | -4.664895 | 0.332952 |
| H | -4.157587 | -5.114516 | -0.496146 |
| H | -4.286910 | -5.032486 | 1.271240 |
| H | -5.744695 | -5.007601 | 0.272311 |
| H | 1.434251 | 3.763740 | 0.611435 |

**Table S#.** Cartesian coordinates for BIP+⦁: E0PT. (-1000.63576249 *E*h)

|  |  |  |  |
| --- | --- | --- | --- |
| atom | x | y | z |
| C | -0.466074 | 2.739723 | 0.447772 |
| C | -1.854058 | 2.951118 | 0.319903 |
| C | -2.391934 | 4.233376 | 0.207908 |
| C | -1.486274 | 5.287507 | 0.227501 |
| C | -0.097537 | 5.074589 | 0.356415 |
| C | 0.441142 | 3.798102 | 0.470540 |
| C | -1.489418 | 0.745897 | 0.439084 |
| H | -3.457367 | 4.390739 | 0.106028 |
| H | -1.856717 | 6.301763 | 0.142565 |
| H | 0.566486 | 5.930269 | 0.367596 |
| N | -2.434650 | 1.695174 | 0.321927 |
| C | -3.103708 | -1.179348 | 0.349603 |
| C | -1.723529 | -0.680580 | 0.453203 |
| C | -0.666042 | -1.561581 | 0.538014 |
| C | -0.868526 | -2.958206 | 0.534195 |
| C | -2.188675 | -3.446638 | 0.445185 |
| C | -3.302983 | -2.633758 | 0.356297 |
| H | 0.349360 | -1.191372 | 0.603130 |
| H | -2.330652 | -4.515531 | 0.445347 |
| C | 0.343791 | -3.876337 | 0.600690 |
| C | -4.713453 | -3.208995 | 0.264086 |
| O | -4.064571 | -0.375411 | 0.253487 |
| N | -0.291768 | 1.366395 | 0.521904 |
| H | 0.595822 | 0.891890 | 0.609864 |
| C | 1.226697 | -3.601069 | -0.638167 |
| H | 1.551270 | -2.558835 | -0.674797 |
| H | 2.117380 | -4.233133 | -0.597240 |
| H | 0.685984 | -3.827008 | -1.560316 |
| C | 1.152204 | -3.560219 | 1.878360 |
| H | 0.556678 | -3.747504 | 2.774723 |
| H | 2.035294 | -4.202976 | 1.912131 |
| H | 1.491157 | -2.522096 | 1.899602 |
| C | -0.042479 | -5.360738 | 0.615579 |
| H | -0.649384 | -5.611748 | 1.489266 |
| H | -0.593772 | -5.643320 | -0.284788 |
| H | 0.865794 | -5.965453 | 0.654552 |
| C | -5.364450 | -2.780987 | -1.071188 |
| H | -6.367107 | -3.212023 | -1.134012 |
| H | -5.445635 | -1.697917 | -1.147513 |
| H | -4.782326 | -3.150539 | -1.919403 |
| C | -5.560336 | -2.696954 | 1.452165 |
| H | -5.663498 | -1.613622 | 1.424783 |
| H | -6.555431 | -3.147082 | 1.405798 |
| H | -5.100567 | -2.981869 | 2.402035 |
| C | -4.702021 | -4.745308 | 0.314682 |
| H | -4.140924 | -5.175143 | -0.519130 |
| H | -4.271843 | -5.116172 | 1.248558 |
| H | -5.729839 | -5.107860 | 0.249878 |
| H | 1.505306 | 3.630573 | 0.571254 |
| H | -3.413478 | 1.421064 | 0.249207 |

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