Electronic Supplementary Material (ESI) for Dalton Transactions.


# Supporting Information

# Theoretical Investigations on P-stabilized Boryl Cation Radicals: From Aufbau Principle to SOMO-HOMO Conversion

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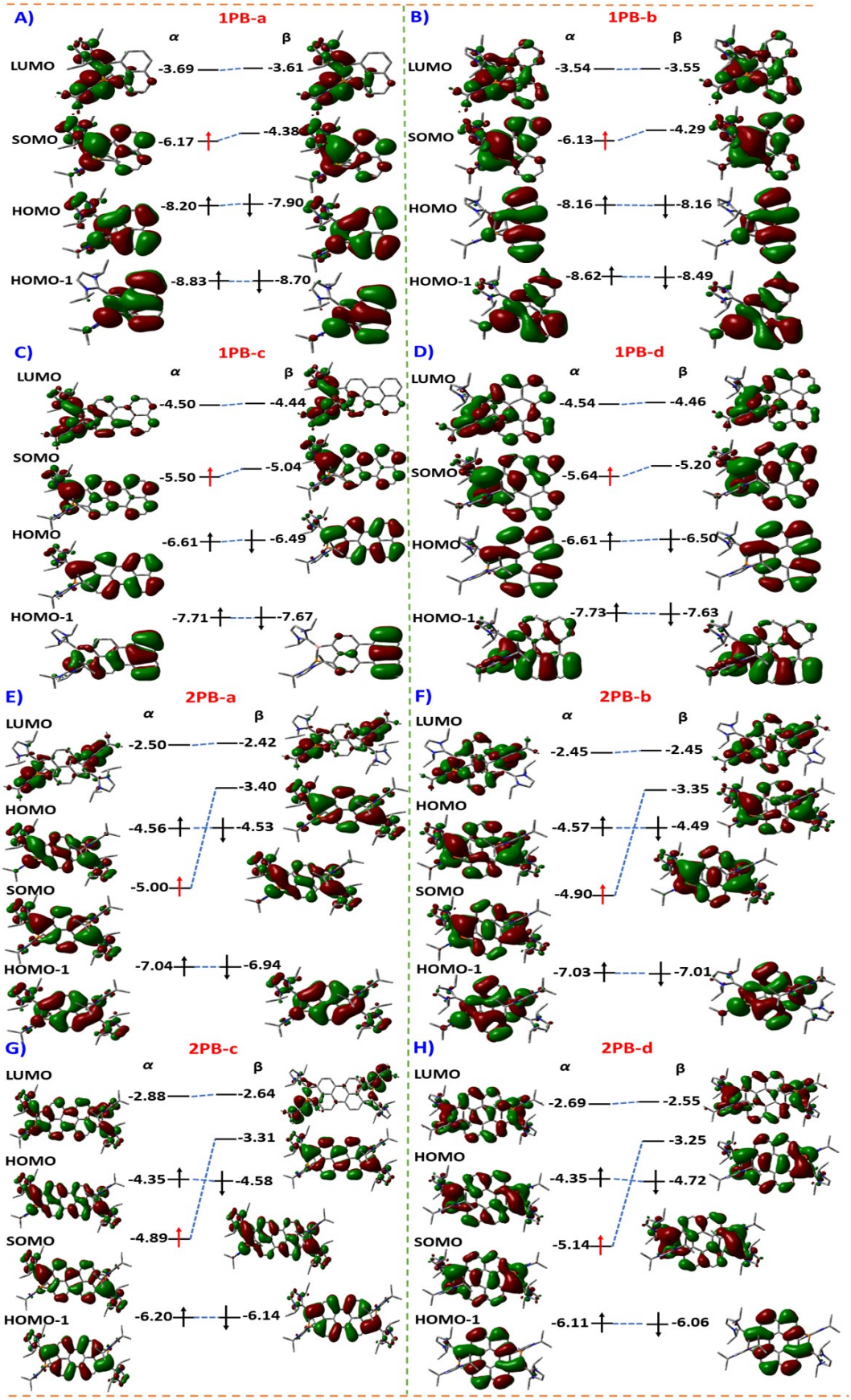



**Figure S1**. Orbital energies (in eV) and isosurfaces (±0.02 a.u.) for the studied compounds at UB3LYP-D3/6-31G(d) level.

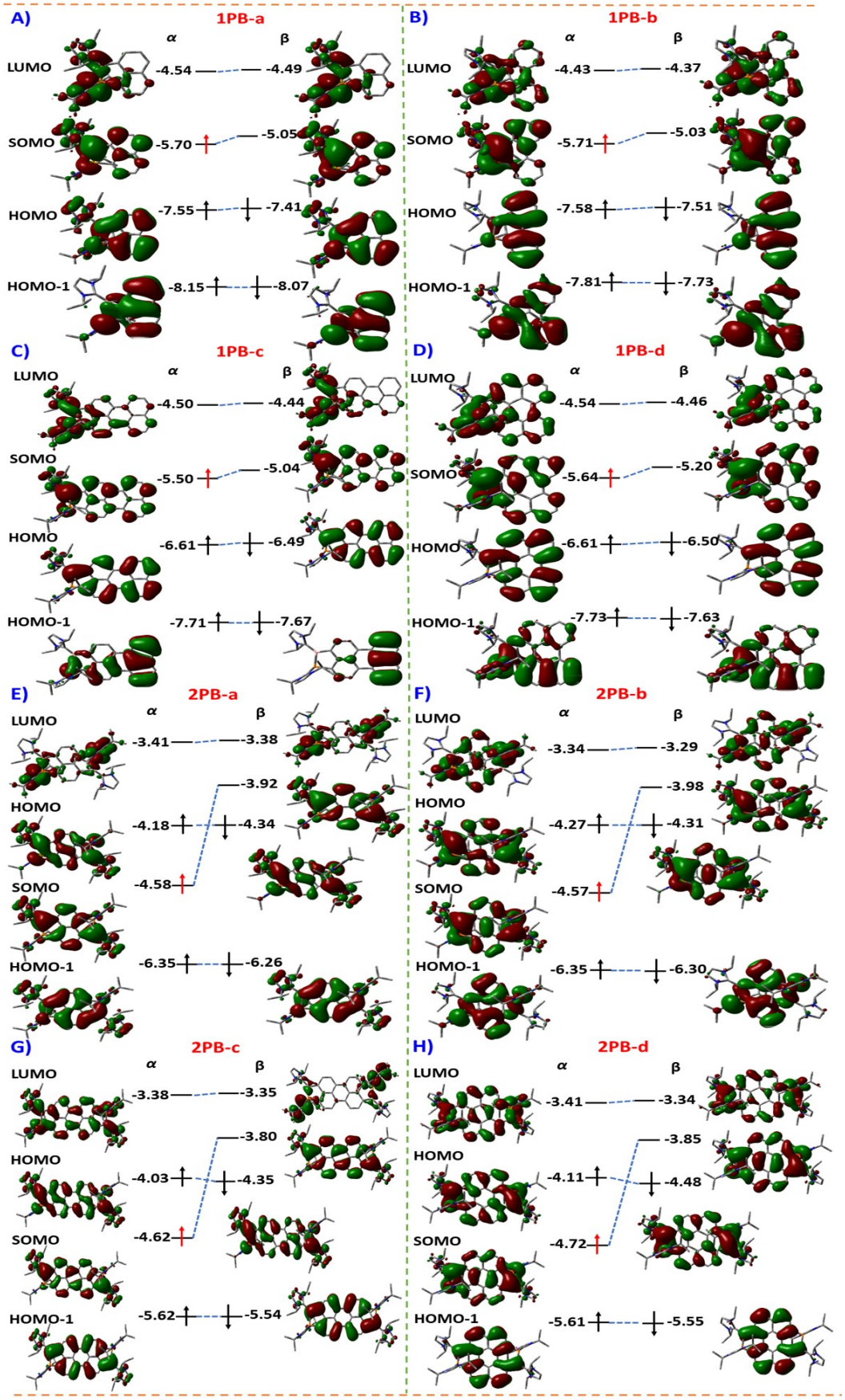



**Figure S2**. Orbital energies (in eV) and isosurfaces (±0.02 a.u.) for the studied compounds at UBP86/6-31G(d) level.

**Table S1** NBO analysis data of the studied compounds from **1PB-a** to **1PB-d** on the basis of UB3LYP/6-31G(d) level.

| | **1PB-a** | **1PB-b** | **1PB-c** | **1PB-d** |
|---|---|---|---|---|
| $d_{(P\text{-}B)}$/Å | 1.96 | 1.91 | 1.96 | 1.90 |
| Occ.$(LP_P)$[a] | 0.93 | 0.92 | 0.93 | 0.91 |
| Occ.$(LP^*_B)$[a] | 0.14 | 0.13 | 0.18 | 0.18 |
| Occ.$(\sigma_{P\text{-}C})$[a] | 0.98 | 0.98 | 0.98 | 0.97 |
| Occ.$(\sigma_{B\text{-}C})$[a] | 0.98 | 0.98 | 0.98 | 0.98 |
| Occ.$(\sigma_{P\text{-}B})$[a] | 0.96 | 0.97 | 0.96 | 0.97 |
| Polarization%[b] | 56.33(P) | 55.27(P) | 56.11(P) | 54.44(P) |
| $(\sigma_{P\text{-}B})$ | 43.67(B) | 44.73(B) | 43.89(B) | 45.56(B) |
| Hybridisation[c] | $sp^{3.50}d^{0.01}$ | $sp^{2.95}d^{0.01}$ | $sp^{3.52}d^{0.01}$ | $sp^{3.06}d^{0.01}$ |
| $(\sigma_{P\text{-}B})$ | $sp^{2.37}d^{0.00}$ | $sp^{2.12}d^{0.00}$ | $sp^{2.39}d^{0.00}$ | $sp^{2.13}d^{0.00}$ |
| $E(2)$[d] $(LP_P \rightarrow LP^*_B)$ | 3.77 | 3.73 | 3.75 | 4.83 |
| $E(2)$[d] $(LP^*_B \rightarrow \sigma^*_{P\text{-}C})$ | 2.15 | 2.64 | 2.52 | 3.04 |

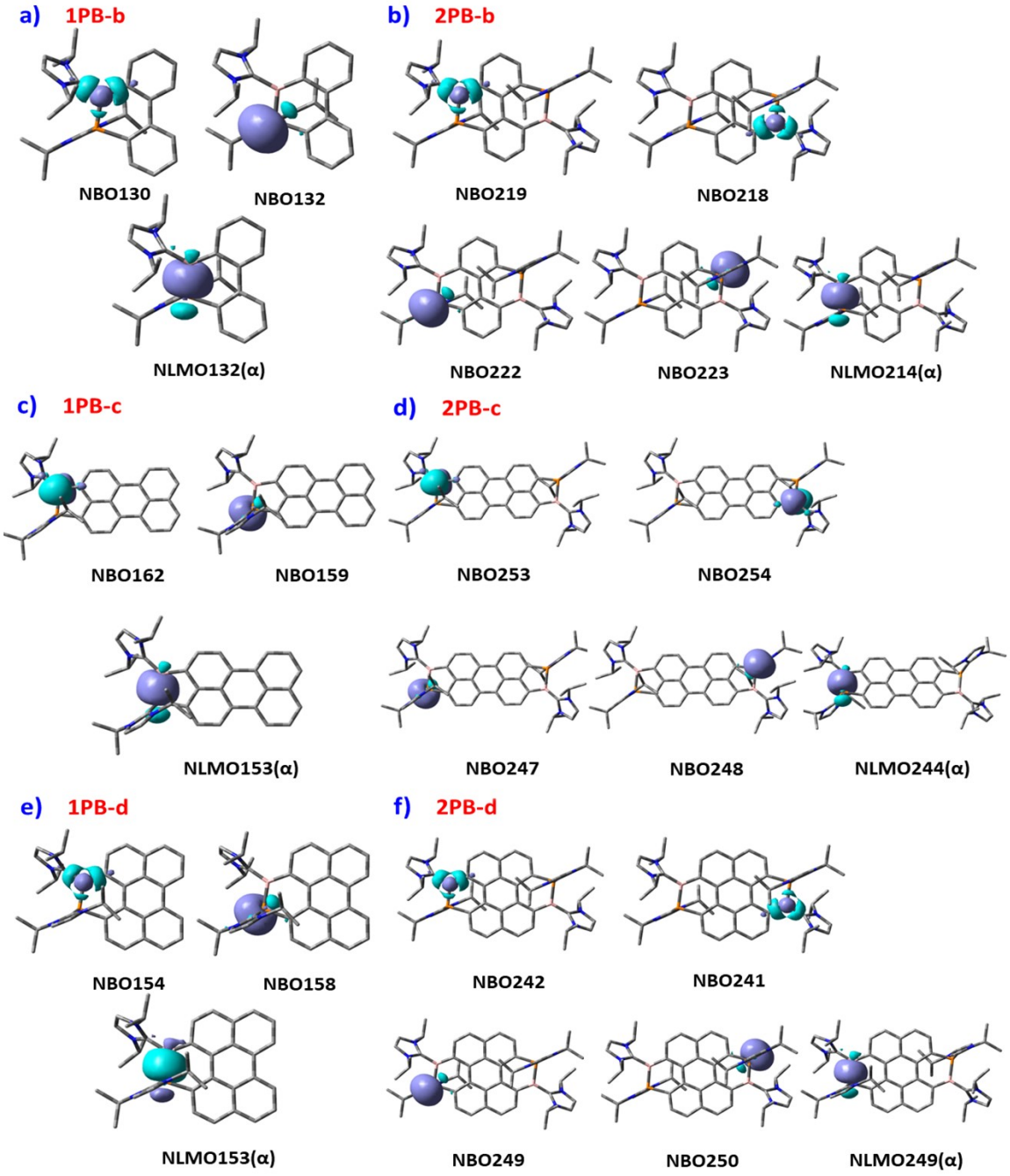



**Figure S3.** Calculated NBOs and NLMOs that show the $LP_P$ and the localized $LP_B$* in the studied compounds.

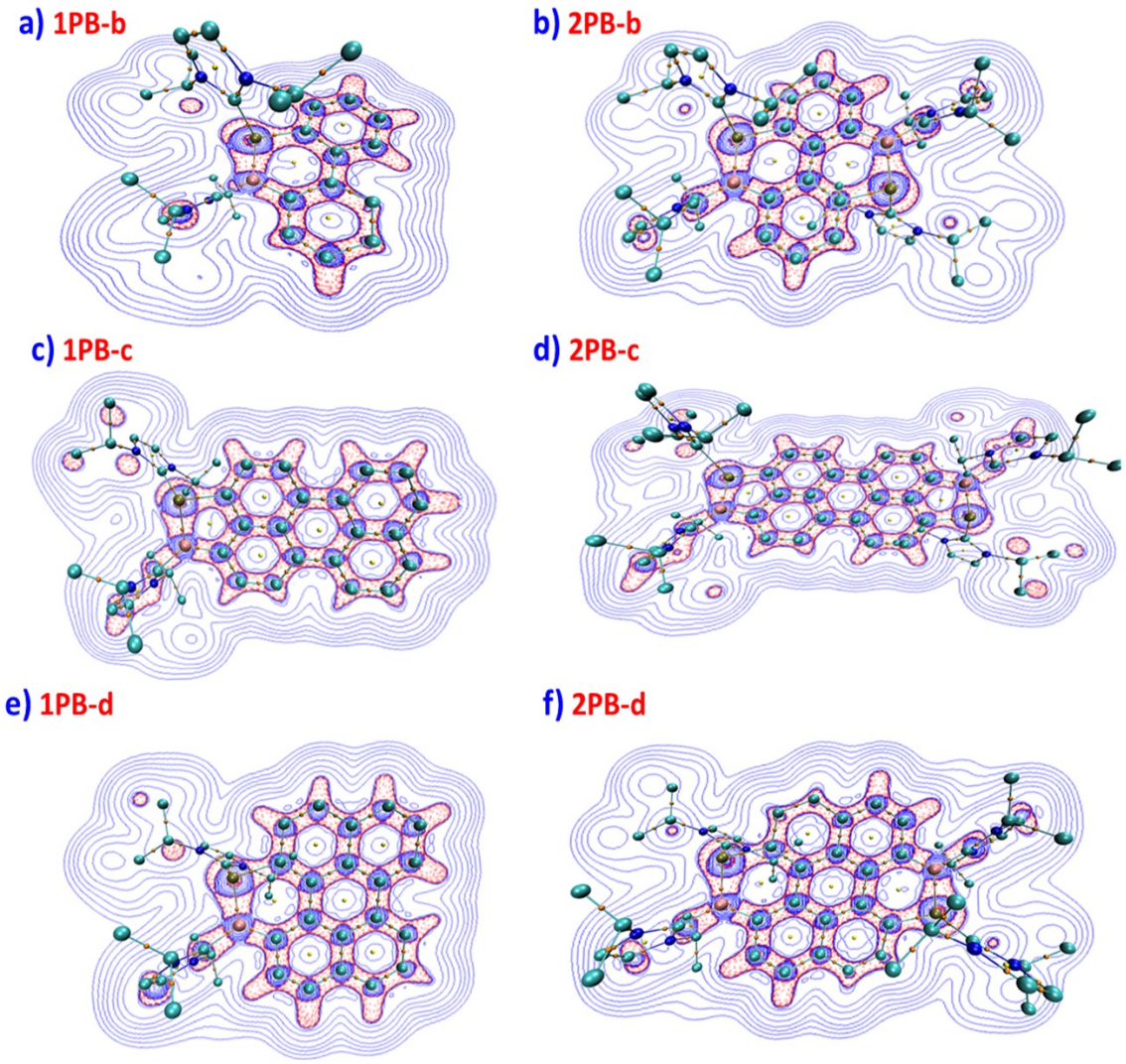



**Figure S4.** Plot of the Laplacian $\nabla^2\rho(r)$ and critical points in the plane containing P and B atoms at the UB3LYP/6-31G(d) level of theory. Red dashed lines indicate areas of charge concentration ($\nabla^2\rho(r)<0$) while solid blue lines show areas of charge depletion ($\nabla^2\rho(r)>0$). Orange dots are bond critical points, yellow dots are ring critical points.

**Table S2** Calculated excited wavelengths (λ), oscillator strengths (*f*) and the transition nature of the selected transitions of studied compounds at TD-DFT//UB3LYP/6-31G(d) level.

| Compounds | Excited state | Wavelength/nm | *f* | Transition nature | |
|---|---|---|---|---|---|
| **1PB-a** | $S_1$ | 692.2 | 0.06 | SOMO(*α*)→LUMO(*α*) | 94% |
| | $S_5$ | 439.7 | 0.14 | HOMO(*β*)→SUMO(*β*) | 66% |
| **1PB-b** | $S_1$ | 676.5 | 0.02 | SOMO(*α*)→LUMO(*α*) | 99% |
| | $S_3$ | 500.8 | 0.04 | HOMO(*α*)→LUMO+3(*α*) | 72% |
| | $S_5$ | 415.3 | 0.04 | HOMO(*β*)→SUMO(*β*) | 57% |
| | $S_{12}$ | 322.7 | 0.12 | HOMO-2(*β*)→SUMO(*β*) | 50% |
| **1PB-c** | $S_1$ | 983.0 | 0.10 | SOMO(*α*)→LUMO(*α*) | 86% |
| | $S_3$ | 612.5 | 0.04 | SOMO(*α*)→LUMO+1(*α*) | 94% |
| | $S_5$ | 496.1 | 0.17 | SOMO(*α*)→LUMO+2(*α*) | 69% |
| | $S_6$ | 480.8 | 0.15 | SOMO(*α*)→LUMO+3(*α*) | 81% |
| | $S_{10}$ | 396.9 | 0.10 | HOMO-1(*β*)→SUMO(*β*) | 57% |

| | | | | | |
|---|---|---|---|---|---|
| | $S_{27}$ | 304.3 | 0.09 | HOMO-1(*β*)→LUMO(*β*) | 36% |
| **1PB-d** | $S_1$ | 890.0 | 0.04 | SOMO(*α*)→LUMO(*α*) | 82% |
| | $S_2$ | 690.4 | 0.11 | HOMO(*β*)→SUMO(*β*) | 69% |
| | $S_8$ | 428.1 | 0.05 | HOMO-1(*β*)→SUMO(*β*) | 70% |
| | $S_{10}$ | 395.2 | 0.11 | HOMO(*β*)→LUMO(*β*) | 34% |
| | | | | HOMO(*α*)→LUMO(*α*) | 22% |
| | | | | SOMO(*α*)→LUMO+6(*α*) | 22% |
| | $S_{16}$ | 346.6 | 0.19 | HOMO-5(*β*)→SUMO(*β*) | 17% |
| | | | | HOMO-2(*β*)→SUMO(*β*) | 17% |
| | | | | HOMO-4(*β*)→SUMO(*β*) | 12% |
| **2PB-a** | $S_1$ | 2339.7 | 0.08 | HOMO(*β*)→SUMO(*β*) | 96% |
| | $S_3$ | 852.1 | 0.20 | HOMO(*α*)→LUMO(*α*) | 91% |
| | $S_6$ | 748.3 | 0.16 | HOMO(*α*)→LUMO+2(*α*) | 53% |
| | | | | HOMO(*β*)→LUMO(*β*) | 44% |
| | $S_{15}$ | 454.4 | 0.44 | SOMO(*α*)→LUMO+3(*α*) | 53% |
| | | | | HOMO(*β*)→LUMO+3(*β*) | 27% |
| | $S_{26}$ | 386.5 | 0.19 | HOMO-2(*β*)→SUMO(*β*) | 68% |
| **2PB-b** | $S_1$ | 2641.3 | 0.07 | HOMO(*β*)→SUMO(*β*) | 97% |
| | $S_3$ | 846.4 | 0.09 | HOMO(*α*)→LUMO(*α*) | 95% |
| | $S_9$ | 612.1 | 0.08 | HOMO(*α*)→LUMO+2(*α*) | 44% |
| | | | | HOMO(*β*)→LUMO+3(*β*) | 17% |
| | $S_{11}$ | 569.0 | 0.23 | HOMO(*α*)→LUMO+4(*α*) | 46% |
| | | | | HOMO(*β*)→LUMO+4(*β*) | 34% |
| **2PB-c** | $S_1$ | 1779.1 | 0.02 | HOMO(*β*)→SUMO(*β*) | 75% |
| | $S_2$ | 1068.0 | 0.89 | HOMO(*α*)→LUMO(*α*) | 73% |
| | $S_7$ | 661.9 | 0.09 | HOMO(*β*)→LUMO+1(*β*) | 96% |
| | $S_{10}$ | 567.6 | 0.13 | HOMO(*β*)→LUMO+3(*β*) | 81% |
| | $S_{17}$ | 506.9 | 0.09 | HOMO(*β*)→LUMO+4(*β*) | 31% |
| | | | | HOMO(*β*)→LUMO+5(*β*) | 29% |
| | $S_{19}$ | 466.8 | 0.12 | HOMO(*α*)→LUMO+9(*α*) | 49% |
| | | | | SOMO(*α*)→LUMO+3(*α*) | 11% |
| | $S_{20}$ | 456.9 | 0.16 | SOMO(*α*)→LUMO+3(*α*) | 32% |
| | | | | HOMO(*β*)→LUMO+5(*β*) | 21% |
| **2PB-d** | $S_1$ | 1519.6 | 0.06 | HOMO(*β*)→SUMO(*β*) | 74% |
| | $S_2$ | 1010.6 | 0.33 | HOMO(*α*)→LUMO(*α*) | 73% |
| | $S_5$ | 662.3 | 0.07 | HOMO(*α*)→LUMO+2(*α*) | 88% |
| | $S_9$ | 590.2 | 0.12 | HOMO(*α*)→LUMO+4(*α*) | 53% |
| | | | | HOMO(*β*)→LUMO+1(*β*) | 34% |
| | $S_{12}$ | 514.2 | 0.08 | HOMO(*β*)→LUMO+3(*β*) | 76% |
| | $S_{21}$ | 439.0 | 0.06 | SOMO(*α*)→LUMO+3(*α*) | 72% |

**Table S3** Calculated excited wavelengths (λ), oscillator strengths (*f*) and the transition nature of the selected transitions of studied compounds at TD-DFT//U$\omega$B97XD/6-31G(d) level.

| Compounds | Excited state | Wavelength/nm | *f* | Transition nature | |
|---|---|---|---|---|---|
| **1PB-a** | $S_1$ | 597.5 | 0.09 | SOMO(*α*)→LUMO(*α*) | 85% |
| | $S_3$ | 414.7 | 0.09 | SOMO(*α*)→LUMO+2(*α*) | 38% |
| | | | | HOMO(*α*)→LUMO(*α*) | 12% |
| **1PB-b** | $S_1$ | 526.2 | 0.04 | SOMO(*α*)→LUMO(*α*) | 91% |
| | $S_3$ | 432.5 | 0.04 | SOMO(*α*)→LUMO+3(*α*) | 60% |
| | $S_8$ | 320.8 | 0.06 | HOMO(*β*)→SUMO(*β*) | 32% |
| | | | | HOMO-1(*β*)→SUMO(*β*) | 15% |
| **1PB-c** | $S_1$ | 820.4 | 0.12 | SOMO(*α*)→LUMO(*α*) | 79% |
| | S2 | 585.6 | 0.36 | HOMO(*β*)→SUMO(*β*) | 46% |
| | $S_5$ | 413.5 | 0.30 | SOMO(*α*)→LUMO+2(*α*) | 43% |
| | $S_9$ | 348.6 | 0.15 | HOMO(*β*)→LUMO(*β*) | 35% |
| | | | | HOMO(*α*)→LUMO(*α*) | 21% |
| **1PB-d** | $S_1$ | 733.2 | 0.05 | SOMO(*α*)→LUMO(*α*) | 71% |
| | $S_2$ | 621.7 | 0.13 | HOMO(*β*)→SUMO(*β*) | 49% |
| | | | | SOMO(*α*)→LUMO(*α*) | 19% |
| | S3 | 451.4 | 0.09 | HOMO(*α*)→LUMO(*α*) | 24% |
| | | | | HOMO(*β*)→SUMO(*β*) | 20% |
| | S5 | 403.9 | 0.05 | SOMO(*α*)→LUMO+2(*α*) | 65% |
| | $S_{12}$ | 331.2 | 0.21 | SOMO(*α*)→LUMO+6(*α*) | 20% |
| | | | | HOMO-2(*β*)→SUMO(*β*) | 16% |
| **2PB-a** | $S_1$ | 2822.3 | 0.13 | HOMO(*β*)→SUMO(*β*) | 98% |
| | $S_2$ | 718.3 | 0.43 | HOMO(*α*)→LUMO(*α*) | 82% |
| | $S_{13}$ | 405.2 | 0.38 | HOMO(*β*)→LUMO+3(*β*) | 38% |
| | | | | SOMO(*α*)→LUMO+3(*α*) | 24% |
| | | | | HOMO(*α*)→LUMO+7(*α*) | 23% |
| | $S_{18}$ | 341.1 | 0.17 | HOMO-2(*β*)→SUMO(*β*) | 74% |
| **2PB-b** | $S_1$ | 3863.6 | 0.12 | HOMO(*β*)→SUMO(*β*) | 98% |
| | $S_3$ | 637.8 | 0.14 | HOMO(*α*)→LUMO(*α*) | 85% |
| | $S_7$ | 517.5 | 0.06 | HOMO(*β*)→LUMO+1(*β*) | 22% |
| | | | | SOMO(*α*)→LUMO+3(*α*) | 16% |
| | $S_9$ | 500.3 | 0.10 | HOMO(*α*)→LUMO+2(*α*) | 47% |
| | | | | SOMO(*α*)→LUMO+1(*α*) | 12% |
| | $S_{11}$ | 449.9 | 0.10 | HOMO(*β*)→LUMO+3(*β*) | 54% |
| | | | | HOMO(*β*)→LUMO+1(*β*) | 18% |
| **2PB-c** | $S_1$ | 1193.3 | 0.24 | HOMO(*β*)→SUMO(*β*) | 91% |
| | $S_2$ | 977.3 | 0.83 | HOMO(*α*)→LUMO(*α*) | 89% |
| | $S_5$ | 530.9 | 0.33 | HOMO(*β*)→LUMO+3(*β*) | 37% |
| | | | | HOMO(*β*)→LUMO+1(*β*) | 22% |
| | $S_6$ | 520.6 | 0.17 | HOMO(*α*)→LUMO+2(*α*) | 39% |
| | | | | HOMO(*β*)→LUMO+3(*β*) | 22% |
| | $S_{15}$ | 399.7 | 0.09 | HOMO(*β*)→LUMO+1(*β*) | 32% |

| | | | | | |
|---|---|---|---|---|---|
| | | | | HOMO(*β*)→LUMO+3(*β*) | 22% |
| | $S_{21}$ | 328.0 | 0.27 | HOMO-2(*β*)→SUMO(*β*) | 40% |
| | | | | HOMO-3(*β*)→LUMO(*β*) | 14% |
| **2PB-d** | $S_1$ | 1294.2 | 0.21 | HOMO(*β*)→SUMO(*β*) | 93% |
| | $S_2$ | 848.0 | 0.30 | HOMO(*α*)→LUMO(*α*) | 86% |
| | $S_5$ | 504.4 | 0.08 | HOMO(*α*)→LUMO+4(*α*) | 28% |
| | | | | HOMO(*α*)→LUMO+2(*α*) | 24% |
| | $S_8$ | 483.6 | 0.17 | HOMO(*α*)→LUMO+4(*α*) | 38% |
| | | | | HOMO(*β*)→LUMO+1(*β*) | 26% |
| | $S_{17}$ | 373.2 | 0.21 | HOMO(*β*)→LUMO+6(*β*) | 35% |
| | | | | HOMO(*β*)→LUMO+4(*β*) | 12% |
| | $S_{19}$ | 360.2 | 0.17 | HOMO(*β*)→LUMO+4(*β*) | 31% |
| | | | | HOMO(*β*)→LUMO+3(*β*) | 12% |

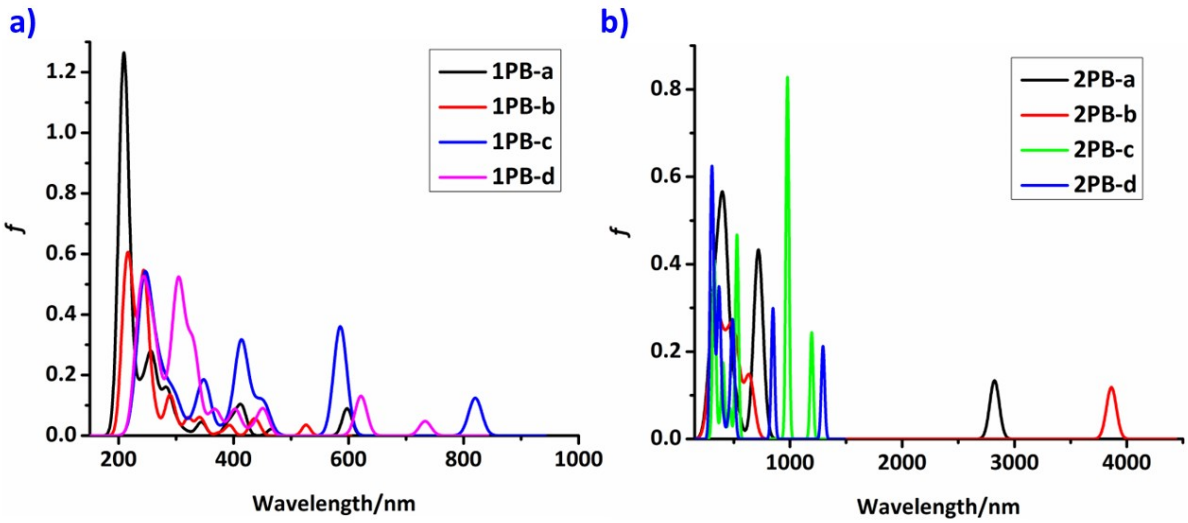
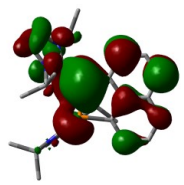
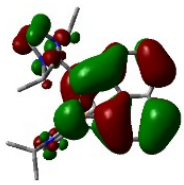
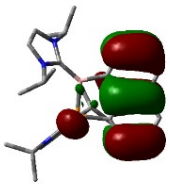
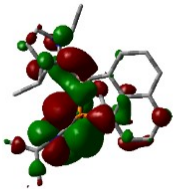
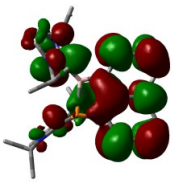
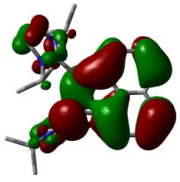
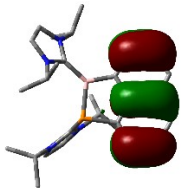
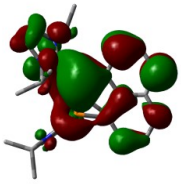
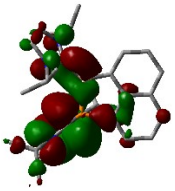
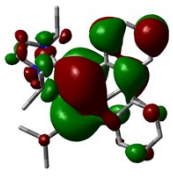
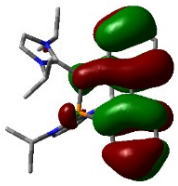
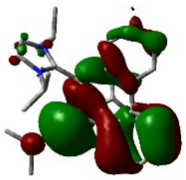
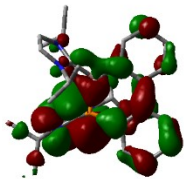
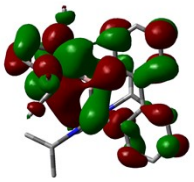
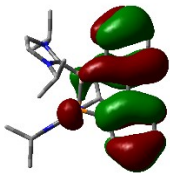
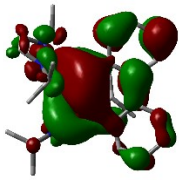
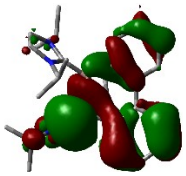
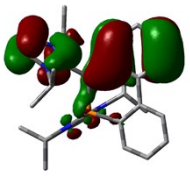
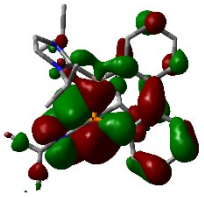
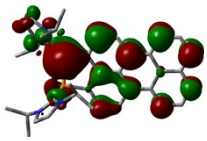
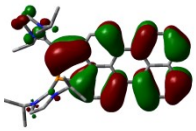
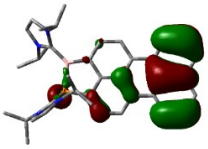
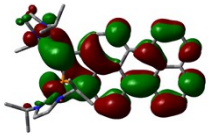
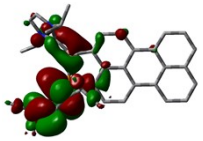
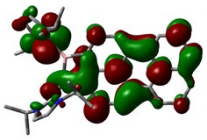
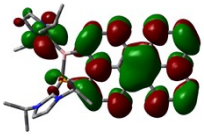
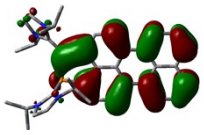
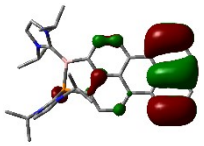
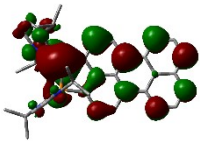
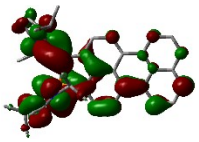
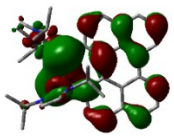
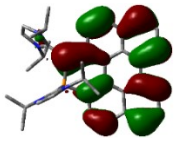
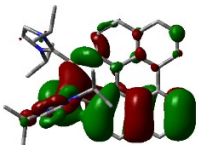
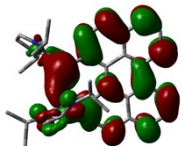
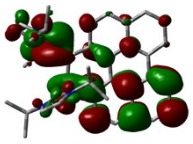
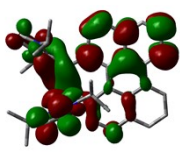
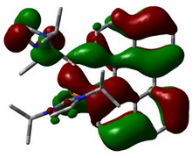
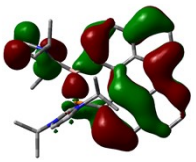
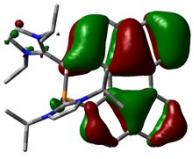
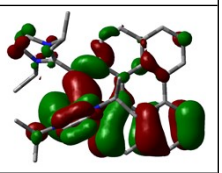
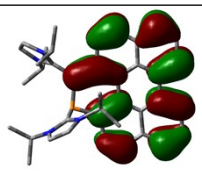
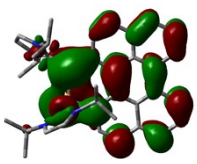
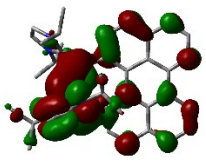
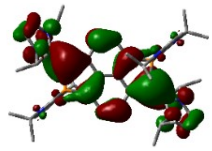
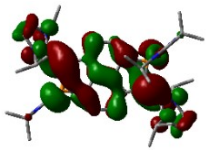
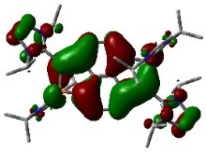
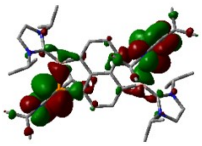
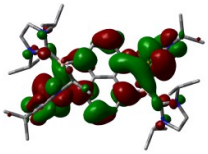
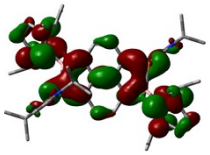
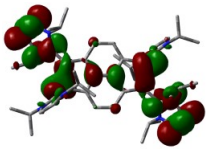
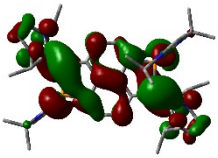
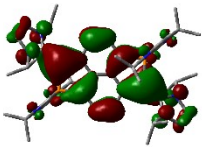
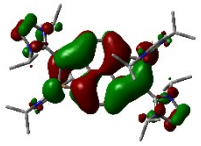
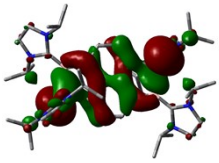
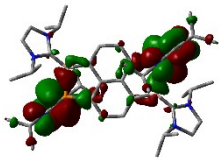
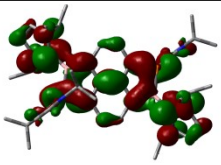
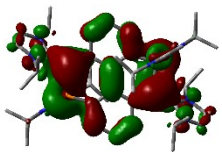
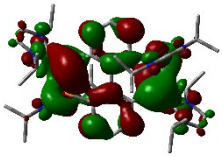
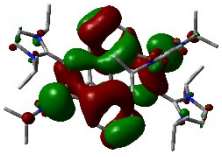
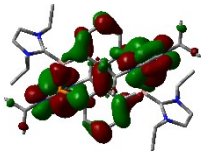
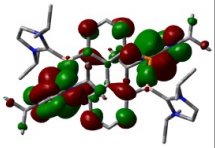
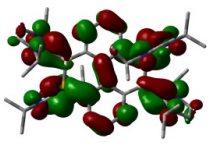
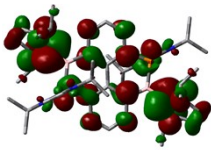
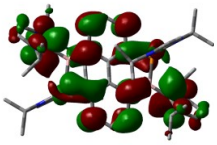
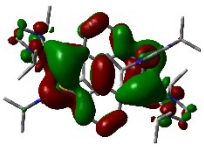
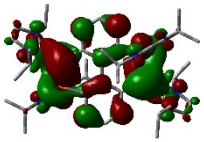
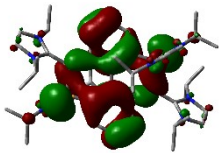
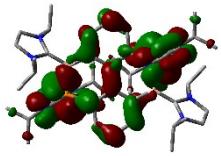
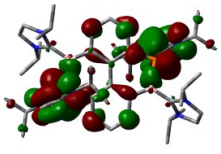
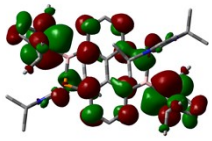
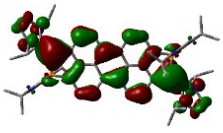
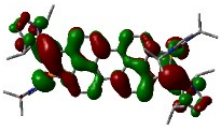
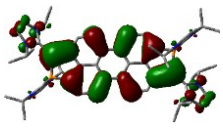
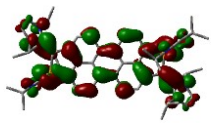
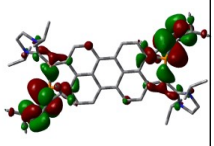
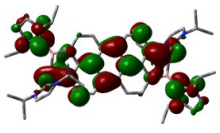
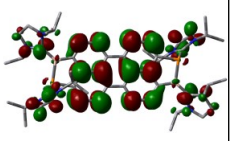
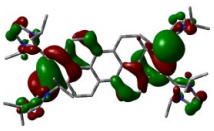
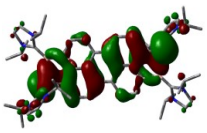
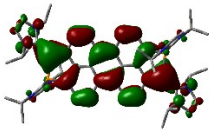


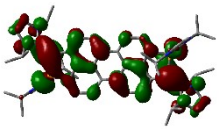
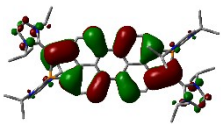
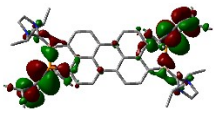
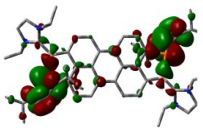
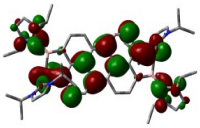
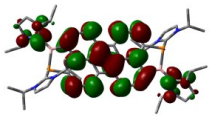
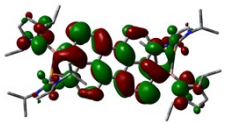
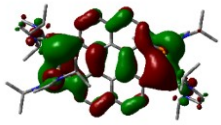
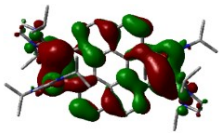
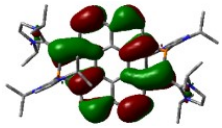
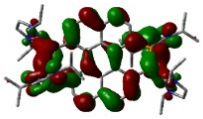
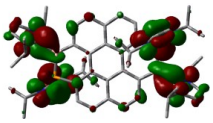
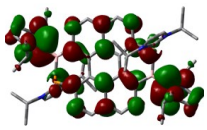
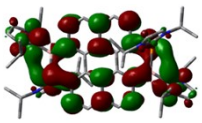
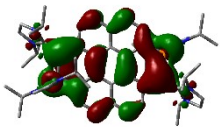
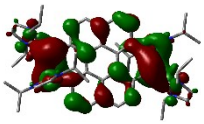
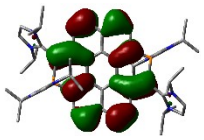
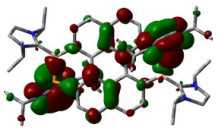
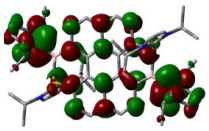
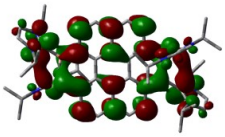
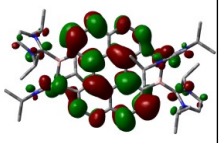

**Figure S5.** Calculated absorption spectra of the studied compounds at TD-DFT//U$\omega$B97XD/6-31G(d).

**Table S4** The molecular orbitals related to electronic configuration and the absorption transitions.

| **1PB-a** | | | | |
|---|---|---|---|---|
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+2(*α*) |
|  |  |  |  | |
| HOMO(*β*) | HOMO-1(*β*) | SUMO(*β*) | LUMO(*β*) | |
| **1PB-b** | | | | |

| | | | | |
|---|---|---|---|---|
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+3(*α*) |
|  |  |  |  |  |
| HOMO(*β*) | SUMO(*β*) | HOMO-1(*β*) | HOMO-2(*β*) | LUMO(*β*) |
| **1PB-c** | | | | |
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+1(*α*) |
|  |  |  |  |  |
| LUMO+2(*α*) | LUMO+3(*α*) | HOMO(*β*) | HOMO-1(*β*) | SUMO(*β*) |
|  | | | | |
| LUMO(*β*) | | | | |
| **1PB-d** | | | | |
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+2(*α*) |
|  |  |  |  |  |
| LUMO+6(*α*) | HOMO-5(*β*) | HOMO-4(*β*) | HOMO-2(*β*) | HOMO-1(*β*) |
|  |  |  | | |
| HOMO(*β*) | SUMO(*β*) | LUMO(*β*) | | |

| **2PB-a** | | | | |
|---|---|---|---|---|
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+2(*α*) |
|  |  |  |  |  |
| LUMO+3(*α*) | LUMO+7(*α*) | HOMO(*β*) | SUMO(*β*) | HOMO-1(*β*) |
|  |  |  | | |
| HOMO-2(*β*) | LUMO(*β*) | LUMO+3(*β*) | | |
| **2PB-b** | | | | |
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+1(*α*) |
|  |  |  |  |  |
| LUMO+2(*α*) | LUMO+3(*α*) | LUMO+4(*α*) | HOMO(*β*) | SUMO(*β*) |
|  |  |  |  | |
| HOMO-1(*β*) | LUMO(*β*) | LUMO+1(*β*) | LUMO+3(*β*) | |
| **2PB-c** | | | | |
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+2(*α*) |
|  |  |  |  |  |
| LUMO+3(*α*) | LUMO+9(*α*) | HOMO-3(*β*) | HOMO-2(*β*) | SUMO(*β*) |

| | | | | |
|---|---|---|---|---|
|  |  |  |  |  |
| HOMO(*β*) | HOMO-1(*β*) | LUMO(*β*) | LUMO+1(*β*) | LUMO+3(*β*) |
|  |  | | | |
| LUMO+4(*β*) | LUMO+5(*β*) | | | |
| **2PB-d** | | | | |
|  |  |  |  |  |
| SOMO(*α*) | HOMO(*α*) | HOMO-1(*α*) | LUMO(*α*) | LUMO+2(*α*) |
|  |  |  |  |  |
| LUMO+3(*α*) | LUMO+4(*α*) | SUMO(*β*) | HOMO(*β*) | HOMO-1(*β*) |
|  |  |  |  | |
| LUMO+1(*β*) | LUMO+3(*β*) | LUMO+4(*β*) | LUMO+6(*β*) | |

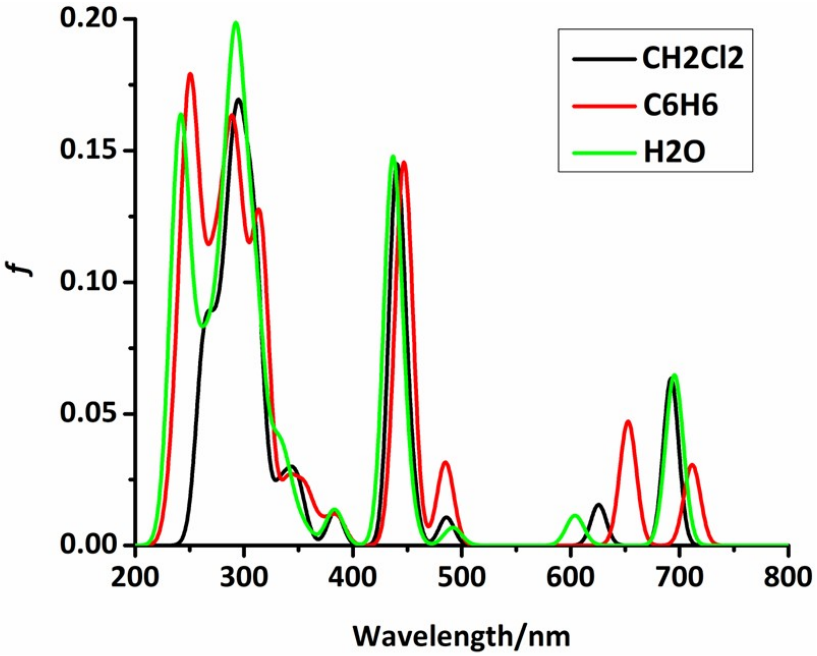
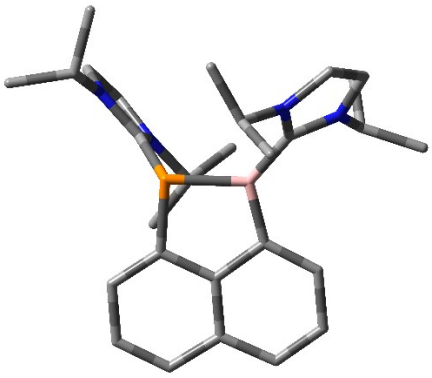



**Figure S6**. Calculated absorption spectra of the compound **1PB-a** in different solvents.

**Coordinates of the studied molecules**

**1PB-a**



**UB3LYP/6-31G***

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.167512 | 2.787044 | -2.133636 |
| 2 | 6 | 0 | -2.284025 | 3.827563 | -1.914207 |
| 3 | 6 | 0 | -0.979159 | 3.585382 | -1.409539 |
| 4 | 6 | 0 | -0.614175 | 2.242861 | -1.106308 |
| 5 | 6 | 0 | -1.534269 | 1.186929 | -1.345025 |
| 6 | 6 | 0 | -2.790664 | 1.450737 | -1.866710 |
| 7 | 6 | 0 | -0.010329 | 4.607506 | -1.199003 |
| 8 | 6 | 0 | 0.690329 | 1.892031 | -0.586673 |
| 9 | 1 | 0 | -3.484870 | 0.643320 | -2.086626 |
| 10 | 6 | 0 | 1.604665 | 2.947552 | -0.437965 |
| 11 | 6 | 0 | 1.251519 | 4.279396 | -0.735780 |
| 12 | 1 | 0 | 2.618161 | 2.745808 | -0.101725 |
| 13 | 1 | 0 | 1.990762 | 5.064567 | -0.599204 |
| 14 | 15 | 0 | -0.766577 | -0.457937 | -1.042264 |
| 15 | 6 | 0 | 4.142091 | -0.981273 | 0.932796 |
| 16 | 6 | 0 | 3.986997 | -1.752826 | -0.170556 |
| 17 | 6 | 0 | -2.980381 | -2.534072 | 1.627028 |
| 18 | 6 | 0 | -2.947649 | -1.357318 | 2.304355 |
| 19 | 6 | 0 | 2.203065 | -0.369360 | -0.057016 |
| 20 | 6 | 0 | -1.765010 | -1.083515 | 0.420118 |
| 21 | 1 | 0 | 4.624340 | -2.520697 | -0.578447 |
| 22 | 1 | 0 | 4.928546 | -0.968843 | 1.669991 |
| 23 | 7 | 0 | 2.799993 | -1.376358 | -0.773903 |
| 24 | 7 | 0 | 3.049177 | -0.134583 | 0.997563 |
| 25 | 6 | 0 | 2.390783 | -1.850639 | -2.119660 |
| 26 | 6 | 0 | 2.266085 | -3.376481 | -2.140205 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 6 | 0 | 3.353573 | -1.315044 | -3.185761 |
| 28 | 1 | 0 | 1.405094 | -1.416149 | -2.286655 |
| 29 | 1 | 0 | 1.581408 | -3.729842 | -1.362172 |
| 30 | 1 | 0 | 1.877389 | -3.695948 | -3.112128 |
| 31 | 1 | 0 | 3.233478 | -3.870695 | -1.996497 |
| 32 | 1 | 0 | 3.407708 | -0.222780 | -3.149239 |
| 33 | 1 | 0 | 4.364120 | -1.718388 | -3.056870 |
| 34 | 1 | 0 | 2.999956 | -1.606821 | -4.179751 |
| 35 | 6 | 0 | 2.776092 | 0.757326 | 2.149212 |
| 36 | 6 | 0 | 3.940383 | 1.725481 | 2.381297 |
| 37 | 6 | 0 | 2.461675 | -0.079673 | 3.395704 |
| 38 | 1 | 0 | 1.889798 | 1.325291 | 1.859221 |
| 39 | 1 | 0 | 4.179129 | 2.292220 | 1.477055 |
| 40 | 1 | 0 | 3.670986 | 2.436217 | 3.168720 |
| 41 | 1 | 0 | 4.845678 | 1.201692 | 2.708001 |
| 42 | 1 | 0 | 1.641162 | -0.778780 | 3.204034 |
| 43 | 1 | 0 | 3.333588 | -0.658369 | 3.719872 |
| 44 | 1 | 0 | 2.173043 | 0.577622 | 4.222162 |
| 45 | 1 | 0 | -3.395739 | -1.082090 | 3.245396 |
| 46 | 1 | 0 | -3.457539 | -3.468966 | 1.872819 |
| 47 | 7 | 0 | -2.193456 | -0.473728 | 1.559300 |
| 48 | 7 | 0 | -2.253225 | -2.355859 | 0.467841 |
| 49 | 6 | 0 | -1.948151 | 0.937626 | 1.973035 |
| 50 | 6 | 0 | -1.350455 | 0.978950 | 3.382492 |
| 51 | 6 | 0 | -3.238964 | 1.754062 | 1.859106 |
| 52 | 1 | 0 | -1.211964 | 1.316359 | 1.266094 |
| 53 | 1 | 0 | -0.457392 | 0.352199 | 3.457252 |
| 54 | 1 | 0 | -1.067937 | 2.009960 | 3.616453 |
| 55 | 1 | 0 | -2.067131 | 0.656642 | 4.145835 |
| 56 | 1 | 0 | -3.636755 | 1.725458 | 0.841977 |
| 57 | 1 | 0 | -4.005726 | 1.389974 | 2.552594 |
| 58 | 1 | 0 | -3.027754 | 2.797759 | 2.111364 |
| 59 | 6 | 0 | -2.085659 | -3.421563 | -0.560901 |
| 60 | 6 | 0 | -3.445741 | -3.804908 | -1.151087 |
| 61 | 6 | 0 | -1.326985 | -4.612798 | 0.030976 |
| 62 | 1 | 0 | -1.479916 | -2.957352 | -1.341314 |
| 63 | 1 | 0 | -3.955860 | -2.931022 | -1.567649 |
| 64 | 1 | 0 | -3.297837 | -4.529577 | -1.957672 |
| 65 | 1 | 0 | -4.100976 | -4.267995 | -0.405098 |
| 66 | 1 | 0 | -0.362935 | -4.303429 | 0.447675 |
| 67 | 1 | 0 | -1.899392 | -5.111173 | 0.821217 |
| 68 | 1 | 0 | -1.140824 | -5.350425 | -0.755753 |
| 69 | 5 | 0 | 0.875834 | 0.380241 | -0.381194 |
| 70 | 1 | 0 | -2.578011 | 4.848609 | -2.144548 |

| | | | | | |
|---|---|---|---|---|---|
| 71 | 1 | 0 | -0.267080 | 5.639525 | -1.422119 |
| 72 | 1 | 0 | -4.155426 | 2.991813 | -2.536470 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.006421 | 2.968880 | -1.986652 |
| 2 | 6 | 0 | -2.030150 | 3.927879 | -1.835440 |
| 3 | 6 | 0 | -0.712959 | 3.573436 | -1.448602 |
| 4 | 6 | 0 | -0.437306 | 2.211596 | -1.191286 |
| 5 | 6 | 0 | -1.455439 | 1.238782 | -1.350058 |
| 6 | 6 | 0 | -2.719065 | 1.604865 | -1.759193 |
| 7 | 6 | 0 | 0.350829 | 4.508775 | -1.313455 |
| 8 | 6 | 0 | 0.864638 | 1.749004 | -0.778697 |
| 9 | 1 | 0 | -3.494829 | 0.858827 | -1.911015 |
| 10 | 6 | 0 | 1.870956 | 2.711187 | -0.705492 |
| 11 | 6 | 0 | 1.609042 | 4.072447 | -0.966032 |
| 12 | 1 | 0 | 2.887021 | 2.417464 | -0.457860 |
| 13 | 1 | 0 | 2.421259 | 4.789567 | -0.889544 |
| 14 | 15 | 0 | -0.837978 | -0.456739 | -1.038869 |
| 15 | 6 | 0 | 4.103583 | -1.344786 | 0.665649 |
| 16 | 6 | 0 | 3.775515 | -2.202736 | -0.325080 |
| 17 | 6 | 0 | -3.112932 | -1.930736 | 1.926042 |
| 18 | 6 | 0 | -2.760409 | -0.770543 | 2.529101 |
| 19 | 6 | 0 | 2.175385 | -0.625418 | -0.240116 |
| 20 | 6 | 0 | -1.755574 | -0.826705 | 0.540578 |
| 21 | 1 | 0 | 4.288242 | -3.078863 | -0.686481 |
| 22 | 1 | 0 | 4.948281 | -1.341669 | 1.335271 |
| 23 | 7 | 0 | 2.597572 | -1.750581 | -0.881081 |
| 24 | 7 | 0 | 3.118721 | -0.380112 | 0.711680 |
| 25 | 6 | 0 | 1.917795 | -2.391391 | -2.019154 |
| 26 | 6 | 0 | 1.104052 | -3.585819 | -1.527247 |
| 27 | 6 | 0 | 2.911579 | -2.763241 | -3.115785 |
| 28 | 1 | 0 | 1.240577 | -1.630522 | -2.411866 |
| 29 | 1 | 0 | 0.415894 | -3.281187 | -0.732224 |
| 30 | 1 | 0 | 0.518521 | -4.005851 | -2.350354 |
| 31 | 1 | 0 | 1.757967 | -4.372201 | -1.134469 |
| 32 | 1 | 0 | 3.522399 | -1.902680 | -3.401660 |
| 33 | 1 | 0 | 3.572899 | -3.582261 | -2.814399 |
| 34 | 1 | 0 | 2.359067 | -3.098756 | -3.997585 |
| 35 | 6 | 0 | 3.006346 | 0.606997 | 1.799022 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | 4.262287 | 1.468801 | 1.888760 |
| 37 | 6 | 0 | 2.709178 | -0.118769 | 3.110704 |
| 38 | 1 | 0 | 2.154997 | 1.235664 | 1.530180 |
| 39 | 1 | 0 | 4.503489 | 1.930025 | 0.927865 |
| 40 | 1 | 0 | 4.105694 | 2.264475 | 2.622281 |
| 41 | 1 | 0 | 5.128833 | 0.884569 | 2.216455 |
| 42 | 1 | 0 | 1.842949 | -0.778219 | 3.000336 |
| 43 | 1 | 0 | 3.562227 | -0.726591 | 3.430143 |
| 44 | 1 | 0 | 2.500353 | 0.607634 | 3.901378 |
| 45 | 1 | 0 | -3.037364 | -0.371635 | 3.491280 |
| 46 | 1 | 0 | -3.751807 | -2.730210 | 2.264430 |
| 47 | 7 | 0 | -1.918409 | -0.103280 | 1.671413 |
| 48 | 7 | 0 | -2.485689 | -1.954592 | 0.702759 |
| 49 | 6 | 0 | -1.331276 | 1.223302 | 1.971932 |
| 50 | 6 | 0 | -0.700429 | 1.216142 | 3.361115 |
| 51 | 6 | 0 | -2.379964 | 2.319352 | 1.814916 |
| 52 | 1 | 0 | -0.542938 | 1.358942 | 1.233235 |
| 53 | 1 | 0 | -0.034341 | 0.360310 | 3.493280 |
| 54 | 1 | 0 | -0.115398 | 2.131782 | 3.485226 |
| 55 | 1 | 0 | -1.452391 | 1.201279 | 4.157050 |
| 56 | 1 | 0 | -2.821342 | 2.307095 | 0.816554 |
| 57 | 1 | 0 | -3.176308 | 2.212188 | 2.560109 |
| 58 | 1 | 0 | -1.904130 | 3.292673 | 1.963088 |
| 59 | 6 | 0 | -2.663371 | -3.046030 | -0.282650 |
| 60 | 6 | 0 | -4.087258 | -3.018309 | -0.829392 |
| 61 | 6 | 0 | -2.279189 | -4.385207 | 0.338510 |
| 62 | 1 | 0 | -1.969765 | -2.812137 | -1.091885 |
| 63 | 1 | 0 | -4.311811 | -2.047432 | -1.280492 |
| 64 | 1 | 0 | -4.198083 | -3.787811 | -1.598208 |
| 65 | 1 | 0 | -4.824265 | -3.218074 | -0.044350 |
| 66 | 1 | 0 | -1.270981 | -4.352097 | 0.761877 |
| 67 | 1 | 0 | -2.977467 | -4.687428 | 1.126027 |
| 68 | 1 | 0 | -2.301777 | -5.158075 | -0.434548 |
| 69 | 5 | 0 | 0.912459 | 0.228019 | -0.545061 |
| 70 | 1 | 0 | -2.259072 | 4.972257 | -2.029854 |
| 71 | 1 | 0 | 0.163384 | 5.561183 | -1.506132 |
| 72 | 1 | 0 | -4.004613 | 3.258169 | -2.300183 |

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**UM06-2X/6-31G***

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| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.383679 | 3.531054 | -1.880231 |
| 2 | 6 | 0 | -1.230131 | 4.272771 | -1.759068 |
| 3 | 6 | 0 | 0.002005 | 3.655853 | -1.419153 |
| 4 | 6 | 0 | 0.005832 | 2.263469 | -1.168347 |
| 5 | 6 | 0 | -1.192753 | 1.515991 | -1.299558 |
| 6 | 6 | 0 | -2.368158 | 2.132108 | -1.669991 |
| 7 | 6 | 0 | 1.238139 | 4.354479 | -1.333380 |
| 8 | 6 | 0 | 1.199787 | 1.544689 | -0.803265 |
| 9 | 1 | 0 | -3.280555 | 1.556693 | -1.806325 |
| 10 | 6 | 0 | 2.382212 | 2.279613 | -0.781129 |
| 11 | 6 | 0 | 2.394311 | 3.668472 | -1.041100 |
| 12 | 1 | 0 | 3.327818 | 1.783498 | -0.577937 |
| 13 | 1 | 0 | 3.339272 | 4.202297 | -1.006647 |
| 14 | 15 | 0 | -0.918166 | -0.279640 | -1.040672 |
| 15 | 6 | 0 | 3.864712 | -2.075511 | 0.506079 |
| 16 | 6 | 0 | 3.291458 | -2.904207 | -0.396944 |
| 17 | 6 | 0 | -3.434334 | -1.279703 | 1.939758 |
| 18 | 6 | 0 | -2.834657 | -0.227691 | 2.551723 |
| 19 | 6 | 0 | 2.032558 | -1.040099 | -0.293510 |
| 20 | 6 | 0 | -1.880413 | -0.475997 | 0.551456 |
| 21 | 1 | 0 | 3.595389 | -3.879175 | -0.741397 |
| 22 | 1 | 0 | 4.752356 | -2.201376 | 1.105505 |
| 23 | 7 | 0 | 2.175282 | -2.259881 | -0.886686 |
| 24 | 7 | 0 | 3.089173 | -0.936292 | 0.563782 |
| 25 | 6 | 0 | 1.251271 | -2.826253 | -1.882949 |
| 26 | 6 | 0 | 0.181326 | -3.648251 | -1.167657 |
| 27 | 6 | 0 | 2.000640 | -3.639527 | -2.932088 |
| 28 | 1 | 0 | 0.790018 | -1.963746 | -2.370041 |
| 29 | 1 | 0 | -0.301367 | -3.054936 | -0.383088 |
| 30 | 1 | 0 | -0.582210 | -3.977652 | -1.879103 |
| 31 | 1 | 0 | 0.626598 | -4.534103 | -0.702073 |
| 32 | 1 | 0 | 2.817025 | -3.061574 | -3.372222 |
| 33 | 1 | 0 | 2.403832 | -4.568470 | -2.517281 |
| 34 | 1 | 0 | 1.305830 | -3.914223 | -3.729384 |
| 35 | 6 | 0 | 3.238820 | 0.078483 | 1.623836 |
| 36 | 6 | 0 | 4.657245 | 0.637046 | 1.647318 |
| 37 | 6 | 0 | 2.843906 | -0.543467 | 2.961920 |
| 38 | 1 | 0 | 2.535184 | 0.873080 | 1.367352 |
| 39 | 1 | 0 | 4.961494 | 1.009126 | 0.666192 |
| 40 | 1 | 0 | 4.710281 | 1.461894 | 2.362402 |
| 41 | 1 | 0 | 5.378765 | -0.121699 | 1.967116 |
| 42 | 1 | 0 | 1.852441 | -1.000625 | 2.893267 |
| 43 | 1 | 0 | 3.558775 | -1.317259 | 3.259758 |
| 44 | 1 | 0 | 2.827518 | 0.221622 | 3.743099 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 1 | 0 | -3.008313 | 0.210945 | 3.521603 |
| 46 | 1 | 0 | -4.228177 | -1.927876 | 2.275460 |
| 47 | 7 | 0 | -1.877238 | 0.252086 | 1.689937 |
| 48 | 7 | 0 | -2.834562 | -1.422917 | 0.710641 |
| 49 | 6 | 0 | -1.013096 | 1.417528 | 1.997249 |
| 50 | 6 | 0 | -0.383276 | 1.244298 | 3.375465 |
| 51 | 6 | 0 | -1.808514 | 2.713077 | 1.884241 |
| 52 | 1 | 0 | -0.228185 | 1.396000 | 1.241603 |
| 53 | 1 | 0 | 0.089012 | 0.264467 | 3.478357 |
| 54 | 1 | 0 | 0.380049 | 2.014865 | 3.513284 |
| 55 | 1 | 0 | -1.117834 | 1.366599 | 4.177795 |
| 56 | 1 | 0 | -2.251173 | 2.823727 | 0.892196 |
| 57 | 1 | 0 | -2.602381 | 2.748977 | 2.638442 |
| 58 | 1 | 0 | -1.137593 | 3.559094 | 2.056443 |
| 59 | 6 | 0 | -3.270710 | -2.422002 | -0.295056 |
| 60 | 6 | 0 | -4.618324 | -2.003344 | -0.872220 |
| 61 | 6 | 0 | -3.292049 | -3.815596 | 0.322001 |
| 62 | 1 | 0 | -2.515238 | -2.381869 | -1.081452 |
| 63 | 1 | 0 | -4.554213 | -1.011359 | -1.327754 |
| 64 | 1 | 0 | -4.925798 | -2.717130 | -1.640565 |
| 65 | 1 | 0 | -5.391162 | -1.984374 | -0.097079 |
| 66 | 1 | 0 | -2.331995 | -4.062631 | 0.783420 |
| 67 | 1 | 0 | -4.079038 | -3.914046 | 1.076260 |
| 68 | 1 | 0 | -3.497686 | -4.548822 | -0.462000 |
| 69 | 5 | 0 | 0.948240 | 0.037161 | -0.564529 |
| 70 | 1 | 0 | -1.247480 | 5.343361 | -1.944497 |
| 71 | 1 | 0 | 1.259366 | 5.423523 | -1.523826 |
| 72 | 1 | 0 | -3.312705 | 4.017297 | -2.160255 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.019394 | 2.990298 | -2.103376 |
| 2 | 6 | 0 | -2.057334 | 3.976297 | -1.900734 |
| 3 | 6 | 0 | -0.760229 | 3.647421 | -1.407493 |
| 4 | 6 | 0 | -0.482808 | 2.275277 | -1.094866 |
| 5 | 6 | 0 | -1.480088 | 1.280054 | -1.319202 |
| 6 | 6 | 0 | -2.731361 | 1.626826 | -1.831991 |
| 7 | 6 | 0 | 0.283937 | 4.604238 | -1.215638 |
| 8 | 6 | 0 | 0.805457 | 1.836983 | -0.585676 |
| 9 | 1 | 0 | -3.485954 | 0.859926 | -2.042088 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 6 | 0 | 1.800480 | 2.833298 | -0.458400 |
| 11 | 6 | 0 | 1.535811 | 4.189346 | -0.764050 |
| 12 | 1 | 0 | 2.810408 | 2.558916 | -0.132290 |
| 13 | 1 | 0 | 2.335965 | 4.928777 | -0.643775 |
| 14 | 15 | 0 | -0.812686 | -0.415870 | -1.024125 |
| 15 | 6 | 0 | 4.107086 | -1.247225 | 0.888197 |
| 16 | 6 | 0 | 3.863595 | -2.040073 | -0.198404 |
| 17 | 6 | 0 | -3.143003 | -2.351509 | 1.664792 |
| 18 | 6 | 0 | -3.003332 | -1.179110 | 2.359044 |
| 19 | 6 | 0 | 2.165311 | -0.531670 | -0.061149 |
| 20 | 6 | 0 | -1.833361 | -0.975817 | 0.439848 |
| 21 | 1 | 0 | 4.440622 | -2.863966 | -0.609335 |
| 22 | 1 | 0 | 4.921612 | -1.269755 | 1.607434 |
| 23 | 7 | 0 | 2.675703 | -1.605015 | -0.771284 |
| 24 | 7 | 0 | 3.069798 | -0.327049 | 0.965552 |
| 25 | 6 | 0 | 2.198778 | -2.052233 | -2.110940 |
| 26 | 6 | 0 | 2.253342 | -3.581498 | -2.229002 |
| 27 | 6 | 0 | 2.993191 | -1.336104 | -3.215553 |
| 28 | 1 | 0 | 1.145924 | -1.730642 | -2.159917 |
| 29 | 1 | 0 | 1.721767 | -4.073201 | -1.396291 |
| 30 | 1 | 0 | 1.772782 | -3.885983 | -3.173899 |
| 31 | 1 | 0 | 3.289430 | -3.963176 | -2.257001 |
| 32 | 1 | 0 | 2.907862 | -0.241260 | -3.113516 |
| 33 | 1 | 0 | 4.062245 | -1.612017 | -3.181864 |
| 34 | 1 | 0 | 2.597186 | -1.622201 | -4.204919 |
| 35 | 6 | 0 | 2.878729 | 0.599491 | 2.112580 |
| 36 | 6 | 0 | 4.114949 | 1.489073 | 2.311940 |
| 37 | 6 | 0 | 2.528681 | -0.202671 | 3.377918 |
| 38 | 1 | 0 | 2.019059 | 1.226511 | 1.821959 |
| 39 | 1 | 0 | 4.382514 | 2.028578 | 1.388492 |
| 40 | 1 | 0 | 3.906746 | 2.234584 | 3.097791 |
| 41 | 1 | 0 | 4.992977 | 0.903436 | 2.638068 |
| 42 | 1 | 0 | 1.652819 | -0.851913 | 3.206963 |
| 43 | 1 | 0 | 3.372206 | -0.840455 | 3.696435 |
| 44 | 1 | 0 | 2.298678 | 0.487135 | 4.207784 |
| 45 | 1 | 0 | -3.412717 | -0.877403 | 3.319614 |
| 46 | 1 | 0 | -3.690241 | -3.257327 | 1.912420 |
| 47 | 7 | 0 | -2.193988 | -0.345445 | 1.604640 |
| 48 | 7 | 0 | -2.425679 | -2.215846 | 0.487556 |
| 49 | 6 | 0 | -1.829450 | 1.044830 | 2.015140 |
| 50 | 6 | 0 | -1.242424 | 1.041124 | 3.434139 |
| 51 | 6 | 0 | -3.047589 | 1.970785 | 1.883249 |
| 52 | 1 | 0 | -1.047853 | 1.350726 | 1.302595 |
| 53 | 1 | 0 | -0.401880 | 0.333297 | 3.523432 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | -0.869761 | 2.052815 | 3.666616 |
| 55 | 1 | 0 | -1.998577 | 0.788783 | 4.198627 |
| 56 | 1 | 0 | -3.438331 | 1.971452 | 0.853364 |
| 57 | 1 | 0 | -3.855353 | 1.673819 | 2.576286 |
| 58 | 1 | 0 | -2.747976 | 3.001898 | 2.135278 |
| 59 | 6 | 0 | -2.354430 | -3.277543 | -0.561629 |
| 60 | 6 | 0 | -3.756668 | -3.570574 | -1.114763 |
| 61 | 6 | 0 | -1.647971 | -4.522821 | -0.006142 |
| 62 | 1 | 0 | -1.738301 | -2.826726 | -1.358561 |
| 63 | 1 | 0 | -4.232577 | -2.654872 | -1.503590 |
| 64 | 1 | 0 | -3.675918 | -4.293819 | -1.943651 |
| 65 | 1 | 0 | -4.418802 | -4.013573 | -0.349828 |
| 66 | 1 | 0 | -0.645998 | -4.275889 | 0.384340 |
| 67 | 1 | 0 | -2.229304 | -4.998563 | 0.803682 |
| 68 | 1 | 0 | -1.532737 | -5.266974 | -0.812191 |
| 69 | 5 | 0 | 0.891031 | 0.309577 | -0.373181 |
| 70 | 1 | 0 | -2.285020 | 5.022119 | -2.138405 |
| 71 | 1 | 0 | 0.094893 | 5.659069 | -1.444551 |
| 72 | 1 | 0 | -4.003541 | 3.262564 | -2.500020 |

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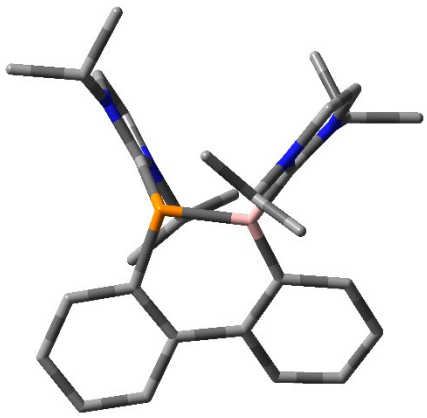
**1PB-b**



**UB3LYP/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.261907 | -4.346388 | 1.160568 |
| 2 | 6 | 0 | -0.785904 | -3.155488 | 0.687283 |
| 3 | 6 | 0 | 0.001003 | -2.156545 | 0.044835 |
| 4 | 6 | 0 | 1.380253 | -2.482979 | -0.213984 |
| 5 | 6 | 0 | 1.898845 | -3.674837 | 0.333798 |
| 6 | 6 | 0 | 1.108465 | -4.592819 | 1.016324 |
| 7 | 6 | 0 | 2.270300 | -1.639854 | -1.063576 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 6 | 0 | 2.015385 | -0.282469 | -1.404314 |
| 9 | 6 | 0 | 2.939990 | 0.436412 | -2.185867 |
| 10 | 1 | 0 | 2.711001 | 1.466069 | -2.451594 |
| 11 | 6 | 0 | 4.119421 | -0.137787 | -2.642886 |
| 12 | 6 | 0 | 4.357650 | -1.484297 | -2.360244 |
| 13 | 6 | 0 | 3.446694 | -2.211127 | -1.605115 |
| 14 | 1 | 0 | -0.904133 | -5.072897 | 1.651433 |
| 15 | 1 | 0 | -1.849906 | -2.972562 | 0.815102 |
| 16 | 1 | 0 | 1.554364 | -5.498396 | 1.416942 |
| 17 | 1 | 0 | 4.820027 | 0.439603 | -3.238841 |
| 18 | 1 | 0 | 5.244842 | -1.977734 | -2.747047 |
| 19 | 15 | 0 | 0.445346 | 0.595208 | -1.040503 |
| 20 | 6 | 0 | 1.792248 | 2.668820 | 2.256879 |
| 21 | 6 | 0 | 1.180221 | 3.649563 | 1.543961 |
| 22 | 1 | 0 | 2.310677 | 2.712923 | 3.201143 |
| 23 | 1 | 0 | 1.065246 | 4.700247 | 1.756560 |
| 24 | 6 | 0 | -4.321108 | -0.104420 | -0.800710 |
| 25 | 6 | 0 | -4.268431 | -0.147677 | 0.555024 |
| 26 | 1 | 0 | -5.156375 | 0.063578 | -1.461559 |
| 27 | 1 | 0 | -5.047324 | -0.015349 | 1.288584 |
| 28 | 6 | 0 | 0.970324 | 1.733118 | 0.391363 |
| 29 | 6 | 0 | -2.186183 | -0.533994 | -0.220765 |
| 30 | 7 | 0 | 1.651035 | 1.494453 | 1.544790 |
| 31 | 7 | 0 | 0.680548 | 3.065814 | 0.396177 |
| 32 | 7 | 0 | -3.041516 | -0.346000 | -1.266163 |
| 33 | 7 | 0 | -2.955269 | -0.415267 | 0.901273 |
| 34 | 6 | 0 | -2.691488 | -0.496665 | -2.702564 |
| 35 | 6 | 0 | -2.944834 | 0.809715 | -3.458145 |
| 36 | 6 | 0 | -3.430989 | -1.695555 | -3.305344 |
| 37 | 1 | 0 | -1.619353 | -0.707734 | -2.699997 |
| 38 | 1 | 0 | -2.384963 | 1.636288 | -3.010301 |
| 39 | 1 | 0 | -2.617520 | 0.698913 | -4.496501 |
| 40 | 1 | 0 | -4.008892 | 1.072524 | -3.472376 |
| 41 | 1 | 0 | -3.222045 | -2.609926 | -2.741836 |
| 42 | 1 | 0 | -4.515144 | -1.537541 | -3.325472 |
| 43 | 1 | 0 | -3.097859 | -1.846423 | -4.336826 |
| 44 | 6 | 0 | -2.449988 | -0.460489 | 2.295056 |
| 45 | 6 | 0 | -3.254879 | -1.454039 | 3.137687 |
| 46 | 6 | 0 | -2.439632 | 0.948478 | 2.899357 |
| 47 | 1 | 0 | -1.423660 | -0.823352 | 2.201820 |
| 48 | 1 | 0 | -3.262950 | -2.448428 | 2.682831 |
| 49 | 1 | 0 | -2.801050 | -1.537901 | 4.129965 |
| 50 | 1 | 0 | -4.291004 | -1.126547 | 3.277788 |
| 51 | 1 | 0 | -1.842953 | 1.634838 | 2.289604 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 1 | 0 | -3.453420 | 1.355055 | 2.985023 |
| 53 | 1 | 0 | -2.008104 | 0.917437 | 3.905174 |
| 54 | 6 | 0 | 2.224663 | 0.193048 | 1.986945 |
| 55 | 6 | 0 | 1.780292 | -0.130468 | 3.416214 |
| 56 | 6 | 0 | 3.747747 | 0.208961 | 1.826579 |
| 57 | 1 | 0 | 1.797107 | -0.549352 | 1.316819 |
| 58 | 1 | 0 | 0.690984 | -0.088600 | 3.515009 |
| 59 | 1 | 0 | 2.104723 | -1.145087 | 3.665121 |
| 60 | 1 | 0 | 2.223695 | 0.547320 | 4.154076 |
| 61 | 1 | 0 | 4.032934 | 0.428048 | 0.794174 |
| 62 | 1 | 0 | 4.212706 | 0.949703 | 2.487343 |
| 63 | 1 | 0 | 4.148742 | -0.774553 | 2.089757 |
| 64 | 6 | 0 | -0.032755 | 3.831578 | -0.664745 |
| 65 | 6 | 0 | 0.880489 | 4.918961 | -1.238180 |
| 66 | 6 | 0 | -1.356205 | 4.380116 | -0.123790 |
| 67 | 1 | 0 | -0.238164 | 3.093536 | -1.442362 |
| 68 | 1 | 0 | 1.817364 | 4.492759 | -1.609928 |
| 69 | 1 | 0 | 0.374280 | 5.411081 | -2.074377 |
| 70 | 1 | 0 | 1.119540 | 5.689375 | -0.496820 |
| 71 | 1 | 0 | -1.990638 | 3.575813 | 0.262817 |
| 72 | 1 | 0 | -1.198605 | 5.111744 | 0.676537 |
| 73 | 1 | 0 | -1.897559 | 4.884287 | -0.930430 |
| 74 | 5 | 0 | -0.631561 | -0.810581 | -0.320349 |
| 75 | 1 | 0 | 2.955444 | -3.896464 | 0.236398 |
| 76 | 1 | 0 | 3.643850 | -3.265730 | -1.456865 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.422382 | -4.083165 | -0.981541 |
| 2 | 6 | 0 | -0.493410 | -3.195408 | -0.474855 |
| 3 | 6 | 0 | -0.854842 | -1.984551 | 0.169152 |
| 4 | 6 | 0 | -2.248882 | -1.754724 | 0.393018 |
| 5 | 6 | 0 | -3.172703 | -2.642689 | -0.182393 |
| 6 | 6 | 0 | -2.780620 | -3.784519 | -0.866219 |
| 7 | 6 | 0 | -2.764708 | -0.604641 | 1.195556 |
| 8 | 6 | 0 | -2.019446 | 0.558072 | 1.503628 |
| 9 | 6 | 0 | -2.616090 | 1.617645 | 2.202710 |
| 10 | 1 | 0 | -2.014926 | 2.491507 | 2.442102 |
| 11 | 6 | 0 | -3.940891 | 1.570278 | 2.605506 |
| 12 | 6 | 0 | -4.668398 | 0.409794 | 2.358900 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | -4.083534 | -0.651404 | 1.686316 |
| 14 | 1 | 0 | -1.098760 | -4.994069 | -1.476499 |
| 15 | 1 | 0 | 0.563456 | -3.430881 | -0.579835 |
| 16 | 1 | 0 | -3.530337 | -4.443220 | -1.292564 |
| 17 | 1 | 0 | -4.386884 | 2.405242 | 3.135944 |
| 18 | 1 | 0 | -5.692159 | 0.320411 | 2.708722 |
| 19 | 15 | 0 | -0.234309 | 0.751625 | 1.180034 |
| 20 | 6 | 0 | -0.563222 | 2.787581 | -2.343791 |
| 21 | 6 | 0 | 0.455896 | 3.444345 | -1.739720 |
| 22 | 1 | 0 | -1.031331 | 2.953527 | -3.300327 |
| 23 | 1 | 0 | 1.043605 | 4.282000 | -2.076618 |
| 24 | 6 | 0 | 3.977406 | -1.372676 | 0.551003 |
| 25 | 6 | 0 | 3.735127 | -1.440924 | -0.779173 |
| 26 | 1 | 0 | 4.905442 | -1.426614 | 1.096923 |
| 27 | 1 | 0 | 4.413295 | -1.557691 | -1.609073 |
| 28 | 6 | 0 | -0.223597 | 1.821510 | -0.363440 |
| 29 | 6 | 0 | 1.761510 | -1.203401 | 0.259905 |
| 30 | 7 | 0 | -0.962344 | 1.783402 | -1.493787 |
| 31 | 7 | 0 | 0.650716 | 2.844662 | -0.515931 |
| 32 | 7 | 0 | 2.757058 | -1.232108 | 1.176474 |
| 33 | 7 | 0 | 2.369934 | -1.337581 | -0.944762 |
| 34 | 6 | 0 | 2.561426 | -1.177092 | 2.637661 |
| 35 | 6 | 0 | 3.114439 | 0.131353 | 3.193107 |
| 36 | 6 | 0 | 3.162384 | -2.414238 | 3.298398 |
| 37 | 1 | 0 | 1.475806 | -1.195884 | 2.769450 |
| 38 | 1 | 0 | 2.620435 | 0.987867 | 2.725400 |
| 39 | 1 | 0 | 2.933121 | 0.179105 | 4.270341 |
| 40 | 1 | 0 | 4.195174 | 0.209520 | 3.029242 |
| 41 | 1 | 0 | 2.762100 | -3.328981 | 2.852712 |
| 42 | 1 | 0 | 4.254388 | -2.430631 | 3.214782 |
| 43 | 1 | 0 | 2.912452 | -2.412822 | 4.362740 |
| 44 | 6 | 0 | 1.686044 | -1.238483 | -2.245789 |
| 45 | 6 | 0 | 2.021125 | -2.434365 | -3.129946 |
| 46 | 6 | 0 | 2.021105 | 0.098925 | -2.901757 |
| 47 | 1 | 0 | 0.621585 | -1.266562 | -2.001421 |
| 48 | 1 | 0 | 1.790476 | -3.374979 | -2.623520 |
| 49 | 1 | 0 | 1.425394 | -2.385658 | -4.045648 |
| 50 | 1 | 0 | 3.076674 | -2.442144 | -3.422202 |
| 51 | 1 | 0 | 1.748438 | 0.932389 | -2.247785 |
| 52 | 1 | 0 | 3.089760 | 0.173644 | -3.130288 |
| 53 | 1 | 0 | 1.470758 | 0.202914 | -3.841534 |
| 54 | 6 | 0 | -2.054726 | 0.831421 | -1.791136 |
| 55 | 6 | 0 | -1.911698 | 0.269079 | -3.201242 |
| 56 | 6 | 0 | -3.410375 | 1.484009 | -1.544981 |

| | | | | | |
|---|---|---|---|---|---|
| 57 | 1 | 0 | -1.912131 | 0.011233 | -1.094140 |
| 58 | 1 | 0 | -0.905730 | -0.124497 | -3.372958 |
| 59 | 1 | 0 | -2.620359 | -0.555225 | -3.316617 |
| 60 | 1 | 0 | -2.137367 | 1.010992 | -3.974538 |
| 61 | 1 | 0 | -3.482339 | 1.868945 | -0.524574 |
| 62 | 1 | 0 | -3.589075 | 2.303581 | -2.249998 |
| 63 | 1 | 0 | -4.197462 | 0.737293 | -1.681795 |
| 64 | 6 | 0 | 1.727032 | 3.207509 | 0.433863 |
| 65 | 6 | 0 | 1.925389 | 4.718173 | 0.481570 |
| 66 | 6 | 0 | 3.003330 | 2.451045 | 0.072485 |
| 67 | 1 | 0 | 1.369077 | 2.864021 | 1.406879 |
| 68 | 1 | 0 | 0.980166 | 5.239706 | 0.655717 |
| 69 | 1 | 0 | 2.602316 | 4.957406 | 1.305842 |
| 70 | 1 | 0 | 2.382565 | 5.105825 | -0.434823 |
| 71 | 1 | 0 | 2.837501 | 1.369238 | 0.090995 |
| 72 | 1 | 0 | 3.356721 | 2.731901 | -0.925743 |
| 73 | 1 | 0 | 3.791242 | 2.688016 | 0.793271 |
| 74 | 5 | 0 | 0.230571 | -0.971601 | 0.535527 |
| 75 | 1 | 0 | -4.235220 | -2.438283 | -0.115020 |
| 76 | 1 | 0 | -4.669765 | -1.553892 | 1.563572 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.444707 | -4.083700 | -1.002074 |
| 2 | 6 | 0 | -0.510537 | -3.188464 | -0.515304 |
| 3 | 6 | 0 | -0.867020 | -1.984377 | 0.142248 |
| 4 | 6 | 0 | -2.256520 | -1.758642 | 0.389787 |
| 5 | 6 | 0 | -3.187806 | -2.653523 | -0.165338 |
| 6 | 6 | 0 | -2.802581 | -3.794718 | -0.854697 |
| 7 | 6 | 0 | -2.761812 | -0.601983 | 1.189387 |
| 8 | 6 | 0 | -2.008404 | 0.557313 | 1.497119 |
| 9 | 6 | 0 | -2.598500 | 1.621030 | 2.197140 |
| 10 | 1 | 0 | -1.989377 | 2.489989 | 2.435507 |
| 11 | 6 | 0 | -3.924350 | 1.583789 | 2.599922 |
| 12 | 6 | 0 | -4.660489 | 0.427373 | 2.352850 |
| 13 | 6 | 0 | -4.082291 | -0.638376 | 1.680697 |
| 14 | 1 | 0 | -1.126080 | -4.991330 | -1.505603 |
| 15 | 1 | 0 | 0.546999 | -3.414025 | -0.644716 |
| 16 | 1 | 0 | -3.556835 | -4.458505 | -1.263957 |
| 17 | 1 | 0 | -4.364296 | 2.422040 | 3.129799 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 1 | 0 | -5.684621 | 0.344687 | 2.702589 |
| 19 | 15 | 0 | -0.218040 | 0.748890 | 1.175724 |
| 20 | 6 | 0 | -0.604520 | 2.790483 | -2.352058 |
| 21 | 6 | 0 | 0.416948 | 3.459955 | -1.759169 |
| 22 | 1 | 0 | -1.086346 | 2.947345 | -3.304188 |
| 23 | 1 | 0 | 0.992458 | 4.304363 | -2.101647 |
| 24 | 6 | 0 | 3.975011 | -1.364165 | 0.597153 |
| 25 | 6 | 0 | 3.752765 | -1.464334 | -0.736683 |
| 26 | 1 | 0 | 4.894981 | -1.399436 | 1.159230 |
| 27 | 1 | 0 | 4.443825 | -1.594846 | -1.554429 |
| 28 | 6 | 0 | -0.234275 | 1.833165 | -0.370713 |
| 29 | 6 | 0 | 1.760426 | -1.222053 | 0.269033 |
| 30 | 7 | 0 | -0.984254 | 1.787412 | -1.492510 |
| 31 | 7 | 0 | 0.628655 | 2.864223 | -0.536046 |
| 32 | 7 | 0 | 2.743726 | -1.222755 | 1.201055 |
| 33 | 7 | 0 | 2.388880 | -1.379986 | -0.922866 |
| 34 | 6 | 0 | 2.537368 | -1.136301 | 2.661693 |
| 35 | 6 | 0 | 3.060364 | 0.196991 | 3.184288 |
| 36 | 6 | 0 | 3.178241 | -2.335912 | 3.352027 |
| 37 | 1 | 0 | 1.452238 | -1.181624 | 2.791491 |
| 38 | 1 | 0 | 2.534559 | 1.030727 | 2.710066 |
| 39 | 1 | 0 | 2.897595 | 0.257736 | 4.263416 |
| 40 | 1 | 0 | 4.135356 | 0.297674 | 2.997597 |
| 41 | 1 | 0 | 2.814736 | -3.274168 | 2.925854 |
| 42 | 1 | 0 | 4.269714 | -2.310498 | 3.270856 |
| 43 | 1 | 0 | 2.925088 | -2.317654 | 4.414822 |
| 44 | 6 | 0 | 1.726887 | -1.294265 | -2.239076 |
| 45 | 6 | 0 | 2.176744 | -2.435054 | -3.143060 |
| 46 | 6 | 0 | 1.987367 | 0.082481 | -2.844839 |
| 47 | 1 | 0 | 0.660597 | -1.405372 | -2.025957 |
| 48 | 1 | 0 | 2.017508 | -3.403887 | -2.662830 |
| 49 | 1 | 0 | 1.596971 | -2.411281 | -4.069191 |
| 50 | 1 | 0 | 3.233810 | -2.345360 | -3.413314 |
| 51 | 1 | 0 | 1.612846 | 0.872129 | -2.184206 |
| 52 | 1 | 0 | 3.059062 | 0.242799 | -3.005407 |
| 53 | 1 | 0 | 1.484479 | 0.169993 | -3.812342 |
| 54 | 6 | 0 | -2.063196 | 0.813208 | -1.772017 |
| 55 | 6 | 0 | -1.927094 | 0.259499 | -3.185195 |
| 56 | 6 | 0 | -3.427755 | 1.438580 | -1.509351 |
| 57 | 1 | 0 | -1.887631 | -0.000888 | -1.074454 |
| 58 | 1 | 0 | -0.914280 | -0.111542 | -3.369063 |
| 59 | 1 | 0 | -2.621411 | -0.577365 | -3.295961 |
| 60 | 1 | 0 | -2.176566 | 1.002927 | -3.949093 |
| 61 | 1 | 0 | -3.494313 | 1.826727 | -0.489442 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -3.628313 | 2.250585 | -2.216814 |
| 63 | 1 | 0 | -4.200280 | 0.674720 | -1.635573 |
| 64 | 6 | 0 | 1.721277 | 3.225299 | 0.398559 |
| 65 | 6 | 0 | 2.009899 | 4.719847 | 0.342145 |
| 66 | 6 | 0 | 2.951925 | 2.379443 | 0.081625 |
| 67 | 1 | 0 | 1.343747 | 2.965426 | 1.390482 |
| 68 | 1 | 0 | 1.098352 | 5.309386 | 0.469546 |
| 69 | 1 | 0 | 2.696924 | 4.974317 | 1.152505 |
| 70 | 1 | 0 | 2.494725 | 5.007095 | -0.596071 |
| 71 | 1 | 0 | 2.724616 | 1.310131 | 0.161921 |
| 72 | 1 | 0 | 3.308213 | 2.585467 | -0.933670 |
| 73 | 1 | 0 | 3.756765 | 2.614377 | 0.784027 |
| 74 | 5 | 0 | 0.225597 | -0.976530 | 0.513490 |
| 75 | 1 | 0 | -4.249374 | -2.453600 | -0.077970 |
| 76 | 1 | 0 | -4.673080 | -1.537760 | 1.558858 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.249820 | -4.412764 | -0.997953 |
| 2 | 6 | 0 | 0.780080 | -3.199320 | -0.565854 |
| 3 | 6 | 0 | -0.011186 | -2.163868 | 0.027127 |
| 4 | 6 | 0 | -1.403346 | -2.472347 | 0.287354 |
| 5 | 6 | 0 | -1.928273 | -3.688111 | -0.221392 |
| 6 | 6 | 0 | -1.132336 | -4.643591 | -0.860982 |
| 7 | 6 | 0 | -2.292983 | -1.592794 | 1.100562 |
| 8 | 6 | 0 | -2.029688 | -0.217126 | 1.395896 |
| 9 | 6 | 0 | -2.957306 | 0.540736 | 2.150063 |
| 10 | 1 | 0 | -2.717906 | 1.586249 | 2.380951 |
| 11 | 6 | 0 | -4.150441 | -0.012400 | 2.623448 |
| 12 | 6 | 0 | -4.397033 | -1.375089 | 2.388775 |
| 13 | 6 | 0 | -3.481576 | -2.139433 | 1.661843 |
| 14 | 1 | 0 | 0.897785 | -5.170734 | -1.452421 |
| 15 | 1 | 0 | 1.856610 | -3.025710 | -0.685273 |
| 16 | 1 | 0 | -1.584289 | -5.568637 | -1.234057 |
| 17 | 1 | 0 | -4.856001 | 0.596032 | 3.198866 |
| 18 | 1 | 0 | -5.295656 | -1.852701 | 2.794134 |
| 19 | 15 | 0 | -0.446995 | 0.639887 | 1.007228 |
| 20 | 6 | 0 | -1.757737 | 2.583907 | -2.391262 |
| 21 | 6 | 0 | -1.153692 | 3.601782 | -1.702044 |
| 22 | 1 | 0 | -2.266387 | 2.589064 | -3.351912 |

| | | | | | |
|---|---|---|---|---|---|
| 23 | 1 | 0 | -1.035536 | 4.652391 | -1.954776 |
| 24 | 6 | 0 | 4.325462 | -0.062989 | 0.855119 |
| 25 | 6 | 0 | 4.302107 | -0.208894 | -0.505807 |
| 26 | 1 | 0 | 5.153019 | 0.152684 | 1.526219 |
| 27 | 1 | 0 | 5.102935 | -0.132222 | -1.236714 |
| 28 | 6 | 0 | -0.955282 | 1.718047 | -0.465627 |
| 29 | 6 | 0 | 2.187637 | -0.536313 | 0.256757 |
| 30 | 7 | 0 | -1.623430 | 1.433922 | -1.629553 |
| 31 | 7 | 0 | -0.668461 | 3.062001 | -0.520841 |
| 32 | 7 | 0 | 3.030675 | -0.269473 | 1.310412 |
| 33 | 7 | 0 | 2.991440 | -0.502687 | -0.860529 |
| 34 | 6 | 0 | 2.645103 | -0.324548 | 2.749173 |
| 35 | 6 | 0 | 2.858711 | 1.040589 | 3.416326 |
| 36 | 6 | 0 | 3.388999 | -1.468820 | 3.455102 |
| 37 | 1 | 0 | 1.565512 | -0.555533 | 2.728004 |
| 38 | 1 | 0 | 2.288510 | 1.827345 | 2.894634 |
| 39 | 1 | 0 | 2.508033 | 0.997239 | 4.461227 |
| 40 | 1 | 0 | 3.925942 | 1.326538 | 3.433826 |
| 41 | 1 | 0 | 3.211554 | -2.431581 | 2.947519 |
| 42 | 1 | 0 | 4.477770 | -1.287109 | 3.496786 |
| 43 | 1 | 0 | 3.025048 | -1.555006 | 4.492826 |
| 44 | 6 | 0 | 2.507601 | -0.635092 | -2.261472 |
| 45 | 6 | 0 | 3.335536 | -1.673931 | -3.031331 |
| 46 | 6 | 0 | 2.499284 | 0.740846 | -2.947677 |
| 47 | 1 | 0 | 1.471861 | -1.001585 | -2.156047 |
| 48 | 1 | 0 | 3.347558 | -2.646328 | -2.512193 |
| 49 | 1 | 0 | 2.893306 | -1.824932 | -4.030438 |
| 50 | 1 | 0 | 4.378592 | -1.342241 | -3.179931 |
| 51 | 1 | 0 | 1.881056 | 1.461269 | -2.385087 |
| 52 | 1 | 0 | 3.520260 | 1.152252 | -3.038165 |
| 53 | 1 | 0 | 2.084922 | 0.647930 | -3.966301 |
| 54 | 6 | 0 | -2.193101 | 0.109960 | -2.020074 |
| 55 | 6 | 0 | -1.755278 | -0.263228 | -3.443617 |
| 56 | 6 | 0 | -3.719294 | 0.125786 | -1.848029 |
| 57 | 1 | 0 | -1.749295 | -0.608463 | -1.315277 |
| 58 | 1 | 0 | -0.658785 | -0.214723 | -3.554582 |
| 59 | 1 | 0 | -2.074784 | -1.297469 | -3.652936 |
| 60 | 1 | 0 | -2.216474 | 0.386032 | -4.209064 |
| 61 | 1 | 0 | -3.999932 | 0.382630 | -0.813732 |
| 62 | 1 | 0 | -4.195254 | 0.845788 | -2.537998 |
| 63 | 1 | 0 | -4.120755 | -0.876193 | -2.074033 |
| 64 | 6 | 0 | 0.024626 | 3.867009 | 0.529668 |
| 65 | 6 | 0 | -0.909629 | 4.965508 | 1.057797 |
| 66 | 6 | 0 | 1.355230 | 4.411576 | -0.009827 |

| | | | | | |
|---|---|---|---|---|---|
| 67 | 1 | 0 | 0.222402 | 3.139240 | 1.335592 |
| 68 | 1 | 0 | -1.856742 | 4.540343 | 1.430038 |
| 69 | 1 | 0 | -0.416882 | 5.490807 | 1.893289 |
| 70 | 1 | 0 | -1.143527 | 5.718000 | 0.283897 |
| 71 | 1 | 0 | 2.006454 | 3.596462 | -0.368670 |
| 72 | 1 | 0 | 1.201520 | 5.126632 | -0.837627 |
| 73 | 1 | 0 | 1.885380 | 4.946601 | 0.796206 |
| 74 | 5 | 0 | 0.632561 | -0.803971 | 0.345808 |
| 75 | 1 | 0 | -2.997809 | -3.897115 | -0.126084 |
| 76 | 1 | 0 | -3.681566 | -3.208552 | 1.553033 |

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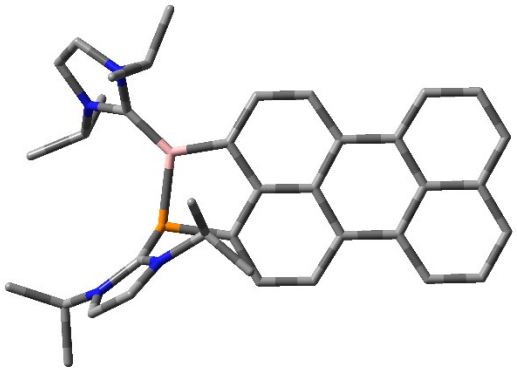
**1PB-c**



**UB3LYP/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.275004 | 2.369979 | 0.071090 |
| 2 | 6 | 0 | 3.070836 | 1.227242 | -0.138992 |
| 3 | 6 | 0 | 2.400095 | -0.006509 | -0.432984 |
| 4 | 6 | 0 | 0.976658 | -0.026919 | -0.463244 |
| 5 | 6 | 0 | 0.168252 | 1.146021 | -0.192789 |
| 6 | 6 | 0 | 0.885291 | 2.339889 | 0.041769 |
| 7 | 6 | 0 | 3.120278 | -1.212137 | -0.705971 |
| 8 | 6 | 0 | 0.285603 | -1.217384 | -0.794843 |
| 9 | 1 | 0 | 0.348110 | 3.272977 | 0.191582 |
| 10 | 6 | 0 | 0.996017 | -2.373428 | -1.092607 |
| 11 | 6 | 0 | 2.394254 | -2.366716 | -1.028936 |
| 12 | 1 | 0 | 0.481711 | -3.284886 | -1.388049 |
| 13 | 6 | 0 | 6.651874 | 2.423976 | 0.256821 |
| 14 | 6 | 0 | 7.366283 | 1.271797 | 0.009010 |
| 15 | 6 | 0 | 6.691945 | 0.061315 | -0.294130 |
| 16 | 6 | 0 | 5.258395 | 0.039677 | -0.345286 |
| 17 | 6 | 0 | 4.529518 | 1.250159 | -0.087232 |

| | | | | | |
|---|---|---|---|---|---|
| 18 | 6 | 0 | 5.249600 | 2.411125 | 0.210494 |
| 19 | 1 | 0 | 7.169114 | 3.350168 | 0.490337 |
| 20 | 6 | 0 | 7.419691 | -1.128477 | -0.546338 |
| 21 | 6 | 0 | 4.589789 | -1.189449 | -0.652282 |
| 22 | 6 | 0 | 5.357786 | -2.330252 | -0.887415 |
| 23 | 6 | 0 | 6.760521 | -2.302720 | -0.836918 |
| 24 | 1 | 0 | 7.319870 | -3.213800 | -1.028604 |
| 25 | 1 | 0 | 4.877329 | -3.274743 | -1.116289 |
| 26 | 1 | 0 | 2.915107 | -3.287216 | -1.265543 |
| 27 | 1 | 0 | 4.725985 | 3.337965 | 0.415712 |
| 28 | 1 | 0 | 2.753633 | 3.324525 | 0.261003 |
| 29 | 15 | 0 | -1.519455 | -0.934482 | -0.943353 |
| 30 | 6 | 0 | -3.519837 | -3.503309 | 1.447458 |
| 31 | 6 | 0 | -2.582988 | -3.113570 | 2.350276 |
| 32 | 1 | 0 | -4.329371 | -4.209059 | 1.540594 |
| 33 | 1 | 0 | -2.427754 | -3.422922 | 3.371208 |
| 34 | 6 | 0 | -4.189093 | 3.309519 | -0.881614 |
| 35 | 6 | 0 | -3.770581 | 3.713249 | 0.342751 |
| 36 | 1 | 0 | -4.977198 | 3.692495 | -1.509632 |
| 37 | 1 | 0 | -4.139427 | 4.499148 | 0.981864 |
| 38 | 6 | 0 | -2.194457 | -1.991484 | 0.449393 |
| 39 | 6 | 0 | -2.456293 | 1.986347 | -0.289047 |
| 40 | 7 | 0 | -1.777007 | -2.179853 | 1.731379 |
| 41 | 7 | 0 | -3.271377 | -2.810841 | 0.279795 |
| 42 | 7 | 0 | -2.708426 | 2.901242 | 0.700564 |
| 43 | 7 | 0 | -3.382842 | 2.252146 | -1.264719 |
| 44 | 6 | 0 | -0.616575 | -1.529080 | 2.404690 |
| 45 | 6 | 0 | 0.512748 | -2.542625 | 2.611171 |
| 46 | 6 | 0 | -1.065304 | -0.876699 | 3.715640 |
| 47 | 1 | 0 | -0.290321 | -0.750848 | 1.716564 |
| 48 | 1 | 0 | 0.829704 | -2.981216 | 1.662159 |
| 49 | 1 | 0 | 1.375103 | -2.034724 | 3.053831 |
| 50 | 1 | 0 | 0.210150 | -3.345863 | 3.292937 |
| 51 | 1 | 0 | -1.904199 | -0.193453 | 3.556161 |
| 52 | 1 | 0 | -1.357538 | -1.617381 | 4.468147 |
| 53 | 1 | 0 | -0.229349 | -0.304752 | 4.129893 |
| 54 | 6 | 0 | -4.073822 | -2.991800 | -0.962817 |
| 55 | 6 | 0 | -5.521409 | -2.551935 | -0.725903 |
| 56 | 6 | 0 | -3.955411 | -4.434052 | -1.463783 |
| 57 | 1 | 0 | -3.607009 | -2.325546 | -1.690797 |
| 58 | 1 | 0 | -5.569637 | -1.518764 | -0.366631 |
| 59 | 1 | 0 | -6.078019 | -2.615514 | -1.666058 |
| 60 | 1 | 0 | -6.029844 | -3.193425 | 0.002455 |
| 61 | 1 | 0 | -2.909144 | -4.711510 | -1.624208 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -4.402342 | -5.149450 | -0.764689 |
| 63 | 1 | 0 | -4.483240 | -4.529240 | -2.417685 |
| 64 | 6 | 0 | -3.399370 | 1.673234 | -2.631772 |
| 65 | 6 | 0 | -2.889133 | 2.701290 | -3.648068 |
| 66 | 6 | 0 | -4.790936 | 1.134299 | -2.973707 |
| 67 | 1 | 0 | -2.699115 | 0.838519 | -2.594931 |
| 68 | 1 | 0 | -1.888254 | 3.051955 | -3.378722 |
| 69 | 1 | 0 | -2.834814 | 2.241411 | -4.639903 |
| 70 | 1 | 0 | -3.556010 | 3.568063 | -3.715424 |
| 71 | 1 | 0 | -5.132580 | 0.412215 | -2.224797 |
| 72 | 1 | 0 | -5.536507 | 1.934168 | -3.044781 |
| 73 | 1 | 0 | -4.756884 | 0.632339 | -3.945624 |
| 74 | 6 | 0 | -2.066877 | 2.936295 | 2.036290 |
| 75 | 6 | 0 | -3.062738 | 2.472210 | 3.106721 |
| 76 | 6 | 0 | -1.501349 | 4.327774 | 2.336928 |
| 77 | 1 | 0 | -1.244396 | 2.221062 | 1.968496 |
| 78 | 1 | 0 | -3.471323 | 1.485830 | 2.864140 |
| 79 | 1 | 0 | -2.562532 | 2.412093 | 4.078566 |
| 80 | 1 | 0 | -3.899408 | 3.172400 | 3.206472 |
| 81 | 1 | 0 | -0.815481 | 4.660912 | 1.553263 |
| 82 | 1 | 0 | -2.295652 | 5.075468 | 2.440746 |
| 83 | 1 | 0 | -0.951258 | 4.300050 | 3.282668 |
| 84 | 5 | 0 | -1.328206 | 0.908412 | -0.309099 |
| 85 | 1 | 0 | 8.452384 | 1.273040 | 0.042804 |
| 86 | 1 | 0 | 8.505237 | -1.097288 | -0.505517 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.223042 | 2.394606 | -0.197366 |
| 2 | 6 | 0 | 3.007172 | 1.244517 | -0.315394 |
| 3 | 6 | 0 | 2.337787 | 0.000832 | -0.548540 |
| 4 | 6 | 0 | 0.925067 | -0.012078 | -0.609384 |
| 5 | 6 | 0 | 0.121589 | 1.171105 | -0.414413 |
| 6 | 6 | 0 | 0.830920 | 2.368335 | -0.248178 |
| 7 | 6 | 0 | 3.049564 | -1.221188 | -0.730044 |
| 8 | 6 | 0 | 0.231654 | -1.213009 | -0.874659 |
| 9 | 1 | 0 | 0.294078 | 3.309404 | -0.167739 |
| 10 | 6 | 0 | 0.931011 | -2.382275 | -1.094112 |
| 11 | 6 | 0 | 2.328341 | -2.380138 | -1.005916 |
| 12 | 1 | 0 | 0.413147 | -3.307341 | -1.334147 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | 6.585360 | 2.430902 | 0.095356 |
| 14 | 6 | 0 | 7.290085 | 1.264961 | -0.054476 |
| 15 | 6 | 0 | 6.611469 | 0.044888 | -0.295668 |
| 16 | 6 | 0 | 5.189611 | 0.032150 | -0.386994 |
| 17 | 6 | 0 | 4.469143 | 1.259919 | -0.228656 |
| 18 | 6 | 0 | 5.184069 | 2.424525 | 0.010837 |
| 19 | 1 | 0 | 7.103714 | 3.366220 | 0.281189 |
| 20 | 6 | 0 | 7.334890 | -1.162839 | -0.444850 |
| 21 | 6 | 0 | 4.520097 | -1.206941 | -0.631825 |
| 22 | 6 | 0 | 5.275260 | -2.360553 | -0.763255 |
| 23 | 6 | 0 | 6.676380 | -2.342921 | -0.672507 |
| 24 | 1 | 0 | 7.230148 | -3.269546 | -0.784383 |
| 25 | 1 | 0 | 4.793945 | -3.315569 | -0.940154 |
| 26 | 1 | 0 | 2.844887 | -3.316707 | -1.179185 |
| 27 | 1 | 0 | 4.666217 | 3.367954 | 0.140536 |
| 28 | 1 | 0 | 2.700548 | 3.358474 | -0.060247 |
| 29 | 15 | 0 | -1.574758 | -0.963396 | -0.964853 |
| 30 | 6 | 0 | -3.154468 | -3.400828 | 1.808735 |
| 31 | 6 | 0 | -2.234780 | -2.798155 | 2.599180 |
| 32 | 1 | 0 | -3.864325 | -4.181404 | 2.029270 |
| 33 | 1 | 0 | -1.994220 | -2.957969 | 3.637565 |
| 34 | 6 | 0 | -4.315039 | 3.212140 | -0.950157 |
| 35 | 6 | 0 | -3.768500 | 3.735077 | 0.169509 |
| 36 | 1 | 0 | -5.177947 | 3.523169 | -1.515606 |
| 37 | 1 | 0 | -4.073150 | 4.578961 | 0.767003 |
| 38 | 6 | 0 | -2.079518 | -1.885370 | 0.571976 |
| 39 | 6 | 0 | -2.509386 | 1.975720 | -0.438724 |
| 40 | 7 | 0 | -1.584983 | -1.861896 | 1.830443 |
| 41 | 7 | 0 | -3.050438 | -2.828236 | 0.562892 |
| 42 | 7 | 0 | -2.661392 | 2.971812 | 0.476475 |
| 43 | 7 | 0 | -3.532400 | 2.139343 | -1.321028 |
| 44 | 6 | 0 | -0.492759 | -1.001333 | 2.342165 |
| 45 | 6 | 0 | 0.795135 | -1.803715 | 2.493824 |
| 46 | 6 | 0 | -0.919375 | -0.333231 | 3.645756 |
| 47 | 1 | 0 | -0.360484 | -0.230824 | 1.584404 |
| 48 | 1 | 0 | 1.080684 | -2.279275 | 1.553674 |
| 49 | 1 | 0 | 1.603372 | -1.129501 | 2.790446 |
| 50 | 1 | 0 | 0.691857 | -2.572873 | 3.267648 |
| 51 | 1 | 0 | -1.895735 | 0.147068 | 3.547245 |
| 52 | 1 | 0 | -0.959879 | -1.041409 | 4.480092 |
| 53 | 1 | 0 | -0.182154 | 0.431773 | 3.905316 |
| 54 | 6 | 0 | -3.858070 | -3.257392 | -0.601700 |
| 55 | 6 | 0 | -5.345468 | -3.137137 | -0.285540 |
| 56 | 6 | 0 | -3.440836 | -4.661600 | -1.027536 |

| | | | | | |
|---|---|---|---|---|---|
| 57 | 1 | 0 | -3.601109 | -2.556453 | -1.397645 |
| 58 | 1 | 0 | -5.597846 | -2.130322 | 0.060137 |
| 59 | 1 | 0 | -5.922145 | -3.344000 | -1.191157 |
| 60 | 1 | 0 | -5.661872 | -3.856236 | 0.477298 |
| 61 | 1 | 0 | -2.372746 | -4.695505 | -1.261099 |
| 62 | 1 | 0 | -3.651597 | -5.399027 | -0.245761 |
| 63 | 1 | 0 | -3.997396 | -4.952186 | -1.922706 |
| 64 | 6 | 0 | -3.771176 | 1.308278 | -2.513140 |
| 65 | 6 | 0 | -4.093536 | 2.170946 | -3.729684 |
| 66 | 6 | 0 | -4.856016 | 0.276900 | -2.213216 |
| 67 | 1 | 0 | -2.825568 | 0.794187 | -2.695809 |
| 68 | 1 | 0 | -3.330611 | 2.939436 | -3.880475 |
| 69 | 1 | 0 | -4.119710 | 1.535741 | -4.619180 |
| 70 | 1 | 0 | -5.072139 | 2.655035 | -3.645848 |
| 71 | 1 | 0 | -4.593874 | -0.310162 | -1.327184 |
| 72 | 1 | 0 | -5.821347 | 0.762303 | -2.032120 |
| 73 | 1 | 0 | -4.968816 | -0.406013 | -3.060368 |
| 74 | 6 | 0 | -1.914353 | 3.102342 | 1.739419 |
| 75 | 6 | 0 | -2.822986 | 2.714573 | 2.905368 |
| 76 | 6 | 0 | -1.345095 | 4.509222 | 1.896571 |
| 77 | 1 | 0 | -1.093625 | 2.386157 | 1.662078 |
| 78 | 1 | 0 | -3.270852 | 1.730486 | 2.737167 |
| 79 | 1 | 0 | -2.246659 | 2.684767 | 3.834516 |
| 80 | 1 | 0 | -3.632786 | 3.440086 | 3.036171 |
| 81 | 1 | 0 | -0.748920 | 4.801442 | 1.028772 |
| 82 | 1 | 0 | -2.138718 | 5.251401 | 2.034515 |
| 83 | 1 | 0 | -0.703687 | 4.544655 | 2.781447 |
| 84 | 5 | 0 | -1.377503 | 0.907680 | -0.479376 |
| 85 | 1 | 0 | 8.374376 | 1.258708 | 0.010056 |
| 86 | 1 | 0 | 8.418606 | -1.137135 | -0.374108 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.259174 | 2.385663 | -0.272616 |
| 2 | 6 | 0 | 3.028177 | 1.225146 | -0.349025 |
| 3 | 6 | 0 | 2.344011 | -0.019072 | -0.527926 |
| 4 | 6 | 0 | 0.929221 | -0.017784 | -0.582316 |
| 5 | 6 | 0 | 0.140859 | 1.178339 | -0.425139 |
| 6 | 6 | 0 | 0.862381 | 2.370692 | -0.309844 |
| 7 | 6 | 0 | 3.042665 | -1.255864 | -0.674625 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 6 | 0 | 0.221930 | -1.219257 | -0.822554 |
| 9 | 1 | 0 | 0.336455 | 3.321139 | -0.265219 |
| 10 | 6 | 0 | 0.909377 | -2.399871 | -1.015891 |
| 11 | 6 | 0 | 2.309308 | -2.412811 | -0.920961 |
| 12 | 1 | 0 | 0.381625 | -3.322869 | -1.243833 |
| 13 | 6 | 0 | 6.625137 | 2.388896 | -0.023337 |
| 14 | 6 | 0 | 7.316164 | 1.209603 | -0.130654 |
| 15 | 6 | 0 | 6.621720 | -0.012137 | -0.313832 |
| 16 | 6 | 0 | 5.198946 | -0.012853 | -0.392936 |
| 17 | 6 | 0 | 4.493359 | 1.228287 | -0.278021 |
| 18 | 6 | 0 | 5.221248 | 2.393776 | -0.093573 |
| 19 | 1 | 0 | 7.154520 | 3.325428 | 0.118195 |
| 20 | 6 | 0 | 7.331677 | -1.233843 | -0.416676 |
| 21 | 6 | 0 | 4.513980 | -1.254402 | -0.581395 |
| 22 | 6 | 0 | 5.254560 | -2.421455 | -0.666011 |
| 23 | 6 | 0 | 6.658392 | -2.415775 | -0.586411 |
| 24 | 1 | 0 | 7.200530 | -3.352664 | -0.660817 |
| 25 | 1 | 0 | 4.758912 | -3.376776 | -0.794210 |
| 26 | 1 | 0 | 2.817370 | -3.357563 | -1.073464 |
| 27 | 1 | 0 | 4.712053 | 3.345727 | 0.003038 |
| 28 | 1 | 0 | 2.748685 | 3.348705 | -0.180972 |
| 29 | 15 | 0 | -1.582010 | -0.948507 | -0.963253 |
| 30 | 6 | 0 | -3.199538 | -3.386793 | 1.801920 |
| 31 | 6 | 0 | -2.298035 | -2.768661 | 2.605725 |
| 32 | 1 | 0 | -3.905634 | -4.173897 | 2.013752 |
| 33 | 1 | 0 | -2.073337 | -2.916277 | 3.650200 |
| 34 | 6 | 0 | -4.276867 | 3.273677 | -0.986106 |
| 35 | 6 | 0 | -3.648007 | 3.873201 | 0.051378 |
| 36 | 1 | 0 | -5.160092 | 3.565500 | -1.530476 |
| 37 | 1 | 0 | -3.890685 | 4.776391 | 0.588425 |
| 38 | 6 | 0 | -2.117978 | -1.866163 | 0.574480 |
| 39 | 6 | 0 | -2.477525 | 2.023093 | -0.470201 |
| 40 | 7 | 0 | -1.645337 | -1.832191 | 1.840038 |
| 41 | 7 | 0 | -3.079765 | -2.818656 | 0.555215 |
| 42 | 7 | 0 | -2.547079 | 3.102347 | 0.360942 |
| 43 | 7 | 0 | -3.549492 | 2.146281 | -1.303193 |
| 44 | 6 | 0 | -0.569224 | -0.955881 | 2.363264 |
| 45 | 6 | 0 | 0.718884 | -1.749253 | 2.550794 |
| 46 | 6 | 0 | -1.030284 | -0.289763 | 3.655567 |
| 47 | 1 | 0 | -0.429187 | -0.191802 | 1.598637 |
| 48 | 1 | 0 | 1.036208 | -2.221188 | 1.618689 |
| 49 | 1 | 0 | 1.511465 | -1.070607 | 2.877603 |
| 50 | 1 | 0 | 0.592300 | -2.519885 | 3.319296 |
| 51 | 1 | 0 | -2.008837 | 0.181074 | 3.535112 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 1 | 0 | -1.082719 | -1.002065 | 4.485134 |
| 53 | 1 | 0 | -0.305188 | 0.479939 | 3.933403 |
| 54 | 6 | 0 | -3.843947 | -3.283663 | -0.627437 |
| 55 | 6 | 0 | -5.336573 | -3.296246 | -0.318831 |
| 56 | 6 | 0 | -3.313492 | -4.642847 | -1.069801 |
| 57 | 1 | 0 | -3.637969 | -2.547488 | -1.406196 |
| 58 | 1 | 0 | -5.674939 | -2.326090 | 0.055348 |
| 59 | 1 | 0 | -5.887525 | -3.524882 | -1.234678 |
| 60 | 1 | 0 | -5.592920 | -4.064545 | 0.417358 |
| 61 | 1 | 0 | -2.247625 | -4.584604 | -1.306971 |
| 62 | 1 | 0 | -3.458888 | -5.396442 | -0.289136 |
| 63 | 1 | 0 | -3.848859 | -4.972401 | -1.963772 |
| 64 | 6 | 0 | -3.901151 | 1.194517 | -2.370032 |
| 65 | 6 | 0 | -4.477933 | 1.914235 | -3.583736 |
| 66 | 6 | 0 | -4.856084 | 0.141687 | -1.812024 |
| 67 | 1 | 0 | -2.958127 | 0.722566 | -2.656054 |
| 68 | 1 | 0 | -3.818952 | 2.720105 | -3.916235 |
| 69 | 1 | 0 | -4.584147 | 1.198168 | -4.402191 |
| 70 | 1 | 0 | -5.471263 | 2.326073 | -3.380378 |
| 71 | 1 | 0 | -4.437495 | -0.321068 | -0.911346 |
| 72 | 1 | 0 | -5.816825 | 0.596902 | -1.548392 |
| 73 | 1 | 0 | -5.035815 | -0.639339 | -2.557239 |
| 74 | 6 | 0 | -1.760251 | 3.291444 | 1.594519 |
| 75 | 6 | 0 | -2.636589 | 2.946443 | 2.797079 |
| 76 | 6 | 0 | -1.208047 | 4.710212 | 1.676520 |
| 77 | 1 | 0 | -0.935649 | 2.579094 | 1.524822 |
| 78 | 1 | 0 | -3.079551 | 1.953787 | 2.675412 |
| 79 | 1 | 0 | -2.039982 | 2.957625 | 3.713460 |
| 80 | 1 | 0 | -3.447725 | 3.672734 | 2.911459 |
| 81 | 1 | 0 | -0.646440 | 4.977950 | 0.778558 |
| 82 | 1 | 0 | -2.010392 | 5.442512 | 1.812805 |
| 83 | 1 | 0 | -0.541127 | 4.789853 | 2.538736 |
| 84 | 5 | 0 | -1.371019 | 0.932035 | -0.486873 |
| 85 | 1 | 0 | 8.400795 | 1.191336 | -0.076095 |
| 86 | 1 | 0 | 8.416053 | -1.214292 | -0.355612 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.278217 | 2.381767 | 0.030976 |
| 2 | 6 | 0 | 3.077368 | 1.225092 | -0.156694 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 6 | 0 | 2.401744 | -0.018117 | -0.427029 |
| 4 | 6 | 0 | 0.969550 | -0.037106 | -0.451245 |
| 5 | 6 | 0 | 0.160206 | 1.145883 | -0.198276 |
| 6 | 6 | 0 | 0.882240 | 2.351982 | 0.006997 |
| 7 | 6 | 0 | 3.123799 | -1.235505 | -0.681286 |
| 8 | 6 | 0 | 0.274049 | -1.238382 | -0.763078 |
| 9 | 1 | 0 | 0.339470 | 3.295742 | 0.137339 |
| 10 | 6 | 0 | 0.985568 | -2.410285 | -1.043342 |
| 11 | 6 | 0 | 2.389832 | -2.403480 | -0.982302 |
| 12 | 1 | 0 | 0.463666 | -3.332665 | -1.324237 |
| 13 | 6 | 0 | 6.672606 | 2.432051 | 0.219452 |
| 14 | 6 | 0 | 7.390501 | 1.266408 | -0.014390 |
| 15 | 6 | 0 | 6.711718 | 0.046902 | -0.298677 |
| 16 | 6 | 0 | 5.268617 | 0.025658 | -0.346719 |
| 17 | 6 | 0 | 4.538029 | 1.246291 | -0.105956 |
| 18 | 6 | 0 | 5.265322 | 2.420114 | 0.175638 |
| 19 | 1 | 0 | 7.196641 | 3.368170 | 0.440119 |
| 20 | 6 | 0 | 7.440946 | -1.152604 | -0.535389 |
| 21 | 6 | 0 | 4.594765 | -1.212838 | -0.633524 |
| 22 | 6 | 0 | 5.367297 | -2.366964 | -0.854972 |
| 23 | 6 | 0 | 6.775323 | -2.339575 | -0.808534 |
| 24 | 1 | 0 | 7.339022 | -3.261012 | -0.989118 |
| 25 | 1 | 0 | 4.879026 | -3.321889 | -1.069625 |
| 26 | 1 | 0 | 2.915169 | -3.336158 | -1.205630 |
| 27 | 1 | 0 | 4.736102 | 3.357362 | 0.370274 |
| 28 | 1 | 0 | 2.764666 | 3.347679 | 0.197767 |
| 29 | 15 | 0 | -1.534349 | -0.946940 | -0.920855 |
| 30 | 6 | 0 | -3.530201 | -3.512481 | 1.492719 |
| 31 | 6 | 0 | -2.609119 | -3.078892 | 2.409043 |
| 32 | 1 | 0 | -4.334139 | -4.237527 | 1.589043 |
| 33 | 1 | 0 | -2.463066 | -3.362748 | 3.447978 |
| 34 | 6 | 0 | -4.222430 | 3.301768 | -0.923305 |
| 35 | 6 | 0 | -3.772208 | 3.757861 | 0.284152 |
| 36 | 1 | 0 | -5.026120 | 3.667142 | -1.556885 |
| 37 | 1 | 0 | -4.126039 | 4.577937 | 0.903471 |
| 38 | 6 | 0 | -2.209229 | -1.986544 | 0.475216 |
| 39 | 6 | 0 | -2.476363 | 1.981334 | -0.303918 |
| 40 | 7 | 0 | -1.808919 | -2.139707 | 1.779277 |
| 41 | 7 | 0 | -3.274759 | -2.839923 | 0.308729 |
| 42 | 7 | 0 | -2.705216 | 2.950127 | 0.655753 |
| 43 | 7 | 0 | -3.433029 | 2.214937 | -1.275827 |
| 44 | 6 | 0 | -0.663065 | -1.448350 | 2.445109 |
| 45 | 6 | 0 | 0.503443 | -2.427365 | 2.643130 |
| 46 | 6 | 0 | -1.124975 | -0.809720 | 3.763155 |

| | | | | | |
|---|---|---|---|---|---|
| 47 | 1 | 0 | -0.370724 | -0.652697 | 1.741848 |
| 48 | 1 | 0 | 0.832537 | -2.856388 | 1.683519 |
| 49 | 1 | 0 | 1.357690 | -1.887916 | 3.085597 |
| 50 | 1 | 0 | 0.227611 | -3.247111 | 3.330925 |
| 51 | 1 | 0 | -1.995760 | -0.150690 | 3.611765 |
| 52 | 1 | 0 | -1.383475 | -1.565752 | 4.525751 |
| 53 | 1 | 0 | -0.298955 | -0.204246 | 4.172493 |
| 54 | 6 | 0 | -4.046896 | -3.062822 | -0.950551 |
| 55 | 6 | 0 | -5.512936 | -2.650605 | -0.752947 |
| 56 | 6 | 0 | -3.882952 | -4.515106 | -1.422125 |
| 57 | 1 | 0 | -3.568035 | -2.389363 | -1.682211 |
| 58 | 1 | 0 | -5.594254 | -1.604920 | -0.410475 |
| 59 | 1 | 0 | -6.050741 | -2.744865 | -1.711394 |
| 60 | 1 | 0 | -6.026919 | -3.297389 | -0.019757 |
| 61 | 1 | 0 | -2.819306 | -4.774316 | -1.554976 |
| 62 | 1 | 0 | -4.334069 | -5.232695 | -0.714058 |
| 63 | 1 | 0 | -4.390865 | -4.641491 | -2.393072 |
| 64 | 6 | 0 | -3.452892 | 1.592991 | -2.630114 |
| 65 | 6 | 0 | -2.741773 | 2.510152 | -3.638632 |
| 66 | 6 | 0 | -4.886961 | 1.239265 | -3.047299 |
| 67 | 1 | 0 | -2.874012 | 0.661688 | -2.522271 |
| 68 | 1 | 0 | -1.708387 | 2.721070 | -3.316279 |
| 69 | 1 | 0 | -2.701381 | 2.017982 | -4.625339 |
| 70 | 1 | 0 | -3.277770 | 3.468740 | -3.756764 |
| 71 | 1 | 0 | -5.388588 | 0.616153 | -2.287168 |
| 72 | 1 | 0 | -5.504740 | 2.137444 | -3.225456 |
| 73 | 1 | 0 | -4.858017 | 0.674261 | -3.994143 |
| 74 | 6 | 0 | -2.043823 | 3.022572 | 1.985442 |
| 75 | 6 | 0 | -3.030658 | 2.587884 | 3.082766 |
| 76 | 6 | 0 | -1.473898 | 4.426066 | 2.239571 |
| 77 | 1 | 0 | -1.215967 | 2.296250 | 1.920998 |
| 78 | 1 | 0 | -3.447841 | 1.588735 | 2.869426 |
| 79 | 1 | 0 | -2.515494 | 2.552917 | 4.057807 |
| 80 | 1 | 0 | -3.871018 | 3.298750 | 3.173637 |
| 81 | 1 | 0 | -0.796161 | 4.743082 | 1.430084 |
| 82 | 1 | 0 | -2.274070 | 5.181256 | 2.338480 |
| 83 | 1 | 0 | -0.903984 | 4.424460 | 3.184005 |
| 84 | 5 | 0 | -1.345860 | 0.906718 | -0.306917 |
| 85 | 1 | 0 | 8.485902 | 1.266836 | 0.017310 |
| 86 | 1 | 0 | 8.535831 | -1.121150 | -0.497254 |

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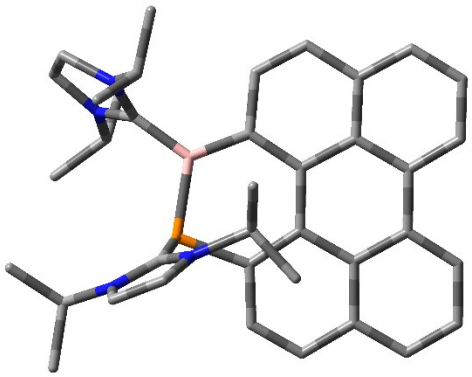
**1PB-d**



**UB3LYP/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.861729 | 1.355174 | -1.050363 |
| 2 | 6 | 0 | -1.946665 | 0.509182 | -0.696472 |
| 3 | 6 | 0 | -3.280085 | 1.063554 | -0.830402 |
| 4 | 6 | 0 | -3.470006 | 2.397823 | -1.332258 |
| 5 | 6 | 0 | -2.344656 | 3.175615 | -1.705273 |
| 6 | 6 | 0 | -1.086616 | 2.657262 | -1.570195 |
| 7 | 6 | 0 | -4.442870 | 0.315347 | -0.463699 |
| 8 | 6 | 0 | -4.767762 | 2.939872 | -1.466189 |
| 9 | 1 | 0 | -2.498891 | 4.174141 | -2.105114 |
| 10 | 1 | 0 | -0.227250 | 3.250732 | -1.874186 |
| 11 | 6 | 0 | -5.872454 | 2.194712 | -1.115140 |
| 12 | 6 | 0 | -5.705281 | 0.897694 | -0.620158 |
| 13 | 1 | 0 | -4.875085 | 3.949060 | -1.854403 |
| 14 | 1 | 0 | -6.872677 | 2.604216 | -1.222434 |
| 15 | 6 | 0 | -0.485897 | -2.923583 | 0.227613 |
| 16 | 6 | 0 | -1.598669 | -3.620358 | 0.570994 |
| 17 | 6 | 0 | -2.876161 | -2.987341 | 0.556964 |
| 18 | 6 | 0 | -2.977530 | -1.620731 | 0.122585 |
| 19 | 6 | 0 | -1.791182 | -0.874467 | -0.224776 |
| 20 | 6 | 0 | -0.505003 | -1.526799 | -0.130732 |
| 21 | 1 | 0 | -3.900544 | -4.739973 | 1.269356 |
| 22 | 1 | 0 | 0.470205 | -3.440076 | 0.226495 |
| 23 | 1 | 0 | -1.539146 | -4.668866 | 0.853127 |
| 24 | 6 | 0 | -4.017305 | -3.708889 | 0.945976 |
| 25 | 6 | 0 | -4.285569 | -1.044400 | 0.053806 |
| 26 | 6 | 0 | -5.389830 | -1.798510 | 0.470636 |
| 27 | 6 | 0 | -5.265925 | -3.114094 | 0.917326 |
| 28 | 1 | 0 | -6.148867 | -3.664518 | 1.228439 |
| 29 | 15 | 0 | 0.907413 | 0.929962 | -0.959958 |
| 30 | 6 | 0 | 1.669047 | 3.011727 | 2.513490 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 6 | 0 | 2.714895 | 3.392202 | 1.734469 |
| 32 | 1 | 0 | 1.406899 | 3.301241 | 3.518354 |
| 33 | 1 | 0 | 3.530143 | 4.067189 | 1.939618 |
| 34 | 6 | 0 | 4.054155 | -2.826527 | 0.149617 |
| 35 | 6 | 0 | 4.033695 | -2.740303 | -1.205211 |
| 36 | 1 | 0 | 4.772665 | -3.284761 | 0.810092 |
| 37 | 1 | 0 | 4.728027 | -3.116554 | -1.939307 |
| 38 | 6 | 0 | 1.464453 | 1.954500 | 0.547550 |
| 39 | 6 | 0 | 2.188998 | -1.705527 | -0.433914 |
| 40 | 7 | 0 | 2.577524 | 2.739982 | 0.524499 |
| 41 | 7 | 0 | 0.911241 | 2.121541 | 1.778601 |
| 42 | 7 | 0 | 2.915657 | -2.189503 | 0.612612 |
| 43 | 7 | 0 | 2.885035 | -2.052229 | -1.552041 |
| 44 | 6 | 0 | 2.567989 | -2.025933 | 2.045003 |
| 45 | 6 | 0 | 3.572486 | -1.093307 | 2.730965 |
| 46 | 6 | 0 | 2.456773 | -3.386872 | 2.738542 |
| 47 | 1 | 0 | 1.582181 | -1.553524 | 2.030150 |
| 48 | 1 | 0 | 3.622654 | -0.123468 | 2.225014 |
| 49 | 1 | 0 | 3.270826 | -0.924516 | 3.769738 |
| 50 | 1 | 0 | 4.578542 | -1.526911 | 2.745646 |
| 51 | 1 | 0 | 1.728386 | -4.028778 | 2.235819 |
| 52 | 1 | 0 | 3.420109 | -3.907830 | 2.771273 |
| 53 | 1 | 0 | 2.125607 | -3.241780 | 3.771528 |
| 54 | 6 | 0 | 2.425757 | -1.841322 | -2.950720 |
| 55 | 6 | 0 | 2.089857 | -3.185891 | -3.603868 |
| 56 | 6 | 0 | 3.454553 | -1.027379 | -3.738328 |
| 57 | 1 | 0 | 1.507382 | -1.258220 | -2.851503 |
| 58 | 1 | 0 | 1.342972 | -3.730365 | -3.018315 |
| 59 | 1 | 0 | 1.679415 | -3.012160 | -4.603373 |
| 60 | 1 | 0 | 2.978471 | -3.817845 | -3.712732 |
| 61 | 1 | 0 | 3.660655 | -0.071918 | -3.246244 |
| 62 | 1 | 0 | 4.398889 | -1.570149 | -3.860536 |
| 63 | 1 | 0 | 3.062597 | -0.818248 | -4.738314 |
| 64 | 6 | 0 | -0.348907 | 1.503753 | 2.283615 |
| 65 | 6 | 0 | -1.464019 | 2.552564 | 2.331692 |
| 66 | 6 | 0 | -0.109934 | 0.835669 | 3.640787 |
| 67 | 1 | 0 | -0.600951 | 0.735404 | 1.554993 |
| 68 | 1 | 0 | -1.614993 | 3.014876 | 1.353033 |
| 69 | 1 | 0 | -2.400448 | 2.070865 | 2.628615 |
| 70 | 1 | 0 | -1.241395 | 3.337362 | 3.064030 |
| 71 | 1 | 0 | 0.722578 | 0.126499 | 3.599236 |
| 72 | 1 | 0 | 0.093589 | 1.564582 | 4.433014 |
| 73 | 1 | 0 | -1.011364 | 0.285437 | 3.926168 |
| 74 | 6 | 0 | 3.520976 | 2.916568 | -0.615017 |

| | | | | | |
|---|---|---|---|---|---|
| 75 | 6 | 0 | 4.889740 | 2.325232 | -0.265457 |
| 76 | 6 | 0 | 3.588683 | 4.390088 | -1.026225 |
| 77 | 1 | 0 | 3.075321 | 2.341030 | -1.428926 |
| 78 | 1 | 0 | 4.807735 | 1.266808 | 0.003168 |
| 79 | 1 | 0 | 5.554276 | 2.407494 | -1.131264 |
| 80 | 1 | 0 | 5.362649 | 2.857948 | 0.567207 |
| 81 | 1 | 0 | 2.593636 | 4.782185 | -1.257713 |
| 82 | 1 | 0 | 4.036715 | 5.016198 | -0.246813 |
| 83 | 1 | 0 | 4.209384 | 4.485259 | -1.922452 |
| 84 | 5 | 0 | 0.832292 | -0.883516 | -0.393202 |
| 85 | 1 | 0 | -6.381579 | -1.364137 | 0.450927 |
| 86 | 1 | 0 | -6.596195 | 0.337856 | -0.365114 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.911943 | 1.392785 | -1.146996 |
| 2 | 6 | 0 | -1.962090 | 0.511877 | -0.816755 |
| 3 | 6 | 0 | -3.306318 | 1.037321 | -0.899781 |
| 4 | 6 | 0 | -3.534911 | 2.373681 | -1.349307 |
| 5 | 6 | 0 | -2.438443 | 3.194725 | -1.710645 |
| 6 | 6 | 0 | -1.171304 | 2.707789 | -1.610680 |
| 7 | 6 | 0 | -4.438712 | 0.254592 | -0.525503 |
| 8 | 6 | 0 | -4.845513 | 2.887180 | -1.442532 |
| 9 | 1 | 0 | -2.624681 | 4.202865 | -2.068869 |
| 10 | 1 | 0 | -0.329032 | 3.334135 | -1.894024 |
| 11 | 6 | 0 | -5.919788 | 2.106291 | -1.100680 |
| 12 | 6 | 0 | -5.710735 | 0.801171 | -0.645417 |
| 13 | 1 | 0 | -4.985158 | 3.904990 | -1.794990 |
| 14 | 1 | 0 | -6.931310 | 2.491384 | -1.180440 |
| 15 | 6 | 0 | -0.399319 | -2.892399 | 0.013737 |
| 16 | 6 | 0 | -1.478073 | -3.615630 | 0.385615 |
| 17 | 6 | 0 | -2.770562 | -3.012436 | 0.411464 |
| 18 | 6 | 0 | -2.920585 | -1.656556 | -0.010774 |
| 19 | 6 | 0 | -1.765806 | -0.881055 | -0.388897 |
| 20 | 6 | 0 | -0.473848 | -1.496831 | -0.334950 |
| 21 | 1 | 0 | -3.727510 | -4.790327 | 1.149966 |
| 22 | 1 | 0 | 0.572295 | -3.379502 | -0.021719 |
| 23 | 1 | 0 | -1.384578 | -4.663050 | 0.660341 |
| 24 | 6 | 0 | -3.878044 | -3.761093 | 0.836160 |
| 25 | 6 | 0 | -4.235783 | -1.109575 | -0.027239 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 6 | 0 | -5.302442 | -1.881925 | 0.425594 |
| 27 | 6 | 0 | -5.134111 | -3.196231 | 0.857610 |
| 28 | 1 | 0 | -5.992219 | -3.766508 | 1.198195 |
| 29 | 15 | 0 | 0.861165 | 1.029565 | -1.051660 |
| 30 | 6 | 0 | 1.471697 | 2.620244 | 2.662336 |
| 31 | 6 | 0 | 2.588373 | 3.020000 | 2.007862 |
| 32 | 1 | 0 | 1.155065 | 2.801780 | 3.676357 |
| 33 | 1 | 0 | 3.426053 | 3.605308 | 2.348951 |
| 34 | 6 | 0 | 4.102077 | -2.436218 | 0.326932 |
| 35 | 6 | 0 | 4.248802 | -2.335017 | -1.015664 |
| 36 | 1 | 0 | 4.770682 | -2.825847 | 1.077608 |
| 37 | 1 | 0 | 5.067498 | -2.624976 | -1.654297 |
| 38 | 6 | 0 | 1.342091 | 1.840257 | 0.578980 |
| 39 | 6 | 0 | 2.231747 | -1.518463 | -0.494197 |
| 40 | 7 | 0 | 2.492687 | 2.538880 | 0.721616 |
| 41 | 7 | 0 | 0.720780 | 1.882040 | 1.778119 |
| 42 | 7 | 0 | 2.855941 | -1.931235 | 0.632562 |
| 43 | 7 | 0 | 3.089582 | -1.772684 | -1.506143 |
| 44 | 6 | 0 | 2.310979 | -1.780036 | 1.992619 |
| 45 | 6 | 0 | 3.127274 | -0.744149 | 2.761107 |
| 46 | 6 | 0 | 2.233276 | -3.128447 | 2.699443 |
| 47 | 1 | 0 | 1.296280 | -1.403624 | 1.837174 |
| 48 | 1 | 0 | 3.148060 | 0.210700 | 2.227089 |
| 49 | 1 | 0 | 2.686000 | -0.578071 | 3.748144 |
| 50 | 1 | 0 | 4.159074 | -1.079946 | 2.910785 |
| 51 | 1 | 0 | 1.637253 | -3.838113 | 2.120278 |
| 52 | 1 | 0 | 3.227135 | -3.556021 | 2.869933 |
| 53 | 1 | 0 | 1.755648 | -2.999503 | 3.674748 |
| 54 | 6 | 0 | 2.807314 | -1.523183 | -2.933540 |
| 55 | 6 | 0 | 2.938689 | -2.817062 | -3.731094 |
| 56 | 6 | 0 | 3.696027 | -0.398347 | -3.454166 |
| 57 | 1 | 0 | 1.763191 | -1.198802 | -2.955074 |
| 58 | 1 | 0 | 2.307211 | -3.603004 | -3.307801 |
| 59 | 1 | 0 | 2.620892 | -2.639437 | -4.761920 |
| 60 | 1 | 0 | 3.973845 | -3.173866 | -3.760416 |
| 61 | 1 | 0 | 3.531023 | 0.519376 | -2.882065 |
| 62 | 1 | 0 | 4.756463 | -0.668546 | -3.397237 |
| 63 | 1 | 0 | 3.455918 | -0.195513 | -4.501385 |
| 64 | 6 | 0 | -0.584622 | 1.267060 | 2.115519 |
| 65 | 6 | 0 | -1.690314 | 2.316468 | 2.070847 |
| 66 | 6 | 0 | -0.511529 | 0.550472 | 3.459977 |
| 67 | 1 | 0 | -0.753454 | 0.518898 | 1.345269 |
| 68 | 1 | 0 | -1.706476 | 2.833794 | 1.108611 |
| 69 | 1 | 0 | -2.658144 | 1.825938 | 2.206608 |

| | | | | | |
|---|---|---|---|---|---|
| 70 | 1 | 0 | -1.563045 | 3.055138 | 2.870319 |
| 71 | 1 | 0 | 0.330809 | -0.145860 | 3.501087 |
| 72 | 1 | 0 | -0.433927 | 1.246358 | 4.301946 |
| 73 | 1 | 0 | -1.431868 | -0.023975 | 3.593630 |
| 74 | 6 | 0 | 3.544961 | 2.679734 | -0.309824 |
| 75 | 6 | 0 | 4.551934 | 1.540233 | -0.170171 |
| 76 | 6 | 0 | 4.194284 | 4.057163 | -0.242176 |
| 77 | 1 | 0 | 3.018796 | 2.579686 | -1.261957 |
| 78 | 1 | 0 | 4.059790 | 0.567211 | -0.266078 |
| 79 | 1 | 0 | 5.310930 | 1.617653 | -0.954015 |
| 80 | 1 | 0 | 5.057648 | 1.580313 | 0.800885 |
| 81 | 1 | 0 | 3.444529 | 4.853024 | -0.256334 |
| 82 | 1 | 0 | 4.823431 | 4.175817 | 0.646181 |
| 83 | 1 | 0 | 4.840687 | 4.183873 | -1.114513 |
| 84 | 5 | 0 | 0.830648 | -0.801240 | -0.595298 |
| 85 | 1 | 0 | -6.303049 | -1.468966 | 0.452145 |
| 86 | 1 | 0 | -6.583787 | 0.212605 | -0.393675 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.910199 | 1.388167 | -1.115477 |
| 2 | 6 | 0 | -1.966288 | 0.513720 | -0.786295 |
| 3 | 6 | 0 | -3.308660 | 1.046410 | -0.877422 |
| 4 | 6 | 0 | -3.527404 | 2.389029 | -1.316268 |
| 5 | 6 | 0 | -2.424482 | 3.206701 | -1.670102 |
| 6 | 6 | 0 | -1.160740 | 2.708777 | -1.575205 |
| 7 | 6 | 0 | -4.450611 | 0.265945 | -0.521575 |
| 8 | 6 | 0 | -4.834021 | 2.914083 | -1.409978 |
| 9 | 1 | 0 | -2.606450 | 4.218512 | -2.020162 |
| 10 | 1 | 0 | -0.312452 | 3.328363 | -1.856521 |
| 11 | 6 | 0 | -5.915735 | 2.138572 | -1.077176 |
| 12 | 6 | 0 | -5.717665 | 0.825572 | -0.635484 |
| 13 | 1 | 0 | -4.961264 | 3.936322 | -1.753863 |
| 14 | 1 | 0 | -6.923889 | 2.532498 | -1.153117 |
| 15 | 6 | 0 | -0.421851 | -2.884055 | 0.111178 |
| 16 | 6 | 0 | -1.510501 | -3.607762 | 0.460713 |
| 17 | 6 | 0 | -2.804731 | -3.009797 | 0.434285 |
| 18 | 6 | 0 | -2.944892 | -1.653422 | 0.007242 |
| 19 | 6 | 0 | -1.781247 | -0.880299 | -0.347274 |
| 20 | 6 | 0 | -0.494910 | -1.497451 | -0.269486 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 1 | 0 | -3.776896 | -4.795050 | 1.132578 |
| 22 | 1 | 0 | 0.554378 | -3.365301 | 0.112833 |
| 23 | 1 | 0 | -1.424560 | -4.650559 | 0.754661 |
| 24 | 6 | 0 | -3.924482 | -3.766661 | 0.815088 |
| 25 | 6 | 0 | -4.261688 | -1.108700 | -0.044673 |
| 26 | 6 | 0 | -5.341294 | -1.891551 | 0.354765 |
| 27 | 6 | 0 | -5.183847 | -3.210212 | 0.784480 |
| 28 | 1 | 0 | -6.052514 | -3.787016 | 1.083840 |
| 29 | 15 | 0 | 0.865657 | 1.012550 | -1.045125 |
| 30 | 6 | 0 | 1.472116 | 2.646579 | 2.662441 |
| 31 | 6 | 0 | 2.587658 | 3.052461 | 2.003572 |
| 32 | 1 | 0 | 1.150738 | 2.832384 | 3.674982 |
| 33 | 1 | 0 | 3.419214 | 3.651117 | 2.337798 |
| 34 | 6 | 0 | 4.116259 | -2.460035 | 0.249811 |
| 35 | 6 | 0 | 4.236465 | -2.311023 | -1.093056 |
| 36 | 1 | 0 | 4.803531 | -2.866028 | 0.975265 |
| 37 | 1 | 0 | 5.045515 | -2.569551 | -1.758012 |
| 38 | 6 | 0 | 1.351623 | 1.847702 | 0.583754 |
| 39 | 6 | 0 | 2.216415 | -1.540926 | -0.505991 |
| 40 | 7 | 0 | 2.495492 | 2.558702 | 0.721857 |
| 41 | 7 | 0 | 0.730139 | 1.895742 | 1.781630 |
| 42 | 7 | 0 | 2.867559 | -1.986758 | 0.593617 |
| 43 | 7 | 0 | 3.059913 | -1.750271 | -1.542259 |
| 44 | 6 | 0 | 2.360410 | -1.869117 | 1.974430 |
| 45 | 6 | 0 | 3.106866 | -0.745820 | 2.689030 |
| 46 | 6 | 0 | 2.460257 | -3.205771 | 2.698535 |
| 47 | 1 | 0 | 1.305876 | -1.599922 | 1.860741 |
| 48 | 1 | 0 | 2.979811 | 0.203836 | 2.157567 |
| 49 | 1 | 0 | 2.727554 | -0.628610 | 3.708129 |
| 50 | 1 | 0 | 4.177731 | -0.967429 | 2.752566 |
| 51 | 1 | 0 | 1.941844 | -3.991661 | 2.143584 |
| 52 | 1 | 0 | 3.501900 | -3.507115 | 2.849201 |
| 53 | 1 | 0 | 1.995687 | -3.117832 | 3.683888 |
| 54 | 6 | 0 | 2.755907 | -1.467732 | -2.961697 |
| 55 | 6 | 0 | 2.918889 | -2.736892 | -3.791450 |
| 56 | 6 | 0 | 3.621129 | -0.315968 | -3.460149 |
| 57 | 1 | 0 | 1.704405 | -1.166816 | -2.966501 |
| 58 | 1 | 0 | 2.317086 | -3.552435 | -3.382930 |
| 59 | 1 | 0 | 2.588960 | -2.542923 | -4.814858 |
| 60 | 1 | 0 | 3.965057 | -3.056585 | -3.835019 |
| 61 | 1 | 0 | 3.430155 | 0.590535 | -2.878467 |
| 62 | 1 | 0 | 4.685649 | -0.566967 | -3.394991 |
| 63 | 1 | 0 | 3.386318 | -0.107631 | -4.507061 |
| 64 | 6 | 0 | -0.564793 | 1.257147 | 2.121369 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 6 | 0 | -1.689466 | 2.285014 | 2.075700 |
| 66 | 6 | 0 | -0.469308 | 0.555666 | 3.471384 |
| 67 | 1 | 0 | -0.714417 | 0.501520 | 1.353006 |
| 68 | 1 | 0 | -1.719764 | 2.797789 | 1.110783 |
| 69 | 1 | 0 | -2.646724 | 1.776450 | 2.222007 |
| 70 | 1 | 0 | -1.568092 | 3.027729 | 2.872047 |
| 71 | 1 | 0 | 0.387162 | -0.124054 | 3.508869 |
| 72 | 1 | 0 | -0.394927 | 1.264097 | 4.302518 |
| 73 | 1 | 0 | -1.378558 | -0.032013 | 3.620045 |
| 74 | 6 | 0 | 3.552206 | 2.682567 | -0.309863 |
| 75 | 6 | 0 | 4.482453 | 1.475452 | -0.219736 |
| 76 | 6 | 0 | 4.295636 | 4.004263 | -0.168325 |
| 77 | 1 | 0 | 3.020178 | 2.664660 | -1.264416 |
| 78 | 1 | 0 | 3.926292 | 0.541010 | -0.357333 |
| 79 | 1 | 0 | 5.250546 | 1.536764 | -0.996027 |
| 80 | 1 | 0 | 4.979103 | 1.445807 | 0.756349 |
| 81 | 1 | 0 | 3.605180 | 4.850848 | -0.133010 |
| 82 | 1 | 0 | 4.930936 | 4.021745 | 0.722704 |
| 83 | 1 | 0 | 4.948936 | 4.132941 | -1.034386 |
| 84 | 5 | 0 | 0.816171 | -0.814214 | -0.559055 |
| 85 | 1 | 0 | -6.344485 | -1.485134 | 0.338904 |
| 86 | 1 | 0 | -6.595024 | 0.242835 | -0.386533 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.846120 | 1.384315 | -1.018780 |
| 2 | 6 | 0 | -1.941703 | 0.524748 | -0.690770 |
| 3 | 6 | 0 | -3.277885 | 1.086674 | -0.820767 |
| 4 | 6 | 0 | -3.464596 | 2.442158 | -1.293552 |
| 5 | 6 | 0 | -2.331543 | 3.230952 | -1.640483 |
| 6 | 6 | 0 | -1.064927 | 2.704034 | -1.509043 |
| 7 | 6 | 0 | -4.449149 | 0.326120 | -0.479435 |
| 8 | 6 | 0 | -4.767798 | 2.990080 | -1.424488 |
| 9 | 1 | 0 | -2.483504 | 4.247671 | -2.020125 |
| 10 | 1 | 0 | -0.194050 | 3.307104 | -1.794844 |
| 11 | 6 | 0 | -5.883391 | 2.230932 | -1.100143 |
| 12 | 6 | 0 | -5.719492 | 0.916292 | -0.634260 |
| 13 | 1 | 0 | -4.872287 | 4.017369 | -1.791437 |
| 14 | 1 | 0 | -6.890815 | 2.646643 | -1.208056 |
| 15 | 6 | 0 | -0.479952 | -2.945798 | 0.136906 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | -1.603489 | -3.656913 | 0.459932 |
| 17 | 6 | 0 | -2.883277 | -3.018501 | 0.465379 |
| 18 | 6 | 0 | -2.981725 | -1.630956 | 0.067136 |
| 19 | 6 | 0 | -1.789582 | -0.873930 | -0.254531 |
| 20 | 6 | 0 | -0.496803 | -1.534049 | -0.173114 |
| 21 | 1 | 0 | -3.918135 | -4.800301 | 1.130598 |
| 22 | 1 | 0 | 0.484700 | -3.466484 | 0.114888 |
| 23 | 1 | 0 | -1.546332 | -4.723326 | 0.709674 |
| 24 | 6 | 0 | -4.033294 | -3.751203 | 0.834463 |
| 25 | 6 | 0 | -4.295676 | -1.047469 | 0.007877 |
| 26 | 6 | 0 | -5.409400 | -1.814392 | 0.407781 |
| 27 | 6 | 0 | -5.288443 | -3.147996 | 0.821991 |
| 28 | 1 | 0 | -6.180031 | -3.708868 | 1.121258 |
| 29 | 15 | 0 | 0.929197 | 0.954842 | -0.922568 |
| 30 | 6 | 0 | 1.621881 | 2.949512 | 2.622621 |
| 31 | 6 | 0 | 2.669329 | 3.385910 | 1.855027 |
| 32 | 1 | 0 | 1.342709 | 3.203493 | 3.642012 |
| 33 | 1 | 0 | 3.471200 | 4.082633 | 2.085590 |
| 34 | 6 | 0 | 4.066108 | -2.880488 | 0.088368 |
| 35 | 6 | 0 | 4.087253 | -2.688256 | -1.266989 |
| 36 | 1 | 0 | 4.768631 | -3.394828 | 0.739105 |
| 37 | 1 | 0 | 4.806935 | -3.013849 | -2.013833 |
| 38 | 6 | 0 | 1.458838 | 1.937247 | 0.612060 |
| 39 | 6 | 0 | 2.208706 | -1.700286 | -0.467220 |
| 40 | 7 | 0 | 2.556620 | 2.762920 | 0.621524 |
| 41 | 7 | 0 | 0.891812 | 2.056051 | 1.854606 |
| 42 | 7 | 0 | 2.910708 | -2.274513 | 0.565852 |
| 43 | 7 | 0 | 2.946565 | -1.968268 | -1.594945 |
| 44 | 6 | 0 | 2.526091 | -2.201664 | 2.001230 |
| 45 | 6 | 0 | 3.506148 | -1.296157 | 2.764659 |
| 46 | 6 | 0 | 2.419710 | -3.607049 | 2.610771 |
| 47 | 1 | 0 | 1.524702 | -1.736171 | 1.985167 |
| 48 | 1 | 0 | 3.551138 | -0.288874 | 2.316440 |
| 49 | 1 | 0 | 3.180759 | -1.195756 | 3.814322 |
| 50 | 1 | 0 | 4.525967 | -1.720148 | 2.772317 |
| 51 | 1 | 0 | 1.712999 | -4.236523 | 2.046126 |
| 52 | 1 | 0 | 3.399236 | -4.116527 | 2.643430 |
| 53 | 1 | 0 | 2.053414 | -3.528325 | 3.648257 |
| 54 | 6 | 0 | 2.517306 | -1.661817 | -2.990197 |
| 55 | 6 | 0 | 2.206612 | -2.963884 | -3.744603 |
| 56 | 6 | 0 | 3.560603 | -0.785374 | -3.695301 |
| 57 | 1 | 0 | 1.583368 | -1.087298 | -2.864849 |
| 58 | 1 | 0 | 1.447421 | -3.559681 | -3.211155 |
| 59 | 1 | 0 | 1.811848 | -2.721161 | -4.745595 |

| | | | | | |
|---|---|---|---|---|---|
| 60 | 1 | 0 | 3.110854 | -3.583467 | -3.881176 |
| 61 | 1 | 0 | 3.744581 | 0.144085 | -3.130821 |
| 62 | 1 | 0 | 4.521041 | -1.314911 | -3.829552 |
| 63 | 1 | 0 | 3.190079 | -0.511121 | -4.697267 |
| 64 | 6 | 0 | -0.360556 | 1.388012 | 2.324721 |
| 65 | 6 | 0 | -1.507538 | 2.407932 | 2.378025 |
| 66 | 6 | 0 | -0.121178 | 0.692536 | 3.672654 |
| 67 | 1 | 0 | -0.576366 | 0.624478 | 1.562049 |
| 68 | 1 | 0 | -1.655940 | 2.892832 | 1.399784 |
| 69 | 1 | 0 | -2.442481 | 1.889917 | 2.648944 |
| 70 | 1 | 0 | -1.316872 | 3.186344 | 3.138986 |
| 71 | 1 | 0 | 0.740818 | 0.005602 | 3.627645 |
| 72 | 1 | 0 | 0.046461 | 1.413534 | 4.492521 |
| 73 | 1 | 0 | -1.016523 | 0.103310 | 3.931427 |
| 74 | 6 | 0 | 3.494949 | 3.000846 | -0.516150 |
| 75 | 6 | 0 | 4.891029 | 2.460093 | -0.174385 |
| 76 | 6 | 0 | 3.498746 | 4.487831 | -0.899567 |
| 77 | 1 | 0 | 3.062626 | 2.412951 | -1.344633 |
| 78 | 1 | 0 | 4.854243 | 1.387463 | 0.081297 |
| 79 | 1 | 0 | 5.555923 | 2.584399 | -1.045883 |
| 80 | 1 | 0 | 5.346021 | 3.005726 | 0.671508 |
| 81 | 1 | 0 | 2.480396 | 4.845261 | -1.126432 |
| 82 | 1 | 0 | 3.923279 | 5.121443 | -0.100730 |
| 83 | 1 | 0 | 4.120611 | 4.628663 | -1.799643 |
| 84 | 5 | 0 | 0.853167 | -0.882207 | -0.406795 |
| 85 | 1 | 0 | -6.407940 | -1.370631 | 0.399592 |
| 86 | 1 | 0 | -6.619157 | 0.342143 | -0.400607 |

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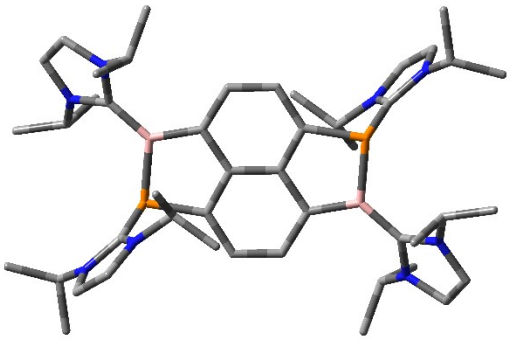
**2PB-a**



**UB3LYP/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.819339 | 2.323450 | -0.620208 |
| 2 | 6 | 0 | 1.528422 | 1.156063 | -0.208488 |
| 3 | 6 | 0 | 0.704400 | -0.007799 | 0.079869 |
| 4 | 6 | 0 | -0.704432 | 0.007832 | -0.079854 |
| 5 | 6 | 0 | -1.335483 | 1.183512 | -0.551205 |
| 6 | 6 | 0 | -0.560501 | 2.329426 | -0.812757 |
| 7 | 1 | 0 | 1.364028 | 3.246354 | -0.799415 |
| 8 | 6 | 0 | 1.335451 | -1.183479 | 0.551223 |
| 9 | 6 | 0 | -1.528453 | -1.156031 | 0.208503 |
| 10 | 1 | 0 | -1.040383 | 3.237833 | -1.174673 |
| 11 | 6 | 0 | -0.819370 | -2.323419 | 0.620217 |
| 12 | 6 | 0 | 0.560470 | -2.329393 | 0.812773 |
| 13 | 1 | 0 | -1.364058 | -3.246326 | 0.799415 |
| 14 | 1 | 0 | 1.040352 | -3.237801 | 1.174690 |
| 15 | 15 | 0 | -3.106917 | 0.886357 | -0.840714 |
| 16 | 15 | 0 | 3.106881 | -0.886317 | 0.840747 |
| 17 | 6 | 0 | 5.978367 | 3.188617 | 0.662225 |
| 18 | 6 | 0 | 5.520793 | 3.674886 | -0.512619 |
| 19 | 6 | 0 | 4.410707 | -3.186782 | -2.292661 |
| 20 | 6 | 0 | 5.253130 | -3.575927 | -1.302477 |
| 21 | 6 | 0 | -5.520785 | -3.674928 | 0.512468 |
| 22 | 6 | 0 | -5.978322 | -3.188653 | -0.662389 |
| 23 | 6 | 0 | -5.253093 | 3.575947 | 1.302613 |
| 24 | 6 | 0 | -4.410674 | 3.186745 | 2.292779 |
| 25 | 6 | 0 | -4.164889 | -1.942042 | -0.076704 |
| 26 | 6 | 0 | -3.888739 | 1.995199 | 0.461389 |
| 27 | 6 | 0 | 3.888727 | -1.995191 | -0.461314 |
| 28 | 6 | 0 | 4.164878 | 1.942043 | 0.076637 |
| 29 | 1 | 0 | 5.893045 | 4.481180 | -1.123931 |
| 30 | 1 | 0 | 6.806039 | 3.512804 | 1.271838 |
| 31 | 1 | 0 | -6.805958 | -3.512853 | -1.272044 |
| 32 | 1 | 0 | -5.893042 | -4.481243 | 1.123751 |
| 33 | 7 | 0 | -5.161765 | -2.125553 | -1.024378 |
| 34 | 7 | 0 | -4.414526 | -2.918426 | 0.874697 |
| 35 | 7 | 0 | 4.414500 | 2.918405 | -0.874790 |
| 36 | 7 | 0 | 5.161799 | 2.125543 | 1.024266 |
| 37 | 6 | 0 | 3.827546 | 2.964447 | -2.228110 |
| 38 | 6 | 0 | 4.841693 | 2.450651 | -3.260239 |
| 39 | 6 | 0 | 3.331289 | 4.373708 | -2.568629 |
| 40 | 1 | 0 | 2.976489 | 2.282879 | -2.192488 |
| 41 | 1 | 0 | 5.209366 | 1.458209 | -2.980716 |
| 42 | 1 | 0 | 4.373549 | 2.383042 | -4.248033 |
| 43 | 1 | 0 | 5.703893 | 3.121941 | -3.343148 |
| 44 | 1 | 0 | 2.634653 | 4.746535 | -1.812498 |

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|---|---|---|---|---|---|
| 45 | 1 | 0 | 4.160051 | 5.086634 | -2.651158 |
| 46 | 1 | 0 | 2.814908 | 4.358824 | -3.533970 |
| 47 | 6 | 0 | 5.150343 | 1.562242 | 2.390918 |
| 48 | 6 | 0 | 4.457604 | 2.529597 | 3.359565 |
| 49 | 6 | 0 | 6.563800 | 1.184429 | 2.843388 |
| 50 | 1 | 0 | 4.555532 | 0.651450 | 2.326172 |
| 51 | 1 | 0 | 3.443739 | 2.753134 | 3.013446 |
| 52 | 1 | 0 | 4.390960 | 2.080567 | 4.356477 |
| 53 | 1 | 0 | 5.012235 | 3.471099 | 3.446613 |
| 54 | 1 | 0 | 7.050247 | 0.523110 | 2.118656 |
| 55 | 1 | 0 | 7.203381 | 2.062292 | 2.989748 |
| 56 | 1 | 0 | 6.509377 | 0.661736 | 3.803856 |
| 57 | 6 | 0 | -5.150259 | -1.562235 | -2.391024 |
| 58 | 6 | 0 | -6.563706 | -1.184467 | -2.843563 |
| 59 | 6 | 0 | -4.457437 | -2.529555 | -3.359646 |
| 60 | 1 | 0 | -4.555482 | -0.651423 | -2.326236 |
| 61 | 1 | 0 | -7.050216 | -0.523176 | -2.118847 |
| 62 | 1 | 0 | -6.509253 | -0.661760 | -3.804021 |
| 63 | 1 | 0 | -7.203248 | -2.062351 | -2.989967 |
| 64 | 1 | 0 | -3.443582 | -2.753061 | -3.013477 |
| 65 | 1 | 0 | -5.012031 | -3.471075 | -3.446733 |
| 66 | 1 | 0 | -4.390757 | -2.080511 | -4.356549 |
| 67 | 6 | 0 | -3.827627 | -2.964476 | 2.228040 |
| 68 | 6 | 0 | -3.331344 | -4.373729 | 2.568553 |
| 69 | 6 | 0 | -4.841832 | -2.450728 | 3.260136 |
| 70 | 1 | 0 | -2.976587 | -2.282883 | 2.192465 |
| 71 | 1 | 0 | -2.634666 | -4.746521 | 1.812445 |
| 72 | 1 | 0 | -2.815004 | -4.358849 | 3.533916 |
| 73 | 1 | 0 | -4.160089 | -5.086681 | 2.651033 |
| 74 | 1 | 0 | -5.209527 | -1.458295 | 2.980612 |
| 75 | 1 | 0 | -5.704013 | -3.122049 | 3.343000 |
| 76 | 1 | 0 | -4.373730 | -2.383118 | 4.247950 |
| 77 | 1 | 0 | -4.336709 | 3.518829 | 3.315554 |
| 78 | 1 | 0 | -6.047070 | 4.305073 | 1.305356 |
| 79 | 7 | 0 | -3.581712 | 2.213100 | 1.771300 |
| 80 | 7 | 0 | -4.923977 | 2.840879 | 0.179115 |
| 81 | 6 | 0 | -2.512117 | 1.538695 | 2.555036 |
| 82 | 6 | 0 | -3.084456 | 0.993976 | 3.867297 |
| 83 | 6 | 0 | -1.335963 | 2.491930 | 2.784656 |
| 84 | 1 | 0 | -2.195789 | 0.699447 | 1.936149 |
| 85 | 1 | 0 | -3.957989 | 0.360811 | 3.689461 |
| 86 | 1 | 0 | -2.318300 | 0.389178 | 4.362336 |
| 87 | 1 | 0 | -3.367415 | 1.793505 | 4.561646 |
| 88 | 1 | 0 | -0.923964 | 2.846862 | 1.837330 |

| | | | | | |
|---|---|---|---|---|---|
| 89 | 1 | 0 | -1.635200 | 3.353329 | 3.394542 |
| 90 | 1 | 0 | -0.542722 | 1.960024 | 3.319596 |
| 91 | 6 | 0 | -5.604631 | 3.003319 | -1.131059 |
| 92 | 6 | 0 | -5.381155 | 4.417868 | -1.674361 |
| 93 | 6 | 0 | -7.085744 | 2.632464 | -1.011037 |
| 94 | 1 | 0 | -5.103782 | 2.290032 | -1.788970 |
| 95 | 1 | 0 | -4.313019 | 4.641184 | -1.756967 |
| 96 | 1 | 0 | -5.825805 | 4.499443 | -2.671310 |
| 97 | 1 | 0 | -5.847342 | 5.179354 | -1.038907 |
| 98 | 1 | 0 | -7.208224 | 1.618918 | -0.615906 |
| 99 | 1 | 0 | -7.629324 | 3.324246 | -0.357437 |
| 100 | 1 | 0 | -7.553867 | 2.675522 | -1.999607 |
| 101 | 1 | 0 | 4.336758 | -3.518900 | -3.315426 |
| 102 | 1 | 0 | 6.047130 | -4.305030 | -1.305192 |
| 103 | 7 | 0 | 3.581711 | -2.213146 | -1.771219 |
| 104 | 7 | 0 | 4.923987 | -2.840831 | -0.179006 |
| 105 | 6 | 0 | 5.604637 | -3.003207 | 1.131178 |
| 106 | 6 | 0 | 7.085741 | -2.632314 | 1.011155 |
| 107 | 6 | 0 | 5.381196 | -4.417743 | 1.674529 |
| 108 | 1 | 0 | 5.103764 | -2.289911 | 1.789061 |
| 109 | 1 | 0 | 7.208195 | -1.618777 | 0.615992 |
| 110 | 1 | 0 | 7.553857 | -2.675326 | 1.999731 |
| 111 | 1 | 0 | 7.629346 | -3.324102 | 0.357583 |
| 112 | 1 | 0 | 4.313065 | -4.641083 | 1.757138 |
| 113 | 1 | 0 | 5.847405 | -5.179239 | 1.039102 |
| 114 | 1 | 0 | 5.825844 | -4.499272 | 2.671482 |
| 115 | 6 | 0 | 2.512099 | -1.538800 | -2.554983 |
| 116 | 6 | 0 | 1.335980 | -2.492082 | -2.784593 |
| 117 | 6 | 0 | 3.084432 | -0.994092 | -3.867250 |
| 118 | 1 | 0 | 2.195736 | -0.699547 | -1.936120 |
| 119 | 1 | 0 | 0.923985 | -2.847010 | -1.837264 |
| 120 | 1 | 0 | 0.542725 | -1.960215 | -3.319553 |
| 121 | 1 | 0 | 1.635255 | -3.353482 | -3.394460 |
| 122 | 1 | 0 | 3.957944 | -0.360894 | -3.689422 |
| 123 | 1 | 0 | 3.367423 | -1.793627 | -4.561579 |
| 124 | 1 | 0 | 2.318261 | -0.389330 | -4.362311 |
| 125 | 5 | 0 | -3.010069 | -0.923801 | -0.080347 |
| 126 | 5 | 0 | 3.010040 | 0.923823 | 0.080339 |

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**UWB97XD/6-31G***

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| Center | Atomic | Atomic | Coordinates (Angstroms) | | |
|---|---|---|---|---|---|
| Number | Number | Type | X | Y | Z |

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| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.026485 | 1.898865 | -1.488307 |
| 2 | 6 | 0 | 1.613711 | 0.916775 | -0.624295 |
| 3 | 6 | 0 | 0.675874 | -0.050716 | -0.065269 |
| 4 | 6 | 0 | -0.690134 | -0.051414 | -0.394097 |
| 5 | 6 | 0 | -1.200869 | 0.928022 | -1.285502 |
| 6 | 6 | 0 | -0.316561 | 1.885443 | -1.820746 |
| 7 | 1 | 0 | 1.652500 | 2.685851 | -1.899633 |
| 8 | 6 | 0 | 1.169412 | -1.014000 | 0.835814 |
| 9 | 6 | 0 | -1.597490 | -1.000782 | 0.192275 |
| 10 | 1 | 0 | -0.702665 | 2.651231 | -2.491571 |
| 11 | 6 | 0 | -1.041126 | -1.977297 | 1.048101 |
| 12 | 6 | 0 | 0.312187 | -1.972103 | 1.387227 |
| 13 | 1 | 0 | -1.679848 | -2.750909 | 1.471559 |
| 14 | 1 | 0 | 0.696798 | -2.714325 | 2.083084 |
| 15 | 15 | 0 | -2.981557 | 0.826190 | -1.440417 |
| 16 | 15 | 0 | 2.935587 | -0.725811 | 1.169743 |
| 17 | 6 | 0 | 6.059935 | 2.937272 | -0.060268 |
| 18 | 6 | 0 | 5.722000 | 3.002581 | -1.362501 |
| 19 | 6 | 0 | 4.298031 | -3.726129 | -1.221495 |
| 20 | 6 | 0 | 5.175808 | -3.775539 | -0.193320 |
| 21 | 6 | 0 | -5.915968 | -2.506311 | 1.353261 |
| 22 | 6 | 0 | -6.323831 | -2.519013 | 0.065507 |
| 23 | 6 | 0 | -5.166879 | 3.093810 | 1.085385 |
| 24 | 6 | 0 | -3.960080 | 3.375250 | 1.619767 |
| 25 | 6 | 0 | -4.321380 | -1.485133 | 0.130289 |
| 26 | 6 | 0 | -3.621113 | 1.953000 | -0.072914 |
| 27 | 6 | 0 | 3.707475 | -2.141351 | 0.235666 |
| 28 | 6 | 0 | 4.234951 | 1.630162 | -0.350708 |
| 29 | 1 | 0 | 6.184460 | 3.538106 | -2.175852 |
| 30 | 1 | 0 | 6.861376 | 3.421474 | 0.471928 |
| 31 | 1 | 0 | -7.217154 | -2.929720 | -0.375266 |
| 32 | 1 | 0 | -6.398025 | -2.886236 | 2.239210 |
| 33 | 7 | 0 | -5.353024 | -1.878911 | -0.681071 |
| 34 | 7 | 0 | -4.686454 | -1.875917 | 1.389278 |
| 35 | 7 | 0 | 4.605384 | 2.203269 | -1.540766 |
| 36 | 7 | 0 | 5.158785 | 2.086542 | 0.560999 |
| 37 | 6 | 0 | 4.150299 | 1.746808 | -2.859197 |
| 38 | 6 | 0 | 5.205875 | 0.822524 | -3.467584 |
| 39 | 6 | 0 | 3.820599 | 2.926646 | -3.768265 |
| 40 | 1 | 0 | 3.241594 | 1.173459 | -2.668858 |
| 41 | 1 | 0 | 5.433481 | 0.002828 | -2.778050 |
| 42 | 1 | 0 | 4.842645 | 0.400116 | -4.409782 |
| 43 | 1 | 0 | 6.135485 | 1.363485 | -3.675924 |

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|---|---|---|---|---|---|
| 44 | 1 | 0 | 3.108953 | 3.606607 | -3.292694 |
| 45 | 1 | 0 | 4.717878 | 3.497345 | -4.033485 |
| 46 | 1 | 0 | 3.377293 | 2.559800 | -4.698493 |
| 47 | 6 | 0 | 5.001296 | 1.969415 | 2.018691 |
| 48 | 6 | 0 | 3.915439 | 2.927183 | 2.507487 |
| 49 | 6 | 0 | 6.329011 | 2.180906 | 2.738626 |
| 50 | 1 | 0 | 4.672583 | 0.945262 | 2.207189 |
| 51 | 1 | 0 | 2.975909 | 2.725698 | 1.983691 |
| 52 | 1 | 0 | 3.754337 | 2.796583 | 3.582155 |
| 53 | 1 | 0 | 4.210211 | 3.966405 | 2.323303 |
| 54 | 1 | 0 | 7.121677 | 1.555718 | 2.315241 |
| 55 | 1 | 0 | 6.652309 | 3.226956 | 2.707642 |
| 56 | 1 | 0 | 6.207246 | 1.911865 | 3.791603 |
| 57 | 6 | 0 | -5.268639 | -1.912413 | -2.150977 |
| 58 | 6 | 0 | -6.642434 | -1.734781 | -2.787437 |
| 59 | 6 | 0 | -4.568958 | -3.194636 | -2.597671 |
| 60 | 1 | 0 | -4.646650 | -1.059154 | -2.428088 |
| 61 | 1 | 0 | -7.149009 | -0.842587 | -2.405872 |
| 62 | 1 | 0 | -6.522057 | -1.620504 | -3.867995 |
| 63 | 1 | 0 | -7.290468 | -2.602297 | -2.623069 |
| 64 | 1 | 0 | -3.576186 | -3.260256 | -2.142418 |
| 65 | 1 | 0 | -5.150654 | -4.076575 | -2.307446 |
| 66 | 1 | 0 | -4.453302 | -3.199948 | -3.685587 |
| 67 | 6 | 0 | -4.021081 | -1.423394 | 2.620643 |
| 68 | 6 | 0 | -3.973320 | -2.539179 | 3.658045 |
| 69 | 6 | 0 | -4.692377 | -0.152607 | 3.136318 |
| 70 | 1 | 0 | -3.000493 | -1.182483 | 2.326030 |
| 71 | 1 | 0 | -3.532598 | -3.447511 | 3.236863 |
| 72 | 1 | 0 | -3.356995 | -2.218816 | 4.502535 |
| 73 | 1 | 0 | -4.966569 | -2.781864 | 4.051621 |
| 74 | 1 | 0 | -4.667502 | 0.627857 | 2.369630 |
| 75 | 1 | 0 | -5.735884 | -0.338971 | 3.415170 |
| 76 | 1 | 0 | -4.162637 | 0.219101 | 4.018745 |
| 77 | 1 | 0 | -3.693679 | 4.011091 | 2.447589 |
| 78 | 1 | 0 | -6.151738 | 3.440743 | 1.351823 |
| 79 | 7 | 0 | -3.012253 | 2.672685 | 0.900538 |
| 80 | 7 | 0 | -4.946462 | 2.214202 | 0.045869 |
| 81 | 6 | 0 | -1.579915 | 2.667857 | 1.286945 |
| 82 | 6 | 0 | -1.377087 | 1.775344 | 2.506514 |
| 83 | 6 | 0 | -1.071034 | 4.091002 | 1.485733 |
| 84 | 1 | 0 | -1.051560 | 2.236869 | 0.444465 |
| 85 | 1 | 0 | -1.728040 | 0.761415 | 2.298335 |
| 86 | 1 | 0 | -0.308827 | 1.714733 | 2.733636 |
| 87 | 1 | 0 | -1.899638 | 2.169888 | 3.386648 |

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| 88 | 1 | 0 | -1.292642 | 4.712840 | 0.613655 |
| 89 | 1 | 0 | -1.485318 | 4.571179 | 2.379532 |
| 90 | 1 | 0 | 0.015187 | 4.052021 | 1.605269 |
| 91 | 6 | 0 | -6.020549 | 1.659084 | -0.796815 |
| 92 | 6 | 0 | -6.571677 | 2.737742 | -1.723619 |
| 93 | 6 | 0 | -7.087307 | 1.006799 | 0.077415 |
| 94 | 1 | 0 | -5.543940 | 0.888033 | -1.403700 |
| 95 | 1 | 0 | -5.774448 | 3.151526 | -2.347248 |
| 96 | 1 | 0 | -7.335579 | 2.308159 | -2.378488 |
| 97 | 1 | 0 | -7.032684 | 3.553006 | -1.155566 |
| 98 | 1 | 0 | -6.645795 | 0.269173 | 0.753353 |
| 99 | 1 | 0 | -7.633759 | 1.746560 | 0.672132 |
| 100 | 1 | 0 | -7.817125 | 0.495614 | -0.556821 |
| 101 | 1 | 0 | 4.234222 | -4.325850 | -2.114523 |
| 102 | 1 | 0 | 6.022289 | -4.420465 | -0.026499 |
| 103 | 7 | 0 | 3.407814 | -2.710953 | -0.954326 |
| 104 | 7 | 0 | 4.795566 | -2.801180 | 0.703541 |
| 105 | 6 | 0 | 5.556981 | -2.430520 | 1.912403 |
| 106 | 6 | 0 | 6.645105 | -1.426366 | 1.536152 |
| 107 | 6 | 0 | 6.105887 | -3.665969 | 2.616623 |
| 108 | 1 | 0 | 4.828852 | -1.942026 | 2.563876 |
| 109 | 1 | 0 | 6.214000 | -0.554579 | 1.032668 |
| 110 | 1 | 0 | 7.164836 | -1.086349 | 2.437139 |
| 111 | 1 | 0 | 7.382565 | -1.881578 | 0.865902 |
| 112 | 1 | 0 | 5.318101 | -4.401865 | 2.800932 |
| 113 | 1 | 0 | 6.911649 | -4.143077 | 2.048540 |
| 114 | 1 | 0 | 6.524780 | -3.365573 | 3.580825 |
| 115 | 6 | 0 | 2.335550 | -2.293654 | -1.883832 |
| 116 | 6 | 0 | 1.154731 | -3.254103 | -1.813432 |
| 117 | 6 | 0 | 2.891393 | -2.148845 | -3.296846 |
| 118 | 1 | 0 | 2.037003 | -1.305591 | -1.543029 |
| 119 | 1 | 0 | 0.771775 | -3.330044 | -0.793725 |
| 120 | 1 | 0 | 0.347779 | -2.874335 | -2.446762 |
| 121 | 1 | 0 | 1.434234 | -4.252106 | -2.171951 |
| 122 | 1 | 0 | 3.785025 | -1.520252 | -3.303065 |
| 123 | 1 | 0 | 3.133101 | -3.114321 | -3.755212 |
| 124 | 1 | 0 | 2.131455 | -1.669739 | -3.920461 |
| 125 | 5 | 0 | -3.030833 | -0.757649 | -0.277541 |
| 126 | 5 | 0 | 3.017748 | 0.727661 | -0.115149 |

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**UM06-2X/6-31G***

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| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.822996 | 2.308925 | -0.528388 |
| 2 | 6 | 0 | 1.507815 | 1.136722 | -0.115212 |
| 3 | 6 | 0 | 0.689866 | -0.032597 | 0.120600 |
| 4 | 6 | 0 | -0.704762 | -0.017565 | -0.099681 |
| 5 | 6 | 0 | -1.314652 | 1.159400 | -0.569274 |
| 6 | 6 | 0 | -0.547680 | 2.316814 | -0.774432 |
| 7 | 1 | 0 | 1.379706 | 3.233681 | -0.665672 |
| 8 | 6 | 0 | 1.309139 | -1.215610 | 0.575873 |
| 9 | 6 | 0 | -1.544270 | -1.179921 | 0.148235 |
| 10 | 1 | 0 | -1.022812 | 3.230932 | -1.126248 |
| 11 | 6 | 0 | -0.842752 | -2.360256 | 0.548237 |
| 12 | 6 | 0 | 0.525327 | -2.366285 | 0.779186 |
| 13 | 1 | 0 | -1.393583 | -3.287897 | 0.681467 |
| 14 | 1 | 0 | 0.999960 | -3.286772 | 1.117737 |
| 15 | 15 | 0 | -3.094269 | 0.882524 | -0.860098 |
| 16 | 15 | 0 | 3.079427 | -0.962618 | 0.853983 |
| 17 | 6 | 0 | 5.867540 | 3.193773 | 0.844956 |
| 18 | 6 | 0 | 5.400749 | 3.695675 | -0.319392 |
| 19 | 6 | 0 | 4.049170 | -3.042980 | -2.521323 |
| 20 | 6 | 0 | 4.918598 | -3.569458 | -1.624164 |
| 21 | 6 | 0 | -5.386115 | -3.764867 | 0.435274 |
| 22 | 6 | 0 | -5.916296 | -3.243766 | -0.691007 |
| 23 | 6 | 0 | -4.828077 | 3.712493 | 1.439638 |
| 24 | 6 | 0 | -4.022574 | 3.168576 | 2.385062 |
| 25 | 6 | 0 | -4.143569 | -1.956798 | -0.122450 |
| 26 | 6 | 0 | -3.714470 | 2.013316 | 0.498652 |
| 27 | 6 | 0 | 3.749548 | -1.965110 | -0.587953 |
| 28 | 6 | 0 | 4.121420 | 1.910752 | 0.209033 |
| 29 | 1 | 0 | 5.743646 | 4.532927 | -0.906250 |
| 30 | 1 | 0 | 6.681694 | 3.525441 | 1.467553 |
| 31 | 1 | 0 | -6.759144 | -3.569505 | -1.277332 |
| 32 | 1 | 0 | -5.691144 | -4.617907 | 1.020300 |
| 33 | 7 | 0 | -5.162622 | -2.131698 | -1.025249 |
| 34 | 7 | 0 | -4.301595 | -2.978205 | 0.781802 |
| 35 | 7 | 0 | 4.330364 | 2.910397 | -0.703901 |
| 36 | 7 | 0 | 5.090042 | 2.095208 | 1.160631 |
| 37 | 6 | 0 | 3.769663 | 2.932965 | -2.063689 |
| 38 | 6 | 0 | 4.807796 | 2.378689 | -3.038046 |
| 39 | 6 | 0 | 3.317284 | 4.338093 | -2.444179 |
| 40 | 1 | 0 | 2.905705 | 2.265623 | -2.033135 |
| 41 | 1 | 0 | 5.142604 | 1.389845 | -2.709566 |
| 42 | 1 | 0 | 4.379793 | 2.292338 | -4.041037 |

| | | | | | |
|---|---|---|---|---|---|
| 43 | 1 | 0 | 5.680883 | 3.037296 | -3.094710 |
| 44 | 1 | 0 | 2.630508 | 4.751123 | -1.701405 |
| 45 | 1 | 0 | 4.169040 | 5.019240 | -2.544450 |
| 46 | 1 | 0 | 2.806385 | 4.307067 | -3.410105 |
| 47 | 6 | 0 | 5.129089 | 1.383938 | 2.450779 |
| 48 | 6 | 0 | 4.022975 | 1.904730 | 3.365195 |
| 49 | 6 | 0 | 6.505442 | 1.496548 | 3.094689 |
| 50 | 1 | 0 | 4.937256 | 0.333249 | 2.221359 |
| 51 | 1 | 0 | 3.045899 | 1.799315 | 2.884579 |
| 52 | 1 | 0 | 4.016419 | 1.340108 | 4.301774 |
| 53 | 1 | 0 | 4.192523 | 2.961833 | 3.596264 |
| 54 | 1 | 0 | 7.300921 | 1.203428 | 2.403251 |
| 55 | 1 | 0 | 6.703208 | 2.511446 | 3.454103 |
| 56 | 1 | 0 | 6.543037 | 0.833112 | 3.962120 |
| 57 | 6 | 0 | -5.283654 | -1.388706 | -2.288671 |
| 58 | 6 | 0 | -6.688677 | -1.513516 | -2.865891 |
| 59 | 6 | 0 | -4.216466 | -1.855173 | -3.275644 |
| 60 | 1 | 0 | -5.105355 | -0.339088 | -2.041253 |
| 61 | 1 | 0 | -7.453757 | -1.256083 | -2.127487 |
| 62 | 1 | 0 | -6.783955 | -0.829135 | -3.712526 |
| 63 | 1 | 0 | -6.883618 | -2.523060 | -3.241541 |
| 64 | 1 | 0 | -3.220341 | -1.755108 | -2.835227 |
| 65 | 1 | 0 | -4.384515 | -2.904748 | -3.540016 |
| 66 | 1 | 0 | -4.261233 | -1.253876 | -4.188238 |
| 67 | 6 | 0 | -3.707997 | -2.997945 | 2.126617 |
| 68 | 6 | 0 | -3.236159 | -4.399511 | 2.496990 |
| 69 | 6 | 0 | -4.726286 | -2.453046 | 3.127457 |
| 70 | 1 | 0 | -2.851531 | -2.323174 | 2.077472 |
| 71 | 1 | 0 | -2.563398 | -4.807908 | 1.739063 |
| 72 | 1 | 0 | -2.704324 | -4.365247 | 3.451581 |
| 73 | 1 | 0 | -4.080438 | -5.087135 | 2.615822 |
| 74 | 1 | 0 | -5.089212 | -1.475268 | 2.796973 |
| 75 | 1 | 0 | -5.584893 | -3.126929 | 3.217521 |
| 76 | 1 | 0 | -4.270629 | -2.345587 | 4.116303 |
| 77 | 1 | 0 | -3.879856 | 3.432731 | 3.420777 |
| 78 | 1 | 0 | -5.518178 | 4.538094 | 1.497191 |
| 79 | 7 | 0 | -3.350102 | 2.123853 | 1.795698 |
| 80 | 7 | 0 | -4.633883 | 2.985814 | 0.285535 |
| 81 | 6 | 0 | -2.387968 | 1.254961 | 2.510309 |
| 82 | 6 | 0 | -3.011578 | 0.765145 | 3.813392 |
| 83 | 6 | 0 | -1.069124 | 1.983348 | 2.739497 |
| 84 | 1 | 0 | -2.241844 | 0.398960 | 1.850144 |
| 85 | 1 | 0 | -3.999549 | 0.331492 | 3.640200 |
| 86 | 1 | 0 | -2.366183 | -0.005633 | 4.243790 |

| | | | | | |
|---|---|---|---|---|---|
| 87 | 1 | 0 | -3.102934 | 1.567798 | 4.553082 |
| 88 | 1 | 0 | -0.642887 | 2.341368 | 1.799823 |
| 89 | 1 | 0 | -1.205572 | 2.830280 | 3.422764 |
| 90 | 1 | 0 | -0.356444 | 1.288622 | 3.194055 |
| 91 | 6 | 0 | -5.261717 | 3.302164 | -1.016691 |
| 92 | 6 | 0 | -4.395757 | 4.306675 | -1.768425 |
| 93 | 6 | 0 | -6.691509 | 3.790732 | -0.818683 |
| 94 | 1 | 0 | -5.273653 | 2.358282 | -1.565311 |
| 95 | 1 | 0 | -3.400640 | 3.891465 | -1.951445 |
| 96 | 1 | 0 | -4.854528 | 4.545968 | -2.731670 |
| 97 | 1 | 0 | -4.294839 | 5.233155 | -1.193597 |
| 98 | 1 | 0 | -7.267073 | 3.103892 | -0.192397 |
| 99 | 1 | 0 | -6.722439 | 4.789686 | -0.372402 |
| 100 | 1 | 0 | -7.178805 | 3.857869 | -1.794335 |
| 101 | 1 | 0 | 3.881035 | -3.283642 | -3.558936 |
| 102 | 1 | 0 | 5.649398 | -4.354050 | -1.732883 |
| 103 | 7 | 0 | 3.343733 | -2.055093 | -1.874674 |
| 104 | 7 | 0 | 4.728054 | -2.890954 | -0.440719 |
| 105 | 6 | 0 | 5.416222 | -3.221710 | 0.827034 |
| 106 | 6 | 0 | 6.878482 | -3.565230 | 0.569558 |
| 107 | 6 | 0 | 4.662270 | -4.341834 | 1.534942 |
| 108 | 1 | 0 | 5.358338 | -2.313482 | 1.429589 |
| 109 | 1 | 0 | 7.373790 | -2.790441 | -0.021686 |
| 110 | 1 | 0 | 7.394910 | -3.650567 | 1.528737 |
| 111 | 1 | 0 | 6.987343 | -4.526267 | 0.057261 |
| 112 | 1 | 0 | 3.635578 | -4.033844 | 1.752346 |
| 113 | 1 | 0 | 4.638296 | -5.242598 | 0.912881 |
| 114 | 1 | 0 | 5.158858 | -4.586882 | 2.477684 |
| 115 | 6 | 0 | 2.304911 | -1.227708 | -2.529711 |
| 116 | 6 | 0 | 1.022363 | -2.026747 | -2.726953 |
| 117 | 6 | 0 | 2.845504 | -0.669710 | -3.842629 |
| 118 | 1 | 0 | 2.128517 | -0.400444 | -1.843353 |
| 119 | 1 | 0 | 0.650885 | -2.424350 | -1.780059 |
| 120 | 1 | 0 | 0.254371 | -1.366169 | -3.140406 |
| 121 | 1 | 0 | 1.182035 | -2.850991 | -3.432327 |
| 122 | 1 | 0 | 3.813787 | -0.183898 | -3.698739 |
| 123 | 1 | 0 | 2.951797 | -1.446933 | -4.606908 |
| 124 | 1 | 0 | 2.138643 | 0.071507 | -4.225736 |
| 125 | 5 | 0 | -3.010543 | -0.915173 | -0.118472 |
| 126 | 5 | 0 | 2.981520 | 0.871429 | 0.182150 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.814661 | 2.356962 | 0.540998 |
| 2 | 6 | 0 | -1.530985 | 1.171460 | 0.177233 |
| 3 | 6 | 0 | -0.708213 | -0.007450 | -0.075040 |
| 4 | 6 | 0 | 0.708201 | 0.007380 | 0.075077 |
| 5 | 6 | 0 | 1.347735 | 1.203163 | 0.510118 |
| 6 | 6 | 0 | 0.575964 | 2.367121 | 0.730619 |
| 7 | 1 | 0 | -1.360946 | 3.295746 | 0.688149 |
| 8 | 6 | 0 | -1.347750 | -1.203237 | -0.510064 |
| 9 | 6 | 0 | 1.530971 | -1.171528 | -0.177202 |
| 10 | 1 | 0 | 1.063812 | 3.294139 | 1.060113 |
| 11 | 6 | 0 | 0.814643 | -2.357033 | -0.540942 |
| 12 | 6 | 0 | -0.575985 | -2.367199 | -0.730550 |
| 13 | 1 | 0 | 1.360920 | -3.295825 | -0.688074 |
| 14 | 1 | 0 | -1.063831 | -3.294223 | -1.060028 |
| 15 | 15 | 0 | 3.125960 | 0.902392 | 0.809122 |
| 16 | 15 | 0 | -3.125974 | -0.902435 | -0.809081 |
| 17 | 6 | 0 | -6.015018 | 3.172540 | -0.755109 |
| 18 | 6 | 0 | -5.530598 | 3.727815 | 0.392061 |
| 19 | 6 | 0 | -4.441118 | -3.101459 | 2.401832 |
| 20 | 6 | 0 | -5.257126 | -3.560508 | 1.403558 |
| 21 | 6 | 0 | 5.530713 | -3.727738 | -0.392097 |
| 22 | 6 | 0 | 6.015061 | -3.172498 | 0.755123 |
| 23 | 6 | 0 | 5.257049 | 3.560474 | -1.403565 |
| 24 | 6 | 0 | 4.441033 | 3.101417 | -2.401831 |
| 25 | 6 | 0 | 4.186145 | -1.944702 | 0.124619 |
| 26 | 6 | 0 | 3.900492 | 1.974941 | -0.515330 |
| 27 | 6 | 0 | -3.900545 | -1.974988 | 0.515338 |
| 28 | 6 | 0 | -4.186129 | 1.944690 | -0.124621 |
| 29 | 1 | 0 | -5.892223 | 4.574957 | 0.969249 |
| 30 | 1 | 0 | -6.860418 | 3.465625 | -1.371187 |
| 31 | 1 | 0 | 6.860450 | -3.465574 | 1.371218 |
| 32 | 1 | 0 | 5.892406 | -4.574830 | -0.969315 |
| 33 | 7 | 0 | 5.208822 | -2.080521 | 1.068208 |
| 34 | 7 | 0 | 4.417631 | -2.984908 | -0.777712 |
| 35 | 7 | 0 | -4.417515 | 2.984971 | 0.777651 |
| 36 | 7 | 0 | -5.208828 | 2.080524 | -1.068189 |
| 37 | 6 | 0 | -3.806311 | 3.096969 | 2.121752 |
| 38 | 6 | 0 | -4.808852 | 2.635357 | 3.195485 |
| 39 | 6 | 0 | -3.302054 | 4.524825 | 2.382803 |
| 40 | 1 | 0 | -2.949683 | 2.403633 | 2.100706 |
| 41 | 1 | 0 | -5.183672 | 1.622652 | 2.968694 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | -4.323695 | 2.616963 | 4.186796 |
| 43 | 1 | 0 | -5.676128 | 3.316985 | 3.255999 |
| 44 | 1 | 0 | -2.613687 | 4.862571 | 1.590312 |
| 45 | 1 | 0 | -4.136047 | 5.247455 | 2.445249 |
| 46 | 1 | 0 | -2.764658 | 4.558418 | 3.346007 |
| 47 | 6 | 0 | -5.214600 | 1.423770 | -2.399145 |
| 48 | 6 | 0 | -4.316086 | 2.201113 | -3.376352 |
| 49 | 6 | 0 | -6.645529 | 1.245085 | -2.925161 |
| 50 | 1 | 0 | -4.774153 | 0.425938 | -2.236397 |
| 51 | 1 | 0 | -3.293558 | 2.283123 | -2.970547 |
| 52 | 1 | 0 | -4.265948 | 1.676446 | -4.346495 |
| 53 | 1 | 0 | -4.711451 | 3.217936 | -3.552432 |
| 54 | 1 | 0 | -7.293071 | 0.745842 | -2.183535 |
| 55 | 1 | 0 | -7.112698 | 2.205787 | -3.207075 |
| 56 | 1 | 0 | -6.619236 | 0.622016 | -3.835240 |
| 57 | 6 | 0 | 5.214518 | -1.423805 | 2.399185 |
| 58 | 6 | 0 | 6.645424 | -1.244963 | 2.925209 |
| 59 | 6 | 0 | 4.316094 | -2.201285 | 3.376365 |
| 60 | 1 | 0 | 4.773953 | -0.426022 | 2.236459 |
| 61 | 1 | 0 | 7.292908 | -0.745620 | 2.183598 |
| 62 | 1 | 0 | 6.619055 | -0.621922 | 3.835306 |
| 63 | 1 | 0 | 7.112709 | -2.205616 | 3.207096 |
| 64 | 1 | 0 | 3.293577 | -2.283405 | 2.970555 |
| 65 | 1 | 0 | 4.711579 | -3.218067 | 3.552413 |
| 66 | 1 | 0 | 4.265891 | -1.676656 | 4.346526 |
| 67 | 6 | 0 | 3.806517 | -3.096833 | -2.121861 |
| 68 | 6 | 0 | 3.302388 | -4.524704 | -2.383069 |
| 69 | 6 | 0 | 4.809091 | -2.635032 | -3.195482 |
| 70 | 1 | 0 | 2.949832 | -2.403568 | -2.100810 |
| 71 | 1 | 0 | 2.614009 | -4.862577 | -1.590642 |
| 72 | 1 | 0 | 2.765041 | -4.558247 | -3.346302 |
| 73 | 1 | 0 | 4.136438 | -5.247265 | -2.445544 |
| 74 | 1 | 0 | 5.183767 | -1.622299 | -2.968578 |
| 75 | 1 | 0 | 5.676448 | -3.316557 | -3.255974 |
| 76 | 1 | 0 | 4.324012 | -2.616617 | -4.186831 |
| 77 | 1 | 0 | 4.382646 | 3.386070 | -3.449016 |
| 78 | 1 | 0 | 6.040676 | 4.313365 | -1.421866 |
| 79 | 7 | 0 | 3.619515 | 2.129337 | -1.852733 |
| 80 | 7 | 0 | 4.916719 | 2.868217 | -0.250038 |
| 81 | 6 | 0 | 2.572548 | 1.393197 | -2.616654 |
| 82 | 6 | 0 | 3.159846 | 0.848138 | -3.927139 |
| 83 | 6 | 0 | 1.351101 | 2.292867 | -2.855121 |
| 84 | 1 | 0 | 2.300069 | 0.544580 | -1.966436 |
| 85 | 1 | 0 | 4.071162 | 0.254476 | -3.746856 |

| | | | | | |
|---|---|---|---|---|---|
| 86 | 1 | 0 | 2.411657 | 0.194441 | -4.406294 |
| 87 | 1 | 0 | 3.398367 | 1.652413 | -4.646487 |
| 88 | 1 | 0 | 0.929041 | 2.653792 | -1.903747 |
| 89 | 1 | 0 | 1.611992 | 3.158757 | -3.491780 |
| 90 | 1 | 0 | 0.570602 | 1.711527 | -3.374789 |
| 91 | 6 | 0 | 5.560764 | 3.099748 | 1.072093 |
| 92 | 6 | 0 | 5.319302 | 4.543519 | 1.537635 |
| 93 | 6 | 0 | 7.049025 | 2.724619 | 1.012892 |
| 94 | 1 | 0 | 5.030774 | 2.408577 | 1.751059 |
| 95 | 1 | 0 | 4.241118 | 4.773030 | 1.573987 |
| 96 | 1 | 0 | 5.734365 | 4.675926 | 2.551331 |
| 97 | 1 | 0 | 5.812207 | 5.278681 | 0.876462 |
| 98 | 1 | 0 | 7.184172 | 1.682722 | 0.676339 |
| 99 | 1 | 0 | 7.612640 | 3.385799 | 0.330218 |
| 100 | 1 | 0 | 7.494749 | 2.826001 | 2.017096 |
| 101 | 1 | 0 | -4.382740 | -3.386124 | 3.449016 |
| 102 | 1 | 0 | -6.040747 | -4.313406 | 1.421844 |
| 103 | 7 | 0 | -3.619572 | -2.129399 | 1.852744 |
| 104 | 7 | 0 | -4.916776 | -2.868252 | 0.250037 |
| 105 | 6 | 0 | -5.560815 | -3.099740 | -1.072104 |
| 106 | 6 | 0 | -7.049035 | -2.724445 | -1.012941 |
| 107 | 6 | 0 | -5.319510 | -4.543549 | -1.537610 |
| 108 | 1 | 0 | -5.030732 | -2.408640 | -1.751070 |
| 109 | 1 | 0 | -7.184071 | -1.682519 | -0.676433 |
| 110 | 1 | 0 | -7.494760 | -2.825819 | -2.017146 |
| 111 | 1 | 0 | -7.612727 | -3.385534 | -0.330242 |
| 112 | 1 | 0 | -4.241353 | -4.773196 | -1.573914 |
| 113 | 1 | 0 | -5.812535 | -5.278640 | -0.876448 |
| 114 | 1 | 0 | -5.734547 | -4.675922 | -2.551320 |
| 115 | 6 | 0 | -2.572604 | -1.393280 | 2.616681 |
| 116 | 6 | 0 | -1.351187 | -2.292982 | 2.855170 |
| 117 | 6 | 0 | -3.159918 | -0.848211 | 3.927153 |
| 118 | 1 | 0 | -2.300102 | -0.544663 | 1.966477 |
| 119 | 1 | 0 | -0.929133 | -2.653939 | 1.903805 |
| 120 | 1 | 0 | -0.570670 | -1.711658 | 3.374830 |
| 121 | 1 | 0 | -1.612105 | -3.158854 | 3.491845 |
| 122 | 1 | 0 | -4.071152 | -0.254438 | 3.746833 |
| 123 | 1 | 0 | -3.398576 | -1.652483 | 4.646459 |
| 124 | 1 | 0 | -2.411678 | -0.194616 | 4.406371 |
| 125 | 5 | 0 | 3.025130 | -0.929374 | 0.098316 |
| 126 | 5 | 0 | -3.025137 | 0.929336 | -0.098313 |

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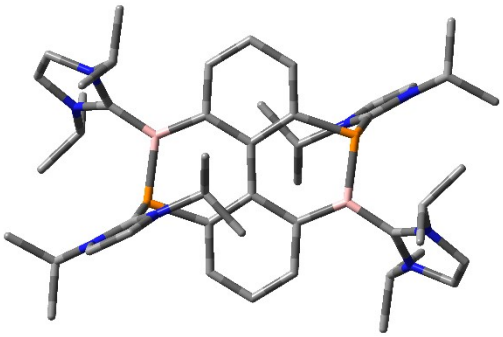
**2PB-b**



**UB3LYP/6-31G***

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.326900 | 2.828241 | 2.275157 |
| 2 | 6 | 0 | 1.386864 | 2.414262 | 1.504069 |
| 3 | 6 | 0 | 1.369687 | 1.255554 | 0.664066 |
| 4 | 6 | 0 | 0.078781 | 0.558831 | 0.470270 |
| 5 | 6 | 0 | -1.029985 | 1.075934 | 1.249215 |
| 6 | 6 | 0 | -0.876111 | 2.118228 | 2.168096 |
| 7 | 6 | 0 | -0.078666 | -0.558890 | -0.470715 |
| 8 | 6 | 0 | 1.030188 | -1.076057 | -1.249511 |
| 9 | 6 | 0 | 0.876268 | -2.118227 | -2.168566 |
| 10 | 1 | 0 | 1.731832 | -2.417496 | -2.769450 |
| 11 | 6 | 0 | -0.326845 | -2.827928 | -2.276071 |
| 12 | 6 | 0 | -1.386902 | -2.413873 | -1.505108 |
| 13 | 6 | 0 | -1.369600 | -1.255455 | -0.664766 |
| 14 | 1 | 0 | 0.410785 | 3.687721 | 2.936183 |
| 15 | 1 | 0 | 2.305269 | 2.993522 | 1.544485 |
| 16 | 1 | 0 | -1.731574 | 2.417384 | 2.769185 |
| 17 | 1 | 0 | -0.410782 | -3.687244 | -2.937303 |
| 18 | 1 | 0 | -2.305418 | -2.992925 | -1.545872 |
| 19 | 15 | 0 | 2.790802 | -0.591941 | -1.132819 |
| 20 | 15 | 0 | -2.790570 | 0.591523 | 1.132826 |
| 21 | 6 | 0 | -5.880495 | -2.714956 | -1.015639 |
| 22 | 6 | 0 | -5.892878 | -2.911980 | 0.324822 |
| 23 | 1 | 0 | -6.585590 | -3.019898 | -1.772209 |
| 24 | 1 | 0 | -6.604094 | -3.431835 | 0.946698 |
| 25 | 6 | 0 | -3.949374 | 3.543291 | -1.586963 |
| 26 | 6 | 0 | -4.955437 | 3.594119 | -0.677664 |
| 27 | 1 | 0 | -3.797728 | 4.109974 | -2.491554 |
| 28 | 1 | 0 | -5.841972 | 4.207141 | -0.648008 |
| 29 | 6 | 0 | 3.949057 | -3.542743 | 1.588612 |
| 30 | 6 | 0 | 4.955369 | -3.593840 | 0.679603 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 1 | 0 | 3.797242 | -4.109039 | 2.493418 |
| 32 | 1 | 0 | 5.841994 | -4.206758 | 0.650461 |
| 33 | 6 | 0 | 5.892936 | 2.911894 | -0.325783 |
| 34 | 6 | 0 | 5.880475 | 2.715223 | 1.014732 |
| 35 | 1 | 0 | 6.604183 | 3.431598 | -0.947751 |
| 36 | 1 | 0 | 6.585505 | 3.020397 | 1.771269 |
| 37 | 6 | 0 | -4.015972 | -1.736397 | -0.168095 |
| 38 | 6 | 0 | 3.485466 | -2.031845 | -0.012142 |
| 39 | 6 | 0 | 4.015998 | 1.736441 | 0.167330 |
| 40 | 6 | 0 | -3.485556 | 2.031639 | 0.012988 |
| 41 | 7 | 0 | 3.058131 | -2.575924 | 1.159634 |
| 42 | 7 | 0 | 4.658724 | -2.664730 | -0.302458 |
| 43 | 7 | 0 | 4.750169 | 2.319727 | -0.838128 |
| 44 | 7 | 0 | 4.731562 | 1.999065 | 1.312315 |
| 45 | 7 | 0 | -4.658659 | 2.664525 | 0.303894 |
| 46 | 7 | 0 | -3.058447 | 2.576172 | -1.158675 |
| 47 | 7 | 0 | -4.750122 | -2.319875 | 0.837263 |
| 48 | 7 | 0 | -4.731626 | -1.998680 | -1.313099 |
| 49 | 6 | 0 | 4.310364 | 2.465330 | -2.242940 |
| 50 | 6 | 0 | 5.306087 | 1.804483 | -3.198891 |
| 51 | 6 | 0 | 4.058966 | 3.941824 | -2.572684 |
| 52 | 1 | 0 | 3.360520 | 1.926751 | -2.284979 |
| 53 | 1 | 0 | 5.441669 | 0.748573 | -2.948194 |
| 54 | 1 | 0 | 4.928183 | 1.865310 | -4.224646 |
| 55 | 1 | 0 | 6.284005 | 2.300452 | -3.175703 |
| 56 | 1 | 0 | 3.337144 | 4.379165 | -1.875686 |
| 57 | 1 | 0 | 4.981003 | 4.532902 | -2.532140 |
| 58 | 1 | 0 | 3.654200 | 4.027795 | -3.586494 |
| 59 | 6 | 0 | 4.437756 | 1.436665 | 2.647919 |
| 60 | 6 | 0 | 4.387505 | 2.537217 | 3.711870 |
| 61 | 6 | 0 | 5.451868 | 0.338320 | 2.993336 |
| 62 | 1 | 0 | 3.445590 | 0.992679 | 2.545986 |
| 63 | 1 | 0 | 3.659686 | 3.309664 | 3.449508 |
| 64 | 1 | 0 | 4.091362 | 2.103241 | 4.672271 |
| 65 | 1 | 0 | 5.364832 | 3.013114 | 3.853696 |
| 66 | 1 | 0 | 5.458605 | -0.443883 | 2.227429 |
| 67 | 1 | 0 | 6.466670 | 0.742179 | 3.083511 |
| 68 | 1 | 0 | 5.191126 | -0.121453 | 3.952606 |
| 69 | 6 | 0 | 1.787206 | -2.259336 | 1.862962 |
| 70 | 6 | 0 | 2.041726 | -2.000821 | 3.350416 |
| 71 | 6 | 0 | 0.765192 | -3.374715 | 1.623812 |
| 72 | 1 | 0 | 1.426753 | -1.339838 | 1.407120 |
| 73 | 1 | 0 | 2.813187 | -1.238960 | 3.496916 |
| 74 | 1 | 0 | 1.116425 | -1.637017 | 3.807108 |

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|---|---|---|---|---|---|
| 75 | 1 | 0 | 2.340718 | -2.908370 | 3.887977 |
| 76 | 1 | 0 | 0.598837 | -3.530496 | 0.554968 |
| 77 | 1 | 0 | 1.091436 | -4.318811 | 2.077575 |
| 78 | 1 | 0 | -0.191118 | -3.090057 | 2.073466 |
| 79 | 6 | 0 | 5.507203 | -2.443331 | -1.501444 |
| 80 | 6 | 0 | 5.636151 | -3.737566 | -2.310206 |
| 81 | 6 | 0 | 6.860140 | -1.851169 | -1.095282 |
| 82 | 1 | 0 | 4.954062 | -1.709284 | -2.091112 |
| 83 | 1 | 0 | 4.651138 | -4.131827 | -2.578457 |
| 84 | 1 | 0 | 6.186831 | -3.534989 | -3.234383 |
| 85 | 1 | 0 | 6.183076 | -4.513656 | -1.762784 |
| 86 | 1 | 0 | 6.730151 | -0.914402 | -0.543580 |
| 87 | 1 | 0 | 7.437267 | -2.543019 | -0.470921 |
| 88 | 1 | 0 | 7.452835 | -1.641303 | -1.991664 |
| 89 | 6 | 0 | -4.310187 | -2.465972 | 2.241992 |
| 90 | 6 | 0 | -4.057953 | -3.942506 | 2.570920 |
| 91 | 6 | 0 | -5.306263 | -1.806191 | 3.198309 |
| 92 | 1 | 0 | -3.360657 | -1.926885 | 2.284323 |
| 93 | 1 | 0 | -3.335823 | -4.379014 | 1.873721 |
| 94 | 1 | 0 | -3.653217 | -4.028832 | 3.584712 |
| 95 | 1 | 0 | -4.979653 | -4.534078 | 2.529943 |
| 96 | 1 | 0 | -5.442608 | -0.750266 | 2.948073 |
| 97 | 1 | 0 | -6.283854 | -2.302797 | 3.175033 |
| 98 | 1 | 0 | -4.928214 | -1.867197 | 4.223999 |
| 99 | 6 | 0 | -4.437924 | -1.435982 | -2.648602 |
| 100 | 6 | 0 | -5.452206 | -0.337712 | -2.993760 |
| 101 | 6 | 0 | -4.387573 | -2.536315 | -3.712779 |
| 102 | 1 | 0 | -3.445803 | -0.991903 | -2.546605 |
| 103 | 1 | 0 | -5.459013 | 0.444358 | -2.227717 |
| 104 | 1 | 0 | -5.191597 | 0.122262 | -3.952968 |
| 105 | 1 | 0 | -6.466955 | -0.741697 | -3.083943 |
| 106 | 1 | 0 | -3.659635 | -3.308713 | -3.450613 |
| 107 | 1 | 0 | -5.364843 | -3.012313 | -3.854653 |
| 108 | 1 | 0 | -4.091534 | -2.102101 | -4.673105 |
| 109 | 6 | 0 | -1.787765 | 2.259803 | -1.862582 |
| 110 | 6 | 0 | -0.765660 | 3.375105 | -1.623478 |
| 111 | 6 | 0 | -2.042858 | 2.001831 | -3.350030 |
| 112 | 1 | 0 | -1.427150 | 1.340149 | -1.407182 |
| 113 | 1 | 0 | -0.598958 | 3.530633 | -0.554655 |
| 114 | 1 | 0 | 0.190501 | 3.090525 | -2.073495 |
| 115 | 1 | 0 | -1.092021 | 4.319311 | -2.076928 |
| 116 | 1 | 0 | -2.814291 | 1.239952 | -3.496526 |
| 117 | 1 | 0 | -2.342167 | 2.909560 | -3.887110 |
| 118 | 1 | 0 | -1.117695 | 1.638325 | -3.807239 |

| | | | | | |
|---|---|---|---|---|---|
| 119 | 6 | 0 | -5.506831 | 2.442678 | 1.503012 |
| 120 | 6 | 0 | -6.860029 | 1.851060 | 1.096927 |
| 121 | 6 | 0 | -5.635225 | 3.736507 | 2.312511 |
| 122 | 1 | 0 | -4.953690 | 1.708178 | 2.092118 |
| 123 | 1 | 0 | -6.730426 | 0.914583 | 0.544641 |
| 124 | 1 | 0 | -7.452494 | 1.640815 | 1.993373 |
| 125 | 1 | 0 | -7.437194 | 2.543399 | 0.473145 |
| 126 | 1 | 0 | -4.650036 | 4.130370 | 2.580702 |
| 127 | 1 | 0 | -6.182095 | 4.513031 | 1.765649 |
| 128 | 1 | 0 | -6.185704 | 3.533577 | 3.236730 |
| 129 | 5 | 0 | -2.688827 | -0.909813 | -0.002256 |
| 130 | 5 | 0 | 2.688875 | 0.909818 | 0.001625 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.442751 | -2.445727 | -2.624055 |
| 2 | 6 | 0 | 1.457627 | -2.155120 | -1.761406 |
| 3 | 6 | 0 | 1.397181 | -1.136764 | -0.749698 |
| 4 | 6 | 0 | 0.102203 | -0.477022 | -0.523048 |
| 5 | 6 | 0 | -0.963193 | -0.876962 | -1.413391 |
| 6 | 6 | 0 | -0.780911 | -1.771848 | -2.456852 |
| 7 | 6 | 0 | -0.088927 | 0.479528 | 0.571277 |
| 8 | 6 | 0 | 0.987872 | 0.874121 | 1.448133 |
| 9 | 6 | 0 | 0.781773 | 1.741423 | 2.527749 |
| 10 | 1 | 0 | 1.623801 | 1.960287 | 3.179737 |
| 11 | 6 | 0 | -0.437837 | 2.370711 | 2.749993 |
| 12 | 6 | 0 | -1.470022 | 2.074671 | 1.887214 |
| 13 | 6 | 0 | -1.379218 | 1.119198 | 0.844539 |
| 14 | 1 | 0 | 0.561254 | -3.195201 | -3.402030 |
| 15 | 1 | 0 | 2.383512 | -2.718971 | -1.848839 |
| 16 | 1 | 0 | -1.612259 | -1.991447 | -3.121884 |
| 17 | 1 | 0 | -0.562696 | 3.084911 | 3.558725 |
| 18 | 1 | 0 | -2.413046 | 2.601783 | 2.015332 |
| 19 | 15 | 0 | 2.750927 | 0.458907 | 1.292104 |
| 20 | 15 | 0 | -2.716551 | -0.412661 | -1.290701 |
| 21 | 6 | 0 | -5.955087 | 2.141828 | 1.417032 |
| 22 | 6 | 0 | -5.963175 | 2.698978 | 0.184435 |
| 23 | 1 | 0 | -6.687826 | 2.178289 | 2.207042 |
| 24 | 1 | 0 | -6.700504 | 3.319653 | -0.298663 |
| 25 | 6 | 0 | -3.879041 | -3.612387 | 0.995255 |

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|---|---|---|---|---|---|
| 26 | 6 | 0 | -4.923465 | -3.491876 | 0.142800 |
| 27 | 1 | 0 | -3.705340 | -4.316865 | 1.792098 |
| 28 | 1 | 0 | -5.833168 | -4.063762 | 0.064769 |
| 29 | 6 | 0 | 3.839908 | 3.568328 | -1.237443 |
| 30 | 6 | 0 | 4.902933 | 3.507493 | -0.402054 |
| 31 | 1 | 0 | 3.653364 | 4.206271 | -2.085920 |
| 32 | 1 | 0 | 5.818972 | 4.074883 | -0.392460 |
| 33 | 6 | 0 | 5.996480 | -2.668327 | -0.047706 |
| 34 | 6 | 0 | 5.940093 | -2.221442 | -1.321737 |
| 35 | 1 | 0 | 6.761573 | -3.229995 | 0.463661 |
| 36 | 1 | 0 | 6.650463 | -2.312897 | -2.127682 |
| 37 | 6 | 0 | -4.030525 | 1.570835 | 0.402589 |
| 38 | 6 | 0 | 3.414281 | 1.970612 | 0.270463 |
| 39 | 6 | 0 | 4.026583 | -1.597207 | -0.299356 |
| 40 | 6 | 0 | -3.431810 | -1.902653 | -0.369052 |
| 41 | 7 | 0 | 2.942354 | 2.610222 | -0.822094 |
| 42 | 7 | 0 | 4.623682 | 2.525538 | 0.525939 |
| 43 | 7 | 0 | 4.818855 | -2.289429 | 0.566833 |
| 44 | 7 | 0 | 4.731723 | -1.567909 | -1.467490 |
| 45 | 7 | 0 | -4.632467 | -2.439261 | -0.697908 |
| 46 | 7 | 0 | -2.977700 | -2.621531 | 0.681915 |
| 47 | 7 | 0 | -4.776542 | 2.346144 | -0.425584 |
| 48 | 7 | 0 | -4.765330 | 1.453412 | 1.539792 |
| 49 | 6 | 0 | 4.433824 | -2.663608 | 1.933230 |
| 50 | 6 | 0 | 5.307506 | -1.940453 | 2.953305 |
| 51 | 6 | 0 | 4.458455 | -4.181904 | 2.094774 |
| 52 | 1 | 0 | 3.401966 | -2.310645 | 2.025361 |
| 53 | 1 | 0 | 5.211072 | -0.857839 | 2.835448 |
| 54 | 1 | 0 | 4.990218 | -2.203067 | 3.966873 |
| 55 | 1 | 0 | 6.362308 | -2.220549 | 2.846492 |
| 56 | 1 | 0 | 3.837701 | -4.662002 | 1.332679 |
| 57 | 1 | 0 | 5.474737 | -4.584859 | 2.021582 |
| 58 | 1 | 0 | 4.066657 | -4.450759 | 3.080134 |
| 59 | 6 | 0 | 4.357909 | -0.763832 | -2.638124 |
| 60 | 6 | 0 | 4.353332 | -1.608531 | -3.907290 |
| 61 | 6 | 0 | 5.273673 | 0.454773 | -2.738406 |
| 62 | 1 | 0 | 3.339916 | -0.430432 | -2.425384 |
| 63 | 1 | 0 | 3.689071 | -2.469751 | -3.800179 |
| 64 | 1 | 0 | 3.995293 | -1.004741 | -4.746308 |
| 65 | 1 | 0 | 5.357300 | -1.967401 | -4.161287 |
| 66 | 1 | 0 | 5.237111 | 1.039735 | -1.814683 |
| 67 | 1 | 0 | 6.313240 | 0.160954 | -2.922094 |
| 68 | 1 | 0 | 4.955974 | 1.097224 | -3.565597 |
| 69 | 6 | 0 | 1.642863 | 2.348161 | -1.469339 |

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|---|---|---|---|---|---|
| 70 | 6 | 0 | 1.786337 | 2.306728 | -2.986271 |
| 71 | 6 | 0 | 0.603247 | 3.358237 | -0.996155 |
| 72 | 1 | 0 | 1.355463 | 1.354181 | -1.140110 |
| 73 | 1 | 0 | 2.589777 | 1.629312 | -3.289597 |
| 74 | 1 | 0 | 0.851423 | 1.928670 | -3.408937 |
| 75 | 1 | 0 | 1.974598 | 3.295313 | -3.420516 |
| 76 | 1 | 0 | 0.542835 | 3.369671 | 0.095385 |
| 77 | 1 | 0 | 0.839553 | 4.367418 | -1.355095 |
| 78 | 1 | 0 | -0.380274 | 3.068522 | -1.378821 |
| 79 | 6 | 0 | 5.564531 | 2.072695 | 1.569154 |
| 80 | 6 | 0 | 6.246857 | 3.259099 | 2.241105 |
| 81 | 6 | 0 | 6.554162 | 1.077382 | 0.967649 |
| 82 | 1 | 0 | 4.938424 | 1.556634 | 2.300256 |
| 83 | 1 | 0 | 5.513283 | 3.989511 | 2.593888 |
| 84 | 1 | 0 | 6.814650 | 2.900295 | 3.104014 |
| 85 | 1 | 0 | 6.954566 | 3.763128 | 1.573987 |
| 86 | 1 | 0 | 6.028347 | 0.221100 | 0.534127 |
| 87 | 1 | 0 | 7.158066 | 1.548225 | 0.183593 |
| 88 | 1 | 0 | 7.230252 | 0.706578 | 1.744050 |
| 89 | 6 | 0 | -4.344170 | 2.813171 | -1.751909 |
| 90 | 6 | 0 | -4.298538 | 4.338492 | -1.785788 |
| 91 | 6 | 0 | -5.226317 | 2.211628 | -2.840740 |
| 92 | 1 | 0 | -3.327201 | 2.424782 | -1.857903 |
| 93 | 1 | 0 | -3.668785 | 4.724966 | -0.979345 |
| 94 | 1 | 0 | -3.879736 | 4.669509 | -2.740360 |
| 95 | 1 | 0 | -5.297474 | 4.778222 | -1.691411 |
| 96 | 1 | 0 | -5.181991 | 1.119540 | -2.807223 |
| 97 | 1 | 0 | -6.269547 | 2.530480 | -2.733215 |
| 98 | 1 | 0 | -4.874426 | 2.537664 | -3.823633 |
| 99 | 6 | 0 | -4.413610 | 0.578350 | 2.668294 |
| 100 | 6 | 0 | -5.344861 | -0.631576 | 2.688623 |
| 101 | 6 | 0 | -4.414648 | 1.351407 | 3.982152 |
| 102 | 1 | 0 | -3.394720 | 0.250221 | 2.450055 |
| 103 | 1 | 0 | -5.310706 | -1.163141 | 1.733179 |
| 104 | 1 | 0 | -5.041570 | -1.324712 | 3.479007 |
| 105 | 1 | 0 | -6.381330 | -0.334453 | 2.883432 |
| 106 | 1 | 0 | -3.739292 | 2.209049 | 3.931716 |
| 107 | 1 | 0 | -5.417528 | 1.706114 | 4.244937 |
| 108 | 1 | 0 | -4.072673 | 0.696435 | 4.788586 |
| 109 | 6 | 0 | -1.690825 | -2.425394 | 1.384757 |
| 110 | 6 | 0 | -0.660587 | -3.437208 | 0.897312 |
| 111 | 6 | 0 | -1.887183 | -2.459837 | 2.896051 |
| 112 | 1 | 0 | -1.364284 | -1.427067 | 1.111049 |
| 113 | 1 | 0 | -0.581208 | -3.416474 | -0.192068 |

| | | | | | |
|---|---|---|---|---|---|
| 114 | 1 | 0 | 0.320352 | -3.170137 | 1.301787 |
| 115 | 1 | 0 | -0.917559 | -4.452525 | 1.223302 |
| 116 | 1 | 0 | -2.676422 | -1.772938 | 3.214448 |
| 117 | 1 | 0 | -2.122521 | -3.463470 | 3.267850 |
| 118 | 1 | 0 | -0.953784 | -2.141314 | 3.367750 |
| 119 | 6 | 0 | -5.549750 | -1.917577 | -1.730552 |
| 120 | 6 | 0 | -6.545634 | -0.953381 | -1.090012 |
| 121 | 6 | 0 | -6.225850 | -3.056489 | -2.485714 |
| 122 | 1 | 0 | -4.906787 | -1.364523 | -2.419050 |
| 123 | 1 | 0 | -6.025187 | -0.128013 | -0.594557 |
| 124 | 1 | 0 | -7.203701 | -0.532498 | -1.856153 |
| 125 | 1 | 0 | -7.168058 | -1.466814 | -0.348537 |
| 126 | 1 | 0 | -5.490710 | -3.772244 | -2.863982 |
| 127 | 1 | 0 | -6.954250 | -3.590380 | -1.866031 |
| 128 | 1 | 0 | -6.769252 | -2.641708 | -3.339011 |
| 129 | 5 | 0 | -2.660558 | 0.883633 | 0.067855 |
| 130 | 5 | 0 | 2.664135 | -0.898487 | 0.016277 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.417877 | 2.332745 | 2.792105 |
| 2 | 6 | 0 | 1.463088 | 2.030683 | 1.941764 |
| 3 | 6 | 0 | 1.368460 | 1.098259 | 0.882707 |
| 4 | 6 | 0 | 0.081386 | 0.470806 | 0.586481 |
| 5 | 6 | 0 | -1.006332 | 0.862584 | 1.451773 |
| 6 | 6 | 0 | -0.804165 | 1.722700 | 2.541669 |
| 7 | 6 | 0 | -0.096220 | -0.485635 | -0.518373 |
| 8 | 6 | 0 | 0.976871 | -0.891414 | -1.394110 |
| 9 | 6 | 0 | 0.806714 | -1.795446 | -2.433768 |
| 10 | 1 | 0 | 1.644994 | -2.019979 | -3.088079 |
| 11 | 6 | 0 | -0.421647 | -2.459615 | -2.615290 |
| 12 | 6 | 0 | -1.449062 | -2.153652 | -1.771475 |
| 13 | 6 | 0 | -1.391359 | -1.136659 | -0.755690 |
| 14 | 1 | 0 | 0.538970 | 3.034729 | 3.611561 |
| 15 | 1 | 0 | 2.414211 | 2.539039 | 2.092926 |
| 16 | 1 | 0 | -1.654122 | 1.944170 | 3.182284 |
| 17 | 1 | 0 | -0.535840 | -3.210074 | -3.392791 |
| 18 | 1 | 0 | -2.382845 | -2.703546 | -1.875462 |
| 19 | 15 | 0 | 2.729746 | -0.398344 | -1.282900 |
| 20 | 15 | 0 | -2.773919 | 0.440211 | 1.295428 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 6 | 0 | -5.941472 | -2.249873 | -1.309025 |
| 22 | 6 | 0 | -6.000688 | -2.670720 | -0.024071 |
| 23 | 1 | 0 | -6.651449 | -2.354298 | -2.114419 |
| 24 | 1 | 0 | -6.768266 | -3.218574 | 0.499616 |
| 25 | 6 | 0 | -3.836867 | 3.585651 | -1.259774 |
| 26 | 6 | 0 | -4.905602 | 3.540665 | -0.425940 |
| 27 | 1 | 0 | -3.641326 | 4.211862 | -2.115833 |
| 28 | 1 | 0 | -5.817664 | 4.115312 | -0.423816 |
| 29 | 6 | 0 | 3.885559 | -3.627256 | 0.980776 |
| 30 | 6 | 0 | 4.925004 | -3.518519 | 0.116030 |
| 31 | 1 | 0 | 3.707948 | -4.330749 | 1.778581 |
| 32 | 1 | 0 | 5.825182 | -4.103900 | 0.023957 |
| 33 | 6 | 0 | 5.949361 | 2.718022 | 0.150752 |
| 34 | 6 | 0 | 5.958115 | 2.176412 | 1.392524 |
| 35 | 1 | 0 | 6.678519 | 3.334703 | -0.350786 |
| 36 | 1 | 0 | 6.700195 | 2.224587 | 2.173848 |
| 37 | 6 | 0 | -4.022658 | -1.614915 | -0.297752 |
| 38 | 6 | 0 | 3.447884 | -1.907229 | -0.376684 |
| 39 | 6 | 0 | 4.020052 | 1.590257 | 0.410082 |
| 40 | 6 | 0 | -3.426687 | 2.000377 | 0.271573 |
| 41 | 7 | 0 | 2.996052 | -2.623766 | 0.676233 |
| 42 | 7 | 0 | 4.638301 | -2.459627 | -0.718427 |
| 43 | 7 | 0 | 4.754387 | 2.356956 | -0.437975 |
| 44 | 7 | 0 | 4.769141 | 1.491728 | 1.539656 |
| 45 | 7 | 0 | -4.633701 | 2.567007 | 0.513736 |
| 46 | 7 | 0 | -2.949182 | 2.626481 | -0.825581 |
| 47 | 7 | 0 | -4.819955 | -2.286973 | 0.581713 |
| 48 | 7 | 0 | -4.727695 | -1.609435 | -1.466603 |
| 49 | 6 | 0 | 4.317262 | 2.806581 | -1.771734 |
| 50 | 6 | 0 | 5.183587 | 2.170389 | -2.852664 |
| 51 | 6 | 0 | 4.313683 | 4.330995 | -1.833197 |
| 52 | 1 | 0 | 3.291454 | 2.438190 | -1.863337 |
| 53 | 1 | 0 | 5.101555 | 1.080478 | -2.815630 |
| 54 | 1 | 0 | 4.850112 | 2.506609 | -3.838031 |
| 55 | 1 | 0 | 6.235053 | 2.456354 | -2.735094 |
| 56 | 1 | 0 | 3.707006 | 4.750862 | -1.026623 |
| 57 | 1 | 0 | 5.327102 | 4.739001 | -1.759711 |
| 58 | 1 | 0 | 3.894325 | 4.655326 | -2.789001 |
| 59 | 6 | 0 | 4.443139 | 0.615821 | 2.678581 |
| 60 | 6 | 0 | 4.556334 | 1.375266 | 3.994165 |
| 61 | 6 | 0 | 5.333016 | -0.623549 | 2.627268 |
| 62 | 1 | 0 | 3.400830 | 0.327604 | 2.517862 |
| 63 | 1 | 0 | 3.922644 | 2.265710 | 3.987117 |
| 64 | 1 | 0 | 4.231384 | 0.729368 | 4.814009 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 1 | 0 | 5.588810 | 1.677530 | 4.199045 |
| 66 | 1 | 0 | 5.199260 | -1.153219 | 1.677846 |
| 67 | 1 | 0 | 6.389661 | -0.352159 | 2.728607 |
| 68 | 1 | 0 | 5.080378 | -1.305673 | 3.444314 |
| 69 | 6 | 0 | 1.718882 | -2.400047 | 1.391994 |
| 70 | 6 | 0 | 1.931420 | -2.473173 | 2.899012 |
| 71 | 6 | 0 | 0.655612 | -3.373528 | 0.899163 |
| 72 | 1 | 0 | 1.428960 | -1.385014 | 1.135392 |
| 73 | 1 | 0 | 2.746372 | -1.818103 | 3.221401 |
| 74 | 1 | 0 | 1.013205 | -2.139322 | 3.389102 |
| 75 | 1 | 0 | 2.140671 | -3.492247 | 3.241529 |
| 76 | 1 | 0 | 0.571663 | -3.341066 | -0.190065 |
| 77 | 1 | 0 | 0.888822 | -4.397022 | 1.216383 |
| 78 | 1 | 0 | -0.314672 | -3.082331 | 1.314620 |
| 79 | 6 | 0 | 5.559483 | -1.929382 | -1.746062 |
| 80 | 6 | 0 | 6.338375 | -3.057243 | -2.410939 |
| 81 | 6 | 0 | 6.471207 | -0.883770 | -1.108777 |
| 82 | 1 | 0 | 4.912663 | -1.449228 | -2.484505 |
| 83 | 1 | 0 | 5.670673 | -3.843830 | -2.771731 |
| 84 | 1 | 0 | 6.884270 | -2.651836 | -3.266202 |
| 85 | 1 | 0 | 7.076817 | -3.498333 | -1.733928 |
| 86 | 1 | 0 | 5.882168 | -0.071898 | -0.667342 |
| 87 | 1 | 0 | 7.084032 | -1.337580 | -0.321853 |
| 88 | 1 | 0 | 7.138775 | -0.456356 | -1.862824 |
| 89 | 6 | 0 | -4.448249 | -2.634343 | 1.960956 |
| 90 | 6 | 0 | -4.518184 | -4.146318 | 2.157923 |
| 91 | 6 | 0 | -5.318348 | -1.872604 | 2.954776 |
| 92 | 1 | 0 | -3.409260 | -2.301404 | 2.050733 |
| 93 | 1 | 0 | -3.910626 | -4.663451 | 1.410559 |
| 94 | 1 | 0 | -4.140893 | -4.402554 | 3.151495 |
| 95 | 1 | 0 | -5.546894 | -4.515535 | 2.089011 |
| 96 | 1 | 0 | -5.188583 | -0.794722 | 2.825356 |
| 97 | 1 | 0 | -6.377229 | -2.126847 | 2.826756 |
| 98 | 1 | 0 | -5.029374 | -2.133209 | 3.976820 |
| 99 | 6 | 0 | -4.355883 | -0.817499 | -2.648485 |
| 100 | 6 | 0 | -5.226971 | 0.435533 | -2.707151 |
| 101 | 6 | 0 | -4.439347 | -1.660057 | -3.915005 |
| 102 | 1 | 0 | -3.317396 | -0.526747 | -2.472104 |
| 103 | 1 | 0 | -5.107063 | 1.024041 | -1.790868 |
| 104 | 1 | 0 | -4.941202 | 1.058175 | -3.560500 |
| 105 | 1 | 0 | -6.285526 | 0.175068 | -2.818130 |
| 106 | 1 | 0 | -3.815864 | -2.553811 | -3.829762 |
| 107 | 1 | 0 | -5.468561 | -1.967841 | -4.129490 |
| 108 | 1 | 0 | -4.084914 | -1.073833 | -4.767103 |

| | | | | | |
|---|---|---|---|---|---|
| 109 | 6 | 0 | -1.649351 | 2.327296 | -1.457169 |
| 110 | 6 | 0 | -0.581524 | 3.292588 | -0.955660 |
| 111 | 6 | 0 | -1.774508 | 2.323030 | -2.975363 |
| 112 | 1 | 0 | -1.414318 | 1.315462 | -1.137047 |
| 113 | 1 | 0 | -0.537693 | 3.291741 | 0.137456 |
| 114 | 1 | 0 | 0.396995 | 2.972734 | -1.329670 |
| 115 | 1 | 0 | -0.781250 | 4.311147 | -1.309317 |
| 116 | 1 | 0 | -2.601173 | 1.684606 | -3.301374 |
| 117 | 1 | 0 | -1.919864 | 3.328410 | -3.385565 |
| 118 | 1 | 0 | -0.849248 | 1.919894 | -3.395714 |
| 119 | 6 | 0 | -5.588397 | 2.109148 | 1.544182 |
| 120 | 6 | 0 | -6.486742 | 1.028047 | 0.948269 |
| 121 | 6 | 0 | -6.379890 | 3.281364 | 2.110437 |
| 122 | 1 | 0 | -4.966614 | 1.672922 | 2.329531 |
| 123 | 1 | 0 | -5.887911 | 0.186852 | 0.580987 |
| 124 | 1 | 0 | -7.180972 | 0.653673 | 1.706664 |
| 125 | 1 | 0 | -7.071046 | 1.431497 | 0.113417 |
| 126 | 1 | 0 | -5.717597 | 4.084891 | 2.443083 |
| 127 | 1 | 0 | -7.089580 | 3.684870 | 1.381063 |
| 128 | 1 | 0 | -6.959613 | 2.935612 | 2.969809 |
| 129 | 5 | 0 | -2.663046 | -0.900395 | 0.007341 |
| 130 | 5 | 0 | 2.654771 | 0.878801 | 0.096449 |

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**UBP86/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.307474 | -2.975327 | -2.114368 |
| 2 | 6 | 0 | 1.379852 | -2.514256 | -1.370124 |
| 3 | 6 | 0 | 1.369123 | -1.298156 | -0.604300 |
| 4 | 6 | 0 | 0.075809 | -0.587419 | -0.442234 |
| 5 | 6 | 0 | -1.041022 | -1.145830 | -1.187339 |
| 6 | 6 | 0 | -0.896283 | -2.248404 | -2.050310 |
| 7 | 6 | 0 | -0.075821 | 0.587377 | 0.442317 |
| 8 | 6 | 0 | 1.041014 | 1.145801 | 1.187405 |
| 9 | 6 | 0 | 0.896281 | 2.248393 | 2.050354 |
| 10 | 1 | 0 | 1.764745 | 2.576285 | 2.634963 |
| 11 | 6 | 0 | -0.307472 | 2.975324 | 2.114398 |
| 12 | 6 | 0 | -1.379852 | 2.514242 | 1.370164 |
| 13 | 6 | 0 | -1.369132 | 1.298123 | 0.604370 |
| 14 | 1 | 0 | 0.385300 | -3.883629 | -2.723854 |
| 15 | 1 | 0 | 2.305575 | -3.102192 | -1.372102 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 1 | 0 | -1.764742 | -2.576284 | -2.634933 |
| 17 | 1 | 0 | -0.385292 | 3.883641 | 2.723861 |
| 18 | 1 | 0 | -2.305571 | 3.102186 | 1.372124 |
| 19 | 15 | 0 | 2.809530 | 0.650654 | 1.090473 |
| 20 | 15 | 0 | -2.809535 | -0.650673 | -1.090422 |
| 21 | 6 | 0 | -5.890509 | 2.803904 | 0.901547 |
| 22 | 6 | 0 | -5.929372 | 2.888947 | -0.461726 |
| 23 | 1 | 0 | -6.586277 | 3.173817 | 1.650438 |
| 24 | 1 | 0 | -6.657581 | 3.360385 | -1.117093 |
| 25 | 6 | 0 | -3.971282 | -3.417389 | 1.811139 |
| 26 | 6 | 0 | -4.966280 | -3.552949 | 0.880934 |
| 27 | 1 | 0 | -3.830814 | -3.912798 | 2.768486 |
| 28 | 1 | 0 | -5.853945 | -4.180633 | 0.881934 |
| 29 | 6 | 0 | 3.971228 | 3.417346 | -1.811128 |
| 30 | 6 | 0 | 4.966267 | 3.552880 | -0.880963 |
| 31 | 1 | 0 | 3.830737 | 3.912757 | -2.768471 |
| 32 | 1 | 0 | 5.853951 | 4.180538 | -0.882000 |
| 33 | 6 | 0 | 5.929445 | -2.888882 | 0.461609 |
| 34 | 6 | 0 | 5.890527 | -2.803798 | -0.901659 |
| 35 | 1 | 0 | 6.657695 | -3.360317 | 1.116934 |
| 36 | 1 | 0 | 6.586279 | -3.173665 | -1.650589 |
| 37 | 6 | 0 | -4.029197 | 1.747852 | 0.096153 |
| 38 | 6 | 0 | 3.488386 | 2.020963 | -0.094074 |
| 39 | 6 | 0 | 4.029211 | -1.747833 | -0.096161 |
| 40 | 6 | 0 | -3.488411 | -2.020989 | 0.094106 |
| 41 | 7 | 0 | 3.079050 | 2.472480 | -1.324142 |
| 42 | 7 | 0 | 4.658125 | 2.696557 | 0.168249 |
| 43 | 7 | 0 | 4.791621 | -2.253782 | 0.946406 |
| 44 | 7 | 0 | 4.730944 | -2.111867 | -1.236455 |
| 45 | 7 | 0 | -4.658119 | -2.696617 | -0.168265 |
| 46 | 7 | 0 | -3.079112 | -2.472496 | 1.324191 |
| 47 | 7 | 0 | -4.791549 | 2.253795 | -0.946459 |
| 48 | 7 | 0 | -4.730962 | 2.111944 | 1.236409 |
| 49 | 6 | 0 | 4.366086 | -2.292939 | 2.366993 |
| 50 | 6 | 0 | 5.354804 | -1.527395 | 3.256399 |
| 51 | 6 | 0 | 4.154267 | -3.747067 | 2.821587 |
| 52 | 1 | 0 | 3.393929 | -1.768287 | 2.366388 |
| 53 | 1 | 0 | 5.453694 | -0.482688 | 2.918255 |
| 54 | 1 | 0 | 4.988882 | -1.517985 | 4.297493 |
| 55 | 1 | 0 | 6.355110 | -1.998432 | 3.257257 |
| 56 | 1 | 0 | 3.439363 | -4.266477 | 2.161319 |
| 57 | 1 | 0 | 5.100040 | -4.318099 | 2.830328 |
| 58 | 1 | 0 | 3.749463 | -3.757682 | 3.848280 |
| 59 | 6 | 0 | 4.412999 | -1.648983 | -2.609116 |

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|---|---|---|---|---|---|
| 60 | 6 | 0 | 4.349001 | -2.829970 | -3.588823 |
| 61 | 6 | 0 | 5.422635 | -0.574994 | -3.050496 |
| 62 | 1 | 0 | 3.410929 | -1.196665 | -2.517373 |
| 63 | 1 | 0 | 3.623537 | -3.589317 | -3.254369 |
| 64 | 1 | 0 | 4.032771 | -2.468072 | -4.582028 |
| 65 | 1 | 0 | 5.334014 | -3.315726 | -3.712302 |
| 66 | 1 | 0 | 5.436028 | 0.269648 | -2.340784 |
| 67 | 1 | 0 | 6.445287 | -0.986862 | -3.122095 |
| 68 | 1 | 0 | 5.148197 | -0.187916 | -4.047351 |
| 69 | 6 | 0 | 1.810666 | 2.093797 | -2.009170 |
| 70 | 6 | 0 | 2.064061 | 1.791928 | -3.492655 |
| 71 | 6 | 0 | 0.757079 | 3.191088 | -1.797901 |
| 72 | 1 | 0 | 1.481557 | 1.170087 | -1.510288 |
| 73 | 1 | 0 | 2.868107 | 1.048175 | -3.622164 |
| 74 | 1 | 0 | 1.141315 | 1.376425 | -3.930665 |
| 75 | 1 | 0 | 2.324815 | 2.698060 | -4.069448 |
| 76 | 1 | 0 | 0.597807 | 3.383873 | -0.724680 |
| 77 | 1 | 0 | 1.054583 | 4.132688 | -2.296025 |
| 78 | 1 | 0 | -0.203835 | 2.859356 | -2.225875 |
| 79 | 6 | 0 | 5.472579 | 2.588156 | 1.410660 |
| 80 | 6 | 0 | 5.503350 | 3.936724 | 2.145247 |
| 81 | 6 | 0 | 6.871547 | 2.043129 | 1.087559 |
| 82 | 1 | 0 | 4.921453 | 1.852354 | 2.022715 |
| 83 | 1 | 0 | 4.482111 | 4.294160 | 2.359397 |
| 84 | 1 | 0 | 6.036476 | 3.820151 | 3.104301 |
| 85 | 1 | 0 | 6.030645 | 4.713444 | 1.562603 |
| 86 | 1 | 0 | 6.810195 | 1.066313 | 0.578461 |
| 87 | 1 | 0 | 7.445391 | 2.736043 | 0.445968 |
| 88 | 1 | 0 | 7.440681 | 1.910052 | 2.023581 |
| 89 | 6 | 0 | -4.365957 | 2.292892 | -2.367030 |
| 90 | 6 | 0 | -4.154069 | 3.746998 | -2.821663 |
| 91 | 6 | 0 | -5.354663 | 1.527352 | -3.256452 |
| 92 | 1 | 0 | -3.393817 | 1.768208 | -2.366368 |
| 93 | 1 | 0 | -3.439176 | 4.266406 | -2.161381 |
| 94 | 1 | 0 | -3.749221 | 3.757566 | -3.848339 |
| 95 | 1 | 0 | -5.099823 | 4.318061 | -2.830464 |
| 96 | 1 | 0 | -5.453601 | 0.482658 | -2.918278 |
| 97 | 1 | 0 | -6.354955 | 1.998422 | -3.257364 |
| 98 | 1 | 0 | -4.988701 | 1.517897 | -4.297530 |
| 99 | 6 | 0 | -4.413084 | 1.649098 | 2.609098 |
| 100 | 6 | 0 | -5.422780 | 0.575166 | 3.050481 |
| 101 | 6 | 0 | -4.349077 | 2.830118 | 3.588764 |
| 102 | 1 | 0 | -3.411029 | 1.196738 | 2.517408 |
| 103 | 1 | 0 | -5.436181 | -0.269503 | 2.340801 |

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|---|---|---|---|---|---|
| 104 | 1 | 0 | -5.148394 | 0.188114 | 4.047360 |
| 105 | 1 | 0 | -6.445418 | 0.987078 | 3.122027 |
| 106 | 1 | 0 | -3.623571 | 3.589424 | 3.254309 |
| 107 | 1 | 0 | -5.334075 | 3.315917 | 3.712190 |
| 108 | 1 | 0 | -4.032897 | 2.468245 | 4.581994 |
| 109 | 6 | 0 | -1.810767 | -2.093779 | 2.009273 |
| 110 | 6 | 0 | -0.757136 | -3.191035 | 1.798037 |
| 111 | 6 | 0 | -2.064231 | -1.791932 | 3.492751 |
| 112 | 1 | 0 | -1.481665 | -1.170055 | 1.510412 |
| 113 | 1 | 0 | -0.597814 | -3.383804 | 0.724821 |
| 114 | 1 | 0 | 0.203749 | -2.859277 | 2.226054 |
| 115 | 1 | 0 | -1.054631 | -4.132649 | 2.296139 |
| 116 | 1 | 0 | -2.868304 | -1.048203 | 3.622234 |
| 117 | 1 | 0 | -2.324983 | -2.698077 | 4.069523 |
| 118 | 1 | 0 | -1.141514 | -1.376406 | 3.930802 |
| 119 | 6 | 0 | -5.472528 | -2.588234 | -1.410707 |
| 120 | 6 | 0 | -6.871518 | -2.043230 | -1.087661 |
| 121 | 6 | 0 | -5.503248 | -3.936804 | -2.145292 |
| 122 | 1 | 0 | -4.921391 | -1.852424 | -2.022743 |
| 123 | 1 | 0 | -6.810202 | -1.066410 | -0.578565 |
| 124 | 1 | 0 | -7.440620 | -1.910168 | -2.023705 |
| 125 | 1 | 0 | -7.445372 | -2.736151 | -0.446087 |
| 126 | 1 | 0 | -4.481995 | -4.294225 | -2.359400 |
| 127 | 1 | 0 | -6.030554 | -4.713531 | -1.562667 |
| 128 | 1 | 0 | -6.036338 | -3.820242 | -3.104367 |
| 129 | 5 | 0 | -2.704726 | 0.913836 | -0.028004 |
| 130 | 5 | 0 | 2.704719 | -0.913862 | 0.028065 |

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**2PB-c**

**UB3LYP/6-31G***

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| Center | Atomic | Atomic | Coordinates (Angstroms) |
|---|---|---|---|

| Number | Number | Type | X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.572962 | -2.358752 | 0.413614 |
| 2 | 6 | 0 | 0.760754 | -1.206417 | 0.236403 |
| 3 | 6 | 0 | 1.411762 | 0.010704 | -0.142008 |
| 4 | 6 | 0 | 2.833910 | 0.023645 | -0.272470 |
| 5 | 6 | 0 | 3.662279 | -1.144424 | -0.012412 |
| 6 | 6 | 0 | 2.947818 | -2.335948 | 0.291186 |
| 7 | 6 | 0 | 0.674473 | 1.219109 | -0.397147 |
| 8 | 6 | 0 | 3.500413 | 1.198180 | -0.691123 |
| 9 | 1 | 0 | 3.490299 | -3.270191 | 0.412166 |
| 10 | 6 | 0 | 2.770729 | 2.355902 | -0.979925 |
| 11 | 6 | 0 | 1.390982 | 2.366682 | -0.816801 |
| 12 | 1 | 0 | 3.273762 | 3.250396 | -1.342267 |
| 13 | 6 | 0 | -2.770750 | -2.355920 | 0.980052 |
| 14 | 6 | 0 | -3.500434 | -1.198195 | 0.691260 |
| 15 | 6 | 0 | -2.833928 | -0.023656 | 0.272621 |
| 16 | 6 | 0 | -1.411779 | -0.010714 | 0.142166 |
| 17 | 6 | 0 | -0.674488 | -1.219121 | 0.397300 |
| 18 | 6 | 0 | -1.391002 | -2.366699 | 0.816939 |
| 19 | 1 | 0 | -3.273787 | -3.250419 | 1.342376 |
| 20 | 6 | 0 | -3.662293 | 1.144411 | 0.012562 |
| 21 | 6 | 0 | -0.760773 | 1.206406 | -0.236247 |
| 22 | 6 | 0 | -1.572978 | 2.358738 | -0.413470 |
| 23 | 6 | 0 | -2.947837 | 2.335929 | -0.291050 |
| 24 | 1 | 0 | -3.490316 | 3.270171 | -0.412044 |
| 25 | 1 | 0 | -1.100255 | 3.307724 | -0.646594 |
| 26 | 1 | 0 | 0.853561 | 3.278453 | -1.053305 |
| 27 | 1 | 0 | -0.853583 | -3.278474 | 1.053432 |
| 28 | 1 | 0 | 1.100236 | -3.307738 | 0.646734 |
| 29 | 15 | 0 | 5.284801 | 0.905650 | -0.931654 |
| 30 | 15 | 0 | -5.284820 | -0.905685 | 0.931759 |
| 31 | 6 | 0 | -7.603066 | 3.714963 | -0.377010 |
| 32 | 6 | 0 | -8.082115 | 3.229982 | 0.790991 |
| 33 | 1 | 0 | -7.953439 | 4.531242 | -0.987912 |
| 34 | 1 | 0 | -8.910914 | 3.563893 | 1.393857 |
| 35 | 6 | 0 | -7.358211 | -3.527506 | -1.356542 |
| 36 | 6 | 0 | -6.475040 | -3.121846 | -2.303933 |
| 37 | 1 | 0 | -8.157892 | -4.248519 | -1.407845 |
| 38 | 1 | 0 | -6.364139 | -3.429446 | -3.331006 |
| 39 | 6 | 0 | 7.358268 | 3.527567 | 1.356479 |
| 40 | 6 | 0 | 6.475237 | 3.121832 | 2.303967 |
| 41 | 1 | 0 | 8.157907 | 4.248631 | 1.407698 |
| 42 | 1 | 0 | 6.364442 | 3.429404 | 3.331060 |

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|---|---|---|---|---|---|
| 43 | 6 | 0 | 8.081847 | -3.230169 | -0.791420 |
| 44 | 6 | 0 | 7.603028 | -3.715106 | 0.376695 |
| 45 | 1 | 0 | 8.910490 | -3.564136 | -1.394473 |
| 46 | 1 | 0 | 7.953479 | -4.531403 | 0.987527 |
| 47 | 6 | 0 | 6.012994 | 1.983376 | 0.424999 |
| 48 | 6 | 0 | 6.285142 | -1.960825 | -0.219300 |
| 49 | 6 | 0 | -6.012959 | -1.983377 | -0.424934 |
| 50 | 6 | 0 | -6.285215 | 1.960739 | 0.219241 |
| 51 | 7 | 0 | 5.658213 | 2.169935 | 1.726984 |
| 52 | 7 | 0 | 7.065351 | 2.824942 | 0.203117 |
| 53 | 7 | 0 | 6.505612 | -2.942911 | 0.728251 |
| 54 | 7 | 0 | 7.284705 | -2.154893 | -1.156210 |
| 55 | 7 | 0 | -6.505524 | 2.942843 | -0.728335 |
| 56 | 7 | 0 | -7.285001 | 2.154735 | 1.155941 |
| 57 | 7 | 0 | -5.658030 | -2.169986 | -1.726869 |
| 58 | 7 | 0 | -7.065389 | -2.824880 | -0.203157 |
| 59 | 6 | 0 | 4.549687 | 1.491422 | 2.453789 |
| 60 | 6 | 0 | 3.382049 | 2.458432 | 2.668415 |
| 61 | 6 | 0 | 5.066251 | 0.900322 | 3.768942 |
| 62 | 1 | 0 | 4.241343 | 0.676003 | 1.800508 |
| 63 | 1 | 0 | 3.014021 | 2.851721 | 1.718214 |
| 64 | 1 | 0 | 2.558493 | 1.925088 | 3.153369 |
| 65 | 1 | 0 | 3.671344 | 3.294425 | 3.317029 |
| 66 | 1 | 0 | 5.933936 | 0.255586 | 3.603959 |
| 67 | 1 | 0 | 5.338989 | 1.675146 | 4.494627 |
| 68 | 1 | 0 | 4.271982 | 0.297426 | 4.219902 |
| 69 | 6 | 0 | 7.795966 | 3.014924 | -1.076890 |
| 70 | 6 | 0 | 9.266175 | 2.618276 | -0.913687 |
| 71 | 6 | 0 | 7.612031 | 4.447627 | -1.586128 |
| 72 | 1 | 0 | 7.310027 | 2.328335 | -1.773188 |
| 73 | 1 | 0 | 9.359934 | 1.591349 | -0.546041 |
| 74 | 1 | 0 | 9.771273 | 2.684471 | -1.882557 |
| 75 | 1 | 0 | 9.794377 | 3.281611 | -0.219282 |
| 76 | 1 | 0 | 6.550927 | 4.690288 | -1.698740 |
| 77 | 1 | 0 | 8.067677 | 5.183507 | -0.913945 |
| 78 | 1 | 0 | 8.091637 | 4.549811 | -2.564756 |
| 79 | 6 | 0 | 7.309173 | -1.565656 | -2.513148 |
| 80 | 6 | 0 | 6.661500 | -2.524204 | -3.520465 |
| 81 | 6 | 0 | 8.731608 | -1.160419 | -2.909941 |
| 82 | 1 | 0 | 6.698963 | -0.665104 | -2.449114 |
| 83 | 1 | 0 | 5.639577 | -2.767602 | -3.214130 |
| 84 | 1 | 0 | 6.621292 | -2.056297 | -4.509871 |
| 85 | 1 | 0 | 7.231620 | -3.456335 | -3.607915 |
| 86 | 1 | 0 | 9.181294 | -0.500722 | -2.160355 |

| | | | | | |
|---|---|---|---|---|---|
| 87 | 1 | 0 | 9.389274 | -2.027046 | -3.042859 |
| 88 | 1 | 0 | 8.703230 | -0.626870 | -3.865457 |
| 89 | 6 | 0 | 5.871101 | -3.009559 | 2.060567 |
| 90 | 6 | 0 | 6.856978 | -2.531557 | 3.135845 |
| 91 | 6 | 0 | 5.344025 | -4.418199 | 2.352626 |
| 92 | 1 | 0 | 5.030466 | -2.315928 | 2.008319 |
| 93 | 1 | 0 | 7.245078 | -1.537244 | 2.892585 |
| 94 | 1 | 0 | 6.357023 | -2.481471 | 4.108866 |
| 95 | 1 | 0 | 7.708176 | -3.215149 | 3.231460 |
| 96 | 1 | 0 | 4.665149 | -4.762244 | 1.567583 |
| 97 | 1 | 0 | 6.158968 | -5.145613 | 2.445625 |
| 98 | 1 | 0 | 4.797105 | -4.415385 | 3.300998 |
| 99 | 6 | 0 | -4.549397 | -1.491515 | -2.453550 |
| 100 | 6 | 0 | -5.065799 | -0.900372 | -3.768750 |
| 101 | 6 | 0 | -3.381779 | -2.458574 | -2.668071 |
| 102 | 1 | 0 | -4.241085 | -0.676121 | -1.800221 |
| 103 | 1 | 0 | -5.933500 | -0.255631 | -3.603857 |
| 104 | 1 | 0 | -4.271473 | -0.297468 | -4.219599 |
| 105 | 1 | 0 | -5.338454 | -1.675175 | -4.494487 |
| 106 | 1 | 0 | -3.013840 | -2.851867 | -1.717838 |
| 107 | 1 | 0 | -3.671062 | -3.294564 | -3.316696 |
| 108 | 1 | 0 | -2.558168 | -1.925271 | -3.152976 |
| 109 | 6 | 0 | -7.796200 | -3.014756 | 1.076753 |
| 110 | 6 | 0 | -7.612682 | -4.447529 | 1.585942 |
| 111 | 6 | 0 | -9.266292 | -2.617738 | 0.913391 |
| 112 | 1 | 0 | -7.310175 | -2.328321 | 1.773144 |
| 113 | 1 | 0 | -6.551652 | -4.690483 | 1.698619 |
| 114 | 1 | 0 | -8.092383 | -4.549618 | 2.564533 |
| 115 | 1 | 0 | -8.068485 | -5.183264 | 0.913706 |
| 116 | 1 | 0 | -9.359753 | -1.590753 | 0.545833 |
| 117 | 1 | 0 | -9.794551 | -3.280879 | 0.218842 |
| 118 | 1 | 0 | -9.771543 | -2.683908 | 1.882184 |
| 119 | 6 | 0 | -7.309629 | 1.565581 | 2.512915 |
| 120 | 6 | 0 | -8.732194 | 1.160910 | 2.909817 |
| 121 | 6 | 0 | -6.661539 | 2.523941 | 3.520145 |
| 122 | 1 | 0 | -6.699776 | 0.664785 | 2.448919 |
| 123 | 1 | 0 | -9.182227 | 0.501426 | 2.160251 |
| 124 | 1 | 0 | -8.703930 | 0.627306 | 3.865305 |
| 125 | 1 | 0 | -9.389497 | 2.027793 | 3.042858 |
| 126 | 1 | 0 | -5.639532 | 2.766911 | 3.213752 |
| 127 | 1 | 0 | -7.231295 | 3.456301 | 3.607532 |
| 128 | 1 | 0 | -6.621481 | 2.056094 | 4.509585 |
| 129 | 6 | 0 | -5.870733 | 3.009543 | -2.060513 |
| 130 | 6 | 0 | -5.343678 | 4.418219 | -2.352447 |

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|---|---|---|---|---|---|
| 131 | 6 | 0 | -6.856336 | 2.531484 | -3.136017 |
| 132 | 1 | 0 | -5.030065 | 2.315966 | -2.008092 |
| 133 | 1 | 0 | -4.664994 | 4.762299 | -1.567254 |
| 134 | 1 | 0 | -4.796554 | 4.415448 | -3.300702 |
| 135 | 1 | 0 | -6.158646 | 5.145584 | -2.445613 |
| 136 | 1 | 0 | -7.244429 | 1.537144 | -2.892849 |
| 137 | 1 | 0 | -7.707555 | 3.215023 | -3.231827 |
| 138 | 1 | 0 | -6.356154 | 2.481429 | -4.108924 |
| 139 | 5 | 0 | 5.146555 | -0.917446 | -0.230777 |
| 140 | 5 | 0 | -5.146578 | 0.917438 | 0.230912 |

**UWB97XD/6-31G***

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
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| 1 | 6 | 0 | 1.656474 | -2.219252 | 0.717126 |
| 2 | 6 | 0 | 0.804391 | -1.135159 | 0.384442 |
| 3 | 6 | 0 | 1.393564 | 0.016308 | -0.216744 |
| 4 | 6 | 0 | 2.801237 | 0.040933 | -0.417964 |
| 5 | 6 | 0 | 3.670547 | -1.038892 | 0.001784 |
| 6 | 6 | 0 | 3.019908 | -2.179408 | 0.533848 |
| 7 | 6 | 0 | 0.617681 | 1.153668 | -0.614770 |
| 8 | 6 | 0 | 3.417701 | 1.160431 | -1.012541 |
| 9 | 1 | 0 | 3.606435 | -3.058573 | 0.791739 |
| 10 | 6 | 0 | 2.648737 | 2.241910 | -1.438575 |
| 11 | 6 | 0 | 1.279788 | 2.239058 | -1.230691 |
| 12 | 1 | 0 | 3.116777 | 3.090179 | -1.932759 |
| 13 | 6 | 0 | -2.648857 | -2.242435 | 1.438039 |
| 14 | 6 | 0 | -3.417777 | -1.160816 | 1.012272 |
| 15 | 6 | 0 | -2.801254 | -0.041189 | 0.418001 |
| 16 | 6 | 0 | -1.393577 | -0.016575 | 0.216805 |
| 17 | 6 | 0 | -0.617709 | -1.153992 | 0.614713 |
| 18 | 6 | 0 | -1.279893 | -2.239553 | 1.230256 |
| 19 | 1 | 0 | -3.116952 | -3.090861 | 1.931903 |
| 20 | 6 | 0 | -3.670500 | 1.038809 | -0.001421 |
| 21 | 6 | 0 | -0.804381 | 1.134960 | -0.384225 |
| 22 | 6 | 0 | -1.656380 | 2.219240 | -0.716494 |
| 23 | 6 | 0 | -3.019809 | 2.179455 | -0.533125 |
| 24 | 1 | 0 | -3.606278 | 3.058767 | -0.790643 |
| 25 | 1 | 0 | -1.226630 | 3.125577 | -1.130122 |
| 26 | 1 | 0 | 0.709053 | 3.095156 | -1.571763 |
| 27 | 1 | 0 | -0.709229 | -3.095814 | 1.571032 |

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|---|---|---|---|---|---|
| 28 | 1 | 0 | 1.226797 | -3.125457 | 1.131119 |
| 29 | 15 | 0 | 5.206094 | 0.930043 | -1.200792 |
| 30 | 15 | 0 | -5.206159 | -0.930438 | 1.200555 |
| 31 | 6 | 0 | -7.685911 | 3.292345 | -0.818520 |
| 32 | 6 | 0 | -8.154582 | 3.011668 | 0.415067 |
| 33 | 1 | 0 | -8.062374 | 3.967857 | -1.569506 |
| 34 | 1 | 0 | -9.003999 | 3.413620 | 0.941166 |
| 35 | 6 | 0 | -7.389382 | -3.306484 | -1.196590 |
| 36 | 6 | 0 | -6.329122 | -3.154266 | -2.021955 |
| 37 | 1 | 0 | -8.304306 | -3.860110 | -1.326351 |
| 38 | 1 | 0 | -6.143428 | -3.559315 | -3.003149 |
| 39 | 6 | 0 | 7.389445 | 3.306742 | 1.195579 |
| 40 | 6 | 0 | 6.329142 | 3.154907 | 2.020959 |
| 41 | 1 | 0 | 8.304437 | 3.860291 | 1.325198 |
| 42 | 1 | 0 | 6.143454 | 3.560298 | 3.002012 |
| 43 | 6 | 0 | 8.154556 | -3.011856 | -0.414200 |
| 44 | 6 | 0 | 7.685952 | -3.292107 | 0.819511 |
| 45 | 1 | 0 | 9.003918 | -3.414024 | -0.940221 |
| 46 | 1 | 0 | 8.062433 | -3.967388 | 1.570696 |
| 47 | 6 | 0 | 5.897955 | 1.994757 | 0.163332 |
| 48 | 6 | 0 | 6.316353 | -1.745153 | -0.085412 |
| 49 | 6 | 0 | -5.897996 | -1.994683 | -0.163961 |
| 50 | 6 | 0 | -6.316319 | 1.745121 | 0.085966 |
| 51 | 7 | 0 | 5.423446 | 2.337353 | 1.382996 |
| 52 | 7 | 0 | 7.107220 | 2.597030 | 0.048601 |
| 53 | 7 | 0 | 6.559048 | -2.516838 | 1.017754 |
| 54 | 7 | 0 | 7.321941 | -2.054260 | -0.965185 |
| 55 | 7 | 0 | -6.558990 | 2.517151 | -1.016968 |
| 56 | 7 | 0 | -7.321970 | 2.053916 | 0.965787 |
| 57 | 7 | 0 | -5.423504 | -2.336800 | -1.383768 |
| 58 | 7 | 0 | -7.107162 | -2.597179 | -0.049359 |
| 59 | 6 | 0 | 4.147008 | 1.907524 | 1.997585 |
| 60 | 6 | 0 | 3.140540 | 3.051720 | 1.985122 |
| 61 | 6 | 0 | 4.394440 | 1.347978 | 3.394074 |
| 62 | 1 | 0 | 3.784883 | 1.098218 | 1.372309 |
| 63 | 1 | 0 | 2.980613 | 3.416489 | 0.968298 |
| 64 | 1 | 0 | 2.180492 | 2.689012 | 2.362640 |
| 65 | 1 | 0 | 3.471205 | 3.881134 | 2.621475 |
| 66 | 1 | 0 | 5.165663 | 0.574304 | 3.372474 |
| 67 | 1 | 0 | 4.688423 | 2.121553 | 4.112252 |
| 68 | 1 | 0 | 3.466472 | 0.896746 | 3.755713 |
| 69 | 6 | 0 | 8.046722 | 2.424029 | -1.075842 |
| 70 | 6 | 0 | 9.024883 | 1.296533 | -0.752903 |
| 71 | 6 | 0 | 8.743239 | 3.737811 | -1.413280 |

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|---|---|---|---|---|---|
| 72 | 1 | 0 | 7.421327 | 2.127764 | -1.921353 |
| 73 | 1 | 0 | 8.490888 | 0.367221 | -0.529069 |
| 74 | 1 | 0 | 9.684573 | 1.122380 | -1.608413 |
| 75 | 1 | 0 | 9.647640 | 1.553646 | 0.111075 |
| 76 | 1 | 0 | 8.018895 | 4.543174 | -1.563266 |
| 77 | 1 | 0 | 9.454929 | 4.040528 | -0.637790 |
| 78 | 1 | 0 | 9.309151 | 3.610250 | -2.340043 |
| 79 | 6 | 0 | 7.328969 | -1.650061 | -2.382513 |
| 80 | 6 | 0 | 6.285226 | -2.449883 | -3.160074 |
| 81 | 6 | 0 | 8.723696 | -1.777354 | -2.985187 |
| 82 | 1 | 0 | 7.044869 | -0.595274 | -2.394500 |
| 83 | 1 | 0 | 5.292697 | -2.315545 | -2.720205 |
| 84 | 1 | 0 | 6.253266 | -2.110260 | -4.199689 |
| 85 | 1 | 0 | 6.535300 | -3.516535 | -3.150351 |
| 86 | 1 | 0 | 9.479463 | -1.280323 | -2.368771 |
| 87 | 1 | 0 | 9.015827 | -2.823568 | -3.125713 |
| 88 | 1 | 0 | 8.724720 | -1.306852 | -3.972117 |
| 89 | 6 | 0 | 5.935993 | -2.314181 | 2.333096 |
| 90 | 6 | 0 | 6.888527 | -1.517813 | 3.225377 |
| 91 | 6 | 0 | 5.524092 | -3.643561 | 2.956626 |
| 92 | 1 | 0 | 5.041732 | -1.718842 | 2.140267 |
| 93 | 1 | 0 | 7.156719 | -0.569704 | 2.746946 |
| 94 | 1 | 0 | 6.413895 | -1.303108 | 4.187923 |
| 95 | 1 | 0 | 7.809601 | -2.077470 | 3.421745 |
| 96 | 1 | 0 | 4.888393 | -4.217890 | 2.277687 |
| 97 | 1 | 0 | 6.393243 | -4.256601 | 3.220370 |
| 98 | 1 | 0 | 4.962375 | -3.455671 | 3.875978 |
| 99 | 6 | 0 | -4.147158 | -1.906569 | -1.998276 |
| 100 | 6 | 0 | -4.394702 | -1.346880 | -3.394691 |
| 101 | 6 | 0 | -3.140400 | -3.050510 | -1.986015 |
| 102 | 1 | 0 | -3.785258 | -1.097252 | -1.372873 |
| 103 | 1 | 0 | -5.166154 | -0.573437 | -3.373031 |
| 104 | 1 | 0 | -3.466847 | -0.895324 | -3.756216 |
| 105 | 1 | 0 | -4.688410 | -2.120439 | -4.112999 |
| 106 | 1 | 0 | -2.980344 | -3.415407 | -0.969259 |
| 107 | 1 | 0 | -3.470879 | -3.879897 | -2.622499 |
| 108 | 1 | 0 | -2.180455 | -2.687498 | -2.363504 |
| 109 | 6 | 0 | -8.046632 | -2.424667 | 1.075189 |
| 110 | 6 | 0 | -8.743060 | -3.738620 | 1.412149 |
| 111 | 6 | 0 | -9.024879 | -1.297112 | 0.752725 |
| 112 | 1 | 0 | -7.421226 | -2.128692 | 1.920793 |
| 113 | 1 | 0 | -8.018668 | -4.544004 | 1.561787 |
| 114 | 1 | 0 | -9.308935 | -3.611453 | 2.338989 |
| 115 | 1 | 0 | -9.454773 | -4.041068 | 0.636573 |

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| 116 | 1 | 0 | -8.490966 | -0.367665 | 0.529263 |
| 117 | 1 | 0 | -9.647633 | -1.553923 | -0.111344 |
| 118 | 1 | 0 | -9.684567 | -1.123362 | 1.608320 |
| 119 | 6 | 0 | -7.329019 | 1.649345 | 2.383009 |
| 120 | 6 | 0 | -8.723790 | 1.776343 | 2.985643 |
| 121 | 6 | 0 | -6.285387 | 2.449067 | 3.160823 |
| 122 | 1 | 0 | -7.044821 | 0.594583 | 2.394732 |
| 123 | 1 | 0 | -9.479475 | 1.279411 | 2.369046 |
| 124 | 1 | 0 | -8.724823 | 1.305564 | 3.972442 |
| 125 | 1 | 0 | -9.016029 | 2.822489 | 3.126447 |
| 126 | 1 | 0 | -5.292824 | 2.314926 | 2.720970 |
| 127 | 1 | 0 | -6.535558 | 3.515699 | 3.151353 |
| 128 | 1 | 0 | -6.253450 | 2.109189 | 4.200355 |
| 129 | 6 | 0 | -5.935892 | 2.314925 | -2.332352 |
| 130 | 6 | 0 | -5.523912 | 3.644506 | -2.955401 |
| 131 | 6 | 0 | -6.888425 | 1.518911 | -3.224949 |
| 132 | 1 | 0 | -5.041665 | 1.719479 | -2.139697 |
| 133 | 1 | 0 | -4.888204 | 4.218564 | -2.276241 |
| 134 | 1 | 0 | -4.962180 | 3.456917 | -3.874806 |
| 135 | 1 | 0 | -6.393028 | 4.257681 | -3.218948 |
| 136 | 1 | 0 | -7.156693 | 0.570654 | -2.746852 |
| 137 | 1 | 0 | -7.809460 | 2.078683 | -3.421174 |
| 138 | 1 | 0 | -6.413754 | 1.304511 | -4.187544 |
| 139 | 5 | 0 | 5.131633 | -0.784988 | -0.290649 |
| 140 | 5 | 0 | -5.131607 | 0.784902 | 0.290958 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.562362 | -2.383503 | 0.252638 |
| 2 | 6 | 0 | 0.756410 | -1.219181 | 0.156625 |
| 3 | 6 | 0 | 1.400042 | 0.009178 | -0.177285 |
| 4 | 6 | 0 | 2.813955 | 0.021395 | -0.340715 |
| 5 | 6 | 0 | 3.641026 | -1.153982 | -0.139517 |
| 6 | 6 | 0 | 2.931197 | -2.359067 | 0.109111 |
| 7 | 6 | 0 | 0.670899 | 1.231200 | -0.354184 |
| 8 | 6 | 0 | 3.477580 | 1.205547 | -0.709680 |
| 9 | 1 | 0 | 3.478271 | -3.297537 | 0.168415 |
| 10 | 6 | 0 | 2.755591 | 2.378725 | -0.928825 |
| 11 | 6 | 0 | 1.382346 | 2.390745 | -0.736767 |
| 12 | 1 | 0 | 3.260909 | 3.287147 | -1.250653 |

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|---|---|---|---|---|---|
| 13 | 6 | 0 | -2.755401 | -2.378571 | 0.929210 |
| 14 | 6 | 0 | -3.477433 | -1.205461 | 0.709849 |
| 15 | 6 | 0 | -2.813833 | -0.021329 | 0.340757 |
| 16 | 6 | 0 | -1.399921 | -0.009099 | 0.177332 |
| 17 | 6 | 0 | -0.670751 | -1.231102 | 0.354312 |
| 18 | 6 | 0 | -1.382161 | -2.390599 | 0.737132 |
| 19 | 1 | 0 | -3.260691 | -3.286938 | 1.251238 |
| 20 | 6 | 0 | -3.640911 | 1.154021 | 0.139473 |
| 21 | 6 | 0 | -0.756299 | 1.219257 | -0.156637 |
| 22 | 6 | 0 | -1.562270 | 2.383534 | -0.252840 |
| 23 | 6 | 0 | -2.931118 | 2.359067 | -0.109324 |
| 24 | 1 | 0 | -3.478210 | 3.297514 | -0.168790 |
| 25 | 1 | 0 | -1.086824 | 3.340986 | -0.438810 |
| 26 | 1 | 0 | 0.845385 | 3.314859 | -0.917302 |
| 27 | 1 | 0 | -0.845155 | -3.314643 | 0.917892 |
| 28 | 1 | 0 | 1.086865 | -3.340967 | 0.438426 |
| 29 | 15 | 0 | 5.266308 | 0.936439 | -0.931984 |
| 30 | 15 | 0 | -5.266159 | -0.936411 | 0.932119 |
| 31 | 6 | 0 | -7.423534 | 3.813238 | -0.231801 |
| 32 | 6 | 0 | -7.997069 | 3.266444 | 0.862499 |
| 33 | 1 | 0 | -7.694974 | 4.689605 | -0.798532 |
| 34 | 1 | 0 | -8.851027 | 3.588925 | 1.434348 |
| 35 | 6 | 0 | -6.963067 | -3.559824 | -1.618479 |
| 36 | 6 | 0 | -6.087625 | -2.994851 | -2.486405 |
| 37 | 1 | 0 | -7.673956 | -4.357392 | -1.759217 |
| 38 | 1 | 0 | -5.892467 | -3.209423 | -3.525029 |
| 39 | 6 | 0 | 6.962859 | 3.560186 | 1.618490 |
| 40 | 6 | 0 | 6.087452 | 2.995158 | 2.486416 |
| 41 | 1 | 0 | 7.673615 | 4.357878 | 1.759195 |
| 42 | 1 | 0 | 5.892204 | 3.209790 | 3.525010 |
| 43 | 6 | 0 | 7.996673 | -3.266976 | -0.862759 |
| 44 | 6 | 0 | 7.422984 | -3.813767 | 0.231457 |
| 45 | 1 | 0 | 8.850564 | -3.589579 | -1.434638 |
| 46 | 1 | 0 | 7.694223 | -4.690253 | 0.798099 |
| 47 | 6 | 0 | 5.851547 | 1.954615 | 0.525831 |
| 48 | 6 | 0 | 6.235812 | -1.969145 | -0.303900 |
| 49 | 6 | 0 | -5.851475 | -1.954488 | -0.525753 |
| 50 | 6 | 0 | -6.235890 | 1.968985 | 0.303782 |
| 51 | 7 | 0 | 5.417760 | 2.006814 | 1.804490 |
| 52 | 7 | 0 | 6.811931 | 2.904151 | 0.417297 |
| 53 | 7 | 0 | 6.344941 | -3.018313 | 0.569263 |
| 54 | 7 | 0 | 7.273975 | -2.132397 | -1.181415 |
| 55 | 7 | 0 | -6.345345 | 3.017970 | -0.569548 |
| 56 | 7 | 0 | -7.274062 | 2.132122 | 1.181316 |

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| 57 | 7 | 0 | -5.417773 | -2.006640 | -1.804443 |
| 58 | 7 | 0 | -6.811970 | -2.903918 | -0.417236 |
| 59 | 6 | 0 | 4.379488 | 1.145557 | 2.416970 |
| 60 | 6 | 0 | 3.085126 | 1.924968 | 2.613750 |
| 61 | 6 | 0 | 4.906319 | 0.558052 | 3.722231 |
| 62 | 1 | 0 | 4.228426 | 0.335850 | 1.702904 |
| 63 | 1 | 0 | 2.729568 | 2.349921 | 1.672728 |
| 64 | 1 | 0 | 2.315139 | 1.246575 | 2.991683 |
| 65 | 1 | 0 | 3.222418 | 2.729343 | 3.346111 |
| 66 | 1 | 0 | 5.881771 | 0.086458 | 3.579568 |
| 67 | 1 | 0 | 4.992416 | 1.315761 | 4.508324 |
| 68 | 1 | 0 | 4.202174 | -0.200689 | 4.074649 |
| 69 | 6 | 0 | 7.519412 | 3.274495 | -0.829359 |
| 70 | 6 | 0 | 8.959189 | 3.674376 | -0.530211 |
| 71 | 6 | 0 | 6.740647 | 4.370086 | -1.548462 |
| 72 | 1 | 0 | 7.514619 | 2.370310 | -1.440979 |
| 73 | 1 | 0 | 9.469435 | 2.916811 | 0.070610 |
| 74 | 1 | 0 | 9.496955 | 3.785083 | -1.474911 |
| 75 | 1 | 0 | 9.015523 | 4.636526 | -0.011570 |
| 76 | 1 | 0 | 5.735558 | 4.022025 | -1.802736 |
| 77 | 1 | 0 | 6.658980 | 5.261319 | -0.917693 |
| 78 | 1 | 0 | 7.255548 | 4.646886 | -2.472392 |
| 79 | 6 | 0 | 7.446722 | -1.345844 | -2.415457 |
| 80 | 6 | 0 | 6.403536 | -1.761015 | -3.449341 |
| 81 | 6 | 0 | 8.867352 | -1.475586 | -2.951099 |
| 82 | 1 | 0 | 7.276468 | -0.303629 | -2.134215 |
| 83 | 1 | 0 | 5.393614 | -1.650340 | -3.044841 |
| 84 | 1 | 0 | 6.493690 | -1.136111 | -4.342263 |
| 85 | 1 | 0 | 6.556846 | -2.806295 | -3.738030 |
| 86 | 1 | 0 | 9.612938 | -1.257178 | -2.180873 |
| 87 | 1 | 0 | 9.056963 | -2.474509 | -3.356627 |
| 88 | 1 | 0 | 9.000241 | -0.763853 | -3.769483 |
| 89 | 6 | 0 | 5.668879 | -3.101979 | 1.873977 |
| 90 | 6 | 0 | 6.636225 | -2.641830 | 2.963531 |
| 91 | 6 | 0 | 5.146661 | -4.510966 | 2.130560 |
| 92 | 1 | 0 | 4.830117 | -2.405990 | 1.811251 |
| 93 | 1 | 0 | 7.041928 | -1.656219 | 2.716684 |
| 94 | 1 | 0 | 6.122142 | -2.581131 | 3.927192 |
| 95 | 1 | 0 | 7.471862 | -3.342316 | 3.065527 |
| 96 | 1 | 0 | 4.509407 | -4.856657 | 1.313406 |
| 97 | 1 | 0 | 5.967634 | -5.224942 | 2.256420 |
| 98 | 1 | 0 | 4.560424 | -4.518334 | 3.053192 |
| 99 | 6 | 0 | -4.379370 | -1.145519 | -2.416887 |
| 100 | 6 | 0 | -4.906002 | -0.558054 | -3.722248 |

| | | | | | |
|---|---|---|---|---|---|
| 101 | 6 | 0 | -3.085056 | -1.925054 | -2.613493 |
| 102 | 1 | 0 | -4.228308 | -0.335777 | -1.702863 |
| 103 | 1 | 0 | -5.881463 | -0.086427 | -3.579754 |
| 104 | 1 | 0 | -4.201783 | 0.200654 | -4.074591 |
| 105 | 1 | 0 | -4.991998 | -1.315786 | -4.508329 |
| 106 | 1 | 0 | -2.729597 | -2.349950 | -1.672409 |
| 107 | 1 | 0 | -3.222371 | -2.729484 | -3.345790 |
| 108 | 1 | 0 | -2.314983 | -1.246761 | -2.991433 |
| 109 | 6 | 0 | -7.519381 | -3.274315 | 0.829444 |
| 110 | 6 | 0 | -6.740583 | -4.369947 | 1.548450 |
| 111 | 6 | 0 | -8.959178 | -3.674173 | 0.530366 |
| 112 | 1 | 0 | -7.514552 | -2.370162 | 1.441111 |
| 113 | 1 | 0 | -5.735474 | -4.021908 | 1.802673 |
| 114 | 1 | 0 | -7.255427 | -4.646783 | 2.472400 |
| 115 | 1 | 0 | -6.658964 | -5.261151 | 0.917633 |
| 116 | 1 | 0 | -9.469453 | -2.916587 | -0.070405 |
| 117 | 1 | 0 | -9.015554 | -4.636309 | 0.011704 |
| 118 | 1 | 0 | -9.496891 | -3.784899 | 1.475093 |
| 119 | 6 | 0 | -7.446659 | 1.345637 | 2.415414 |
| 120 | 6 | 0 | -8.867359 | 1.474983 | 2.950973 |
| 121 | 6 | 0 | -6.403607 | 1.761161 | 3.449291 |
| 122 | 1 | 0 | -7.276070 | 0.303456 | 2.134276 |
| 123 | 1 | 0 | -9.612825 | 1.256353 | 2.180693 |
| 124 | 1 | 0 | -9.000093 | 0.763237 | 3.769371 |
| 125 | 1 | 0 | -9.057295 | 2.473856 | 3.356471 |
| 126 | 1 | 0 | -5.393659 | 1.650686 | 3.044788 |
| 127 | 1 | 0 | -6.557158 | 2.806423 | 3.737914 |
| 128 | 1 | 0 | -6.493593 | 1.136296 | 4.342256 |
| 129 | 6 | 0 | -5.669074 | 3.101898 | -1.874126 |
| 130 | 6 | 0 | -5.146861 | 4.510955 | -2.130352 |
| 131 | 6 | 0 | -6.636213 | 2.641964 | -2.963956 |
| 132 | 1 | 0 | -4.830321 | 2.405889 | -1.811389 |
| 133 | 1 | 0 | -4.509772 | 4.856538 | -1.313028 |
| 134 | 1 | 0 | -4.560478 | 4.518537 | -3.052889 |
| 135 | 1 | 0 | -5.967866 | 5.224899 | -2.256196 |
| 136 | 1 | 0 | -7.042009 | 1.656324 | -2.717387 |
| 137 | 1 | 0 | -7.471809 | 3.342489 | -3.066028 |
| 138 | 1 | 0 | -6.121923 | 2.581424 | -3.927517 |
| 139 | 5 | 0 | 5.120095 | -0.900084 | -0.308756 |
| 140 | 5 | 0 | -5.119979 | 0.900108 | 0.308799 |

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**BP86/6-31G(d)**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.575152 | -2.382827 | -0.352567 |
| 2 | 6 | 0 | -0.762087 | -1.219529 | -0.207183 |
| 3 | 6 | 0 | -1.418843 | 0.013369 | 0.138398 |
| 4 | 6 | 0 | -2.847949 | 0.027334 | 0.263123 |
| 5 | 6 | 0 | -3.677809 | -1.151229 | 0.029579 |
| 6 | 6 | 0 | -2.960289 | -2.356831 | -0.235734 |
| 7 | 6 | 0 | -0.679718 | 1.234448 | 0.365585 |
| 8 | 6 | 0 | -3.519855 | 1.217670 | 0.657091 |
| 9 | 1 | 0 | -3.507590 | -3.302359 | -0.330392 |
| 10 | 6 | 0 | -2.789779 | 2.390502 | 0.920075 |
| 11 | 6 | 0 | -1.401190 | 2.397625 | 0.756710 |
| 12 | 1 | 0 | -3.298952 | 3.299607 | 1.263780 |
| 13 | 6 | 0 | 2.789760 | -2.390506 | -0.919929 |
| 14 | 6 | 0 | 3.519834 | -1.217664 | -0.656987 |
| 15 | 6 | 0 | 2.847927 | -0.027325 | -0.263027 |
| 16 | 6 | 0 | 1.418822 | -0.013366 | -0.138287 |
| 17 | 6 | 0 | 0.679698 | -1.234451 | -0.365456 |
| 18 | 6 | 0 | 1.401173 | -2.397635 | -0.756550 |
| 19 | 1 | 0 | 3.298934 | -3.299621 | -1.263609 |
| 20 | 6 | 0 | 3.677782 | 1.151246 | -0.029521 |
| 21 | 6 | 0 | 0.762065 | 1.219530 | 0.207292 |
| 22 | 6 | 0 | 1.575123 | 2.382836 | 0.352644 |
| 23 | 6 | 0 | 2.960257 | 2.356848 | 0.235781 |
| 24 | 1 | 0 | 3.507552 | 3.302381 | 0.330408 |
| 25 | 1 | 0 | 1.095336 | 3.346166 | 0.556186 |
| 26 | 1 | 0 | -0.858609 | 3.322518 | 0.974699 |
| 27 | 1 | 0 | 0.858597 | -3.322539 | -0.974506 |
| 28 | 1 | 0 | -1.095369 | -3.346158 | -0.556113 |
| 29 | 15 | 0 | -5.309916 | 0.921262 | 0.907398 |
| 30 | 15 | 0 | 5.309876 | -0.921243 | -0.907376 |
| 31 | 6 | 0 | 7.626930 | 3.753941 | 0.287581 |
| 32 | 6 | 0 | 8.133529 | 3.208613 | -0.855882 |
| 33 | 1 | 0 | 7.967019 | 4.606061 | 0.870402 |
| 34 | 1 | 0 | 8.980999 | 3.515780 | -1.462154 |
| 35 | 6 | 0 | 7.377983 | -3.518614 | 1.428951 |
| 36 | 6 | 0 | 6.514884 | -3.057724 | 2.386157 |
| 37 | 1 | 0 | 8.172409 | -4.257713 | 1.490638 |
| 38 | 1 | 0 | 6.418003 | -3.327224 | 3.434484 |
| 39 | 6 | 0 | -7.377851 | 3.518715 | -1.428998 |
| 40 | 6 | 0 | -6.514710 | 3.057826 | -2.386167 |
| 41 | 1 | 0 | -8.172255 | 4.257834 | -1.490715 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | -6.417749 | 3.327362 | -3.434478 |
| 43 | 6 | 0 | -8.133512 | -3.208695 | 0.855810 |
| 44 | 6 | 0 | -7.626960 | -3.753882 | -0.287740 |
| 45 | 1 | 0 | -8.980945 | -3.515947 | 1.462092 |
| 46 | 1 | 0 | -7.967068 | -4.605933 | -0.870651 |
| 47 | 6 | 0 | -6.032506 | 1.972400 | -0.461950 |
| 48 | 6 | 0 | -6.319518 | -1.954052 | 0.248945 |
| 49 | 6 | 0 | 6.032550 | -1.972354 | 0.461943 |
| 50 | 6 | 0 | 6.319488 | 1.954068 | -0.248958 |
| 51 | 7 | 0 | -5.700372 | 2.108712 | -1.788624 |
| 52 | 7 | 0 | -7.072510 | 2.851369 | -0.251719 |
| 53 | 7 | 0 | -6.521586 | -2.993226 | -0.656858 |
| 54 | 7 | 0 | -7.346826 | -2.106889 | 1.179928 |
| 55 | 7 | 0 | 6.521532 | 2.993340 | 0.656741 |
| 56 | 7 | 0 | 7.346852 | 2.106772 | -1.179899 |
| 57 | 7 | 0 | 5.700526 | -2.108605 | 1.788650 |
| 58 | 7 | 0 | 7.072561 | -2.851304 | 0.251671 |
| 59 | 6 | 0 | -4.608195 | 1.382243 | -2.499892 |
| 60 | 6 | 0 | -3.400061 | 2.306560 | -2.709768 |
| 61 | 6 | 0 | -5.133972 | 0.799225 | -3.819954 |
| 62 | 1 | 0 | -4.339833 | 0.553114 | -1.824309 |
| 63 | 1 | 0 | -3.025347 | 2.698482 | -1.751012 |
| 64 | 1 | 0 | -2.584574 | 1.734605 | -3.183775 |
| 65 | 1 | 0 | -3.655258 | 3.152218 | -3.375078 |
| 66 | 1 | 0 | -6.036342 | 0.185819 | -3.661762 |
| 67 | 1 | 0 | -5.365363 | 1.584157 | -4.562557 |
| 68 | 1 | 0 | -4.352312 | 0.156569 | -4.258793 |
| 69 | 6 | 0 | -7.771805 | 3.094149 | 1.040808 |
| 70 | 6 | 0 | -9.247681 | 2.682908 | 0.932670 |
| 71 | 6 | 0 | -7.580413 | 4.551927 | 1.485063 |
| 72 | 1 | 0 | -7.253309 | 2.428878 | 1.753523 |
| 73 | 1 | 0 | -9.346041 | 1.630960 | 0.615039 |
| 74 | 1 | 0 | -9.734040 | 2.795675 | 1.916563 |
| 75 | 1 | 0 | -9.798945 | 3.315766 | 0.214039 |
| 76 | 1 | 0 | -6.509958 | 4.807977 | 1.555187 |
| 77 | 1 | 0 | -8.066598 | 5.262426 | 0.792708 |
| 78 | 1 | 0 | -8.034218 | 4.693307 | 2.480725 |
| 79 | 6 | 0 | -7.381609 | -1.441637 | 2.507946 |
| 80 | 6 | 0 | -6.492682 | -2.205270 | 3.504257 |
| 81 | 6 | 0 | -8.823510 | -1.273712 | 3.006468 |
| 82 | 1 | 0 | -6.947867 | -0.441137 | 2.344858 |
| 83 | 1 | 0 | -5.460880 | -2.277785 | 3.121085 |
| 84 | 1 | 0 | -6.467193 | -1.675482 | 4.472398 |
| 85 | 1 | 0 | -6.880305 | -3.225437 | 3.677898 |

| | | | | | |
|---|---|---|---|---|---|
| 86 | 1 | 0 | -9.462117 | -0.783548 | 2.251137 |
| 87 | 1 | 0 | -9.286533 | -2.237516 | 3.284554 |
| 88 | 1 | 0 | -8.818923 | -0.646468 | 3.913948 |
| 89 | 6 | 0 | -5.864881 | -3.112032 | -1.980104 |
| 90 | 6 | 0 | -6.837899 | -2.671829 | -3.089025 |
| 91 | 6 | 0 | -5.336324 | -4.536199 | -2.209474 |
| 92 | 1 | 0 | -5.016477 | -2.409478 | -1.935897 |
| 93 | 1 | 0 | -7.229169 | -1.660017 | -2.886933 |
| 94 | 1 | 0 | -6.321651 | -2.660713 | -4.064517 |
| 95 | 1 | 0 | -7.696448 | -3.362510 | -3.168943 |
| 96 | 1 | 0 | -4.667263 | -4.856052 | -1.393718 |
| 97 | 1 | 0 | -6.158988 | -5.269887 | -2.290317 |
| 98 | 1 | 0 | -4.768814 | -4.571751 | -3.155066 |
| 99 | 6 | 0 | 4.608421 | -1.382080 | 2.499971 |
| 100 | 6 | 0 | 5.134268 | -0.799142 | 3.820040 |
| 101 | 6 | 0 | 3.400225 | -2.306318 | 2.709836 |
| 102 | 1 | 0 | 4.340101 | -0.552912 | 1.824414 |
| 103 | 1 | 0 | 6.036720 | -0.185852 | 3.661859 |
| 104 | 1 | 0 | 4.352692 | -0.156390 | 4.258887 |
| 105 | 1 | 0 | 5.365554 | -1.584112 | 4.562636 |
| 106 | 1 | 0 | 3.025459 | -2.698166 | 1.751069 |
| 107 | 1 | 0 | 3.655380 | -3.152025 | 3.375098 |
| 108 | 1 | 0 | 2.584791 | -1.734328 | 3.183889 |
| 109 | 6 | 0 | 7.771689 | -3.094219 | -1.040922 |
| 110 | 6 | 0 | 7.579865 | -4.551933 | -1.485202 |
| 111 | 6 | 0 | 9.247684 | -2.683377 | -0.932902 |
| 112 | 1 | 0 | 7.253307 | -2.428794 | -1.753574 |
| 113 | 1 | 0 | 6.509332 | -4.807669 | -1.555292 |
| 114 | 1 | 0 | 8.033594 | -4.693433 | -2.480882 |
| 115 | 1 | 0 | 8.065861 | -5.262578 | -0.792864 |
| 116 | 1 | 0 | 9.346362 | -1.631477 | -0.615212 |
| 117 | 1 | 0 | 9.798864 | -3.316432 | -0.214381 |
| 118 | 1 | 0 | 9.733907 | -2.796208 | -1.916855 |
| 119 | 6 | 0 | 7.381727 | 1.441281 | -2.507798 |
| 120 | 6 | 0 | 8.823638 | 1.273588 | -3.006367 |
| 121 | 6 | 0 | 6.492578 | 2.204522 | -3.504211 |
| 122 | 1 | 0 | 6.948223 | 0.440708 | -2.344508 |
| 123 | 1 | 0 | 9.462417 | 0.783753 | -2.250968 |
| 124 | 1 | 0 | 8.819138 | 0.646130 | -3.913699 |
| 125 | 1 | 0 | 9.286406 | 2.237438 | -3.284717 |
| 126 | 1 | 0 | 5.460779 | 2.276880 | -3.121000 |
| 127 | 1 | 0 | 6.879970 | 3.224741 | -3.678060 |
| 128 | 1 | 0 | 6.467160 | 1.674542 | -4.472249 |
| 129 | 6 | 0 | 5.864788 | 3.112299 | 1.979955 |

| | | | | | |
|---|---|---|---|---|---|
| 130 | 6 | 0 | 5.336284 | 4.536510 | 2.209174 |
| 131 | 6 | 0 | 6.837751 | 2.672167 | 3.088951 |
| 132 | 1 | 0 | 5.016358 | 2.409774 | 1.935787 |
| 133 | 1 | 0 | 4.667274 | 4.856326 | 1.393363 |
| 134 | 1 | 0 | 4.768736 | 4.572171 | 3.154739 |
| 135 | 1 | 0 | 6.158979 | 5.270166 | 2.289988 |
| 136 | 1 | 0 | 7.228989 | 1.660321 | 2.886972 |
| 137 | 1 | 0 | 7.696323 | 3.362824 | 3.168829 |
| 138 | 1 | 0 | 6.321471 | 2.661166 | 4.064427 |
| 139 | 5 | 0 | -5.173887 | -0.916150 | 0.238969 |
| 140 | 5 | 0 | 5.173860 | 0.916166 | -0.238928 |

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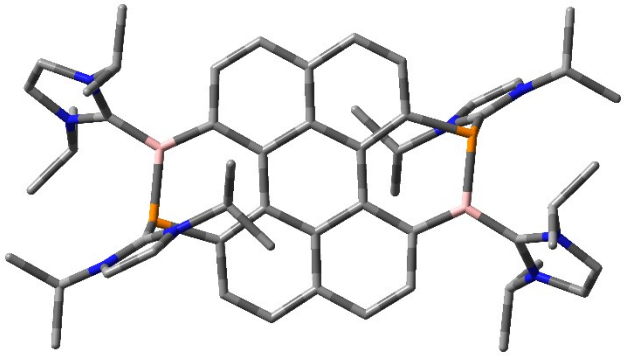
**2PB-d**



**UB3LYP/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.316982 | -1.185834 | -1.267415 |
| 2 | 6 | 0 | -1.193880 | -0.561510 | -0.616822 |
| 3 | 6 | 0 | 0.106316 | -1.193102 | -0.763882 |
| 4 | 6 | 0 | 0.195033 | -2.416593 | -1.525342 |
| 5 | 6 | 0 | -0.916886 | -2.931939 | -2.207409 |
| 6 | 6 | 0 | -2.140861 | -2.312212 | -2.090564 |
| 7 | 6 | 0 | 1.301994 | -0.656591 | -0.162543 |
| 8 | 6 | 0 | 1.421626 | -3.137017 | -1.573064 |
| 9 | 1 | 0 | -0.799608 | -3.830427 | -2.808568 |
| 10 | 1 | 0 | -3.003556 | -2.716913 | -2.615363 |
| 11 | 6 | 0 | 2.531639 | -2.647135 | -0.965001 |
| 12 | 6 | 0 | 2.571239 | -1.371343 | -0.309108 |
| 13 | 1 | 0 | 1.439929 | -4.092082 | -2.094065 |
| 14 | 1 | 0 | 3.440043 | -3.243835 | -0.985005 |
| 15 | 6 | 0 | -2.531630 | 2.647102 | 0.965109 |
| 16 | 6 | 0 | -1.421617 | 3.136981 | 1.573175 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 6 | 0 | -0.195021 | 2.416564 | 1.525437 |
| 18 | 6 | 0 | -0.106305 | 1.193077 | 0.763971 |
| 19 | 6 | 0 | -1.301984 | 0.656568 | 0.162631 |
| 20 | 6 | 0 | -2.571228 | 1.371321 | 0.309198 |
| 21 | 1 | 0 | 0.799625 | 3.830402 | 2.808657 |
| 22 | 1 | 0 | -3.440035 | 3.243800 | 0.985121 |
| 23 | 1 | 0 | -1.439922 | 4.092040 | 2.094186 |
| 24 | 6 | 0 | 0.916903 | 2.931916 | 2.207494 |
| 25 | 6 | 0 | 1.193893 | 0.561491 | 0.616901 |
| 26 | 6 | 0 | 2.317001 | 1.185826 | 1.267475 |
| 27 | 6 | 0 | 2.140882 | 2.312203 | 2.090627 |
| 28 | 1 | 0 | 3.003582 | 2.716913 | 2.615410 |
| 29 | 15 | 0 | 4.066683 | 0.726918 | 1.114942 |
| 30 | 15 | 0 | -4.066662 | -0.726904 | -1.114916 |
| 31 | 6 | 0 | 7.050968 | -2.888858 | -0.656030 |
| 32 | 6 | 0 | 7.080000 | -2.946763 | 0.698505 |
| 33 | 1 | 0 | 7.737394 | -3.285273 | -1.386895 |
| 34 | 1 | 0 | 7.791007 | -3.412456 | 1.362076 |
| 35 | 6 | 0 | 6.083177 | 3.501099 | -1.176076 |
| 36 | 6 | 0 | 5.024990 | 3.332099 | -2.009159 |
| 37 | 1 | 0 | 6.952921 | 4.131741 | -1.268118 |
| 38 | 1 | 0 | 4.802749 | 3.794771 | -2.957258 |
| 39 | 6 | 0 | -5.025069 | -3.332167 | 2.009084 |
| 40 | 6 | 0 | -6.083267 | -3.501086 | 1.175998 |
| 41 | 1 | 0 | -4.802845 | -3.794890 | 2.957161 |
| 42 | 1 | 0 | -6.953037 | -4.131695 | 1.268015 |
| 43 | 6 | 0 | -7.050929 | 2.888953 | 0.655961 |
| 44 | 6 | 0 | -7.079934 | 2.946804 | -0.698577 |
| 45 | 1 | 0 | -7.737360 | 3.285414 | 1.386796 |
| 46 | 1 | 0 | -7.790918 | 3.412486 | -1.362180 |
| 47 | 6 | 0 | 5.222413 | -1.796676 | 0.110900 |
| 48 | 6 | 0 | 4.701294 | 1.993322 | -0.232456 |
| 49 | 6 | 0 | -4.701320 | -1.993333 | 0.232433 |
| 50 | 6 | 0 | -5.222385 | 1.796698 | -0.110890 |
| 51 | 7 | 0 | 5.910121 | -2.186127 | -1.008883 |
| 52 | 7 | 0 | 5.956599 | -2.281906 | 1.160089 |
| 53 | 7 | 0 | 4.188769 | 2.398555 | -1.424834 |
| 54 | 7 | 0 | 5.872107 | 2.676699 | -0.084812 |
| 55 | 7 | 0 | -5.872161 | -2.676655 | 0.084764 |
| 56 | 7 | 0 | -4.188809 | -2.398635 | 1.424795 |
| 57 | 7 | 0 | -5.910108 | 2.186208 | 1.008865 |
| 58 | 7 | 0 | -5.956543 | 2.281898 | -1.160112 |
| 59 | 6 | 0 | 5.569156 | -1.797594 | -2.395679 |
| 60 | 6 | 0 | 5.468072 | -3.027429 | -3.302597 |

| | | | | | |
|---|---|---|---|---|---|
| 61 | 6 | 0 | 6.576025 | -0.765383 | -2.918337 |
| 62 | 1 | 0 | 4.583950 | -1.333422 | -2.312882 |
| 63 | 1 | 0 | 4.742398 | -3.746818 | -2.913954 |
| 64 | 1 | 0 | 5.138859 | -2.718133 | -4.299704 |
| 65 | 1 | 0 | 6.434578 | -3.532004 | -3.416652 |
| 66 | 1 | 0 | 6.616003 | 0.110963 | -2.263269 |
| 67 | 1 | 0 | 7.584438 | -1.188304 | -2.991919 |
| 68 | 1 | 0 | 6.281530 | -0.432997 | -3.919415 |
| 69 | 6 | 0 | 5.540776 | -2.243943 | 2.581622 |
| 70 | 6 | 0 | 6.568862 | -1.490365 | 3.428339 |
| 71 | 6 | 0 | 5.267416 | -3.662830 | 3.093365 |
| 72 | 1 | 0 | 4.602131 | -1.684573 | 2.573988 |
| 73 | 1 | 0 | 6.715489 | -0.475359 | 3.047786 |
| 74 | 1 | 0 | 6.211829 | -1.418559 | 4.460673 |
| 75 | 1 | 0 | 7.537547 | -2.004181 | 3.446647 |
| 76 | 1 | 0 | 4.523421 | -4.166019 | 2.468166 |
| 77 | 1 | 0 | 6.177536 | -4.273384 | 3.111561 |
| 78 | 1 | 0 | 4.879141 | -3.613770 | 4.115788 |
| 79 | 6 | 0 | 6.799088 | 2.595922 | 1.073452 |
| 80 | 6 | 0 | 6.959515 | 3.972223 | 1.725885 |
| 81 | 6 | 0 | 8.132376 | 1.974538 | 0.646668 |
| 82 | 1 | 0 | 6.296055 | 1.927136 | 1.775125 |
| 83 | 1 | 0 | 5.987836 | 4.385526 | 2.013199 |
| 84 | 1 | 0 | 7.570790 | 3.876478 | 2.628927 |
| 85 | 1 | 0 | 7.459023 | 4.687791 | 1.062915 |
| 86 | 1 | 0 | 7.982542 | 0.982303 | 0.208596 |
| 87 | 1 | 0 | 8.657528 | 2.599502 | -0.084914 |
| 88 | 1 | 0 | 8.783965 | 1.868057 | 1.520087 |
| 89 | 6 | 0 | 2.890513 | 1.973689 | -2.014910 |
| 90 | 6 | 0 | 3.075837 | 1.547577 | -3.473931 |
| 91 | 6 | 0 | 1.851781 | 3.086954 | -1.851316 |
| 92 | 1 | 0 | 2.583894 | 1.104396 | -1.437309 |
| 93 | 1 | 0 | 3.858482 | 0.788858 | -3.572291 |
| 94 | 1 | 0 | 2.137881 | 1.115617 | -3.835336 |
| 95 | 1 | 0 | 3.323997 | 2.391566 | -4.128044 |
| 96 | 1 | 0 | 1.737188 | 3.364670 | -0.800471 |
| 97 | 1 | 0 | 2.128975 | 3.978177 | -2.427833 |
| 98 | 1 | 0 | 0.881738 | 2.733870 | -2.213899 |
| 99 | 6 | 0 | -5.569182 | 1.797727 | 2.395685 |
| 100 | 6 | 0 | -6.576098 | 0.765577 | 2.918373 |
| 101 | 6 | 0 | -5.468072 | 3.027601 | 3.302548 |
| 102 | 1 | 0 | -4.583990 | 1.333518 | 2.312928 |
| 103 | 1 | 0 | -6.616093 | -0.110801 | 2.263348 |
| 104 | 1 | 0 | -6.281638 | 0.433232 | 3.919475 |

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|---|---|---|---|---|---|
| 105 | 1 | 0 | -7.584498 | 1.188538 | 2.991910 |
| 106 | 1 | 0 | -4.742367 | 3.746949 | 2.913885 |
| 107 | 1 | 0 | -6.434563 | 3.532213 | 3.416563 |
| 108 | 1 | 0 | -5.138886 | 2.718340 | 4.299675 |
| 109 | 6 | 0 | -5.540696 | 2.243867 | -2.581637 |
| 110 | 6 | 0 | -5.267296 | 3.662727 | -3.093434 |
| 111 | 6 | 0 | -6.568783 | 1.490276 | -3.428341 |
| 112 | 1 | 0 | -4.602063 | 1.684477 | -2.573963 |
| 113 | 1 | 0 | -4.523303 | 4.165927 | -2.468242 |
| 114 | 1 | 0 | -4.879003 | 3.613616 | -4.115847 |
| 115 | 1 | 0 | -6.177403 | 4.273299 | -3.111674 |
| 116 | 1 | 0 | -6.715437 | 0.475288 | -3.047748 |
| 117 | 1 | 0 | -7.537456 | 2.004111 | -3.446685 |
| 118 | 1 | 0 | -6.211734 | 1.418419 | -4.460665 |
| 119 | 6 | 0 | -2.890527 | -1.973862 | 2.014885 |
| 120 | 6 | 0 | -1.851850 | -3.087168 | 1.851217 |
| 121 | 6 | 0 | -3.075817 | -1.547831 | 3.473933 |
| 122 | 1 | 0 | -2.583874 | -1.104550 | 1.437333 |
| 123 | 1 | 0 | -1.737278 | -3.364829 | 0.800356 |
| 124 | 1 | 0 | -0.881787 | -2.734151 | 2.213813 |
| 125 | 1 | 0 | -2.129084 | -3.978411 | 2.427685 |
| 126 | 1 | 0 | -3.858426 | -0.789083 | 3.572349 |
| 127 | 1 | 0 | -3.324009 | -2.391849 | 4.127997 |
| 128 | 1 | 0 | -2.137837 | -1.115938 | 3.835354 |
| 129 | 6 | 0 | -6.799139 | -2.595793 | -1.073496 |
| 130 | 6 | 0 | -8.132400 | -1.974366 | -0.646690 |
| 131 | 6 | 0 | -6.959628 | -3.972064 | -1.725979 |
| 132 | 1 | 0 | -6.296076 | -1.927004 | -1.775145 |
| 133 | 1 | 0 | -7.982523 | -0.982153 | -0.208584 |
| 134 | 1 | 0 | -8.783985 | -1.867827 | -1.520105 |
| 135 | 1 | 0 | -8.657577 | -2.599333 | 0.084871 |
| 136 | 1 | 0 | -5.987968 | -4.385401 | -2.013307 |
| 137 | 1 | 0 | -7.459169 | -4.687632 | -1.063036 |
| 138 | 1 | 0 | -7.570896 | -3.876257 | -2.629019 |
| 139 | 5 | 0 | -3.909550 | 0.926893 | -0.205829 |
| 140 | 5 | 0 | 3.909564 | -0.926900 | 0.205894 |

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**UWB97XD/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.246402 | -1.112402 | -1.423807 |

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|---|---|---|---|---|---|
| 2 | 6 | 0 | -1.154395 | -0.514828 | -0.711155 |
| 3 | 6 | 0 | 0.143798 | -1.137633 | -0.832569 |
| 4 | 6 | 0 | 0.273535 | -2.301411 | -1.666525 |
| 5 | 6 | 0 | -0.805133 | -2.784848 | -2.413140 |
| 6 | 6 | 0 | -2.038174 | -2.190490 | -2.293435 |
| 7 | 6 | 0 | 1.297884 | -0.649126 | -0.132809 |
| 8 | 6 | 0 | 1.511340 | -3.004537 | -1.721916 |
| 9 | 1 | 0 | -0.659960 | -3.644234 | -3.062151 |
| 10 | 1 | 0 | -2.882987 | -2.580637 | -2.856223 |
| 11 | 6 | 0 | 2.584630 | -2.552429 | -1.036309 |
| 12 | 6 | 0 | 2.573144 | -1.336144 | -0.278672 |
| 13 | 1 | 0 | 1.562425 | -3.916883 | -2.311374 |
| 14 | 1 | 0 | 3.506017 | -3.130481 | -1.068890 |
| 15 | 6 | 0 | -2.584592 | 2.552491 | 1.036769 |
| 16 | 6 | 0 | -1.511258 | 3.004665 | 1.722286 |
| 17 | 6 | 0 | -0.273435 | 2.301623 | 1.666781 |
| 18 | 6 | 0 | -0.143725 | 1.137813 | 0.832869 |
| 19 | 6 | 0 | -1.297832 | 0.649280 | 0.133156 |
| 20 | 6 | 0 | -2.573088 | 1.336262 | 0.279074 |
| 21 | 1 | 0 | 0.660159 | 3.644600 | 3.062212 |
| 22 | 1 | 0 | -3.506005 | 3.130490 | 1.069451 |
| 23 | 1 | 0 | -1.562350 | 3.917010 | 2.311746 |
| 24 | 6 | 0 | 0.805310 | 2.785182 | 2.413241 |
| 25 | 6 | 0 | 1.154480 | 0.515015 | 0.711416 |
| 26 | 6 | 0 | 2.246562 | 1.112719 | 1.423863 |
| 27 | 6 | 0 | 2.038359 | 2.190901 | 2.293410 |
| 28 | 1 | 0 | 2.883225 | 2.581157 | 2.856045 |
| 29 | 15 | 0 | 3.999027 | 0.705308 | 1.269936 |
| 30 | 15 | 0 | -3.998865 | -0.704890 | -1.270042 |
| 31 | 6 | 0 | 7.090591 | -2.436191 | -0.958248 |
| 32 | 6 | 0 | 7.208499 | -2.674546 | 0.368317 |
| 33 | 1 | 0 | 7.760703 | -2.660028 | -1.772617 |
| 34 | 1 | 0 | 7.997510 | -3.151738 | 0.926831 |
| 35 | 6 | 0 | 6.015791 | 3.332724 | -1.097384 |
| 36 | 6 | 0 | 4.902348 | 3.230668 | -1.860498 |
| 37 | 1 | 0 | 6.915718 | 3.906295 | -1.245717 |
| 38 | 1 | 0 | 4.648452 | 3.707408 | -2.793060 |
| 39 | 6 | 0 | -4.902532 | -3.230570 | 1.859952 |
| 40 | 6 | 0 | -6.015845 | -3.332623 | 1.096646 |
| 41 | 1 | 0 | -4.648792 | -3.707332 | 2.792542 |
| 42 | 1 | 0 | -6.915798 | -3.906193 | 1.244815 |
| 43 | 6 | 0 | -7.090607 | 2.436116 | 0.958722 |
| 44 | 6 | 0 | -7.208618 | 2.674363 | -0.367852 |
| 45 | 1 | 0 | -7.760671 | 2.659989 | 1.773121 |

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|---|---|---|---|---|---|
| 46 | 1 | 0 | -7.997689 | 3.151475 | -0.926349 |
| 47 | 6 | 0 | 5.234918 | -1.651904 | 0.039383 |
| 48 | 6 | 0 | 4.607964 | 1.923942 | -0.073099 |
| 49 | 6 | 0 | -4.607903 | -1.923742 | 0.072674 |
| 50 | 6 | 0 | -5.234922 | 1.651914 | -0.038966 |
| 51 | 7 | 0 | 5.875987 | -1.809093 | -1.147860 |
| 52 | 7 | 0 | 6.062228 | -2.193570 | 0.967465 |
| 53 | 7 | 0 | 4.053484 | 2.350981 | -1.228488 |
| 54 | 7 | 0 | 5.817911 | 2.528900 | 0.004960 |
| 55 | 7 | 0 | -5.817783 | -2.528785 | -0.005660 |
| 56 | 7 | 0 | -4.053532 | -2.350918 | 1.228068 |
| 57 | 7 | 0 | -5.875973 | 1.809062 | 1.148302 |
| 58 | 7 | 0 | -6.062365 | 2.193396 | -0.967036 |
| 59 | 6 | 0 | 5.406702 | -1.255352 | -2.427520 |
| 60 | 6 | 0 | 5.304827 | -2.343941 | -3.489764 |
| 61 | 6 | 0 | 6.306584 | -0.094930 | -2.846092 |
| 62 | 1 | 0 | 4.405184 | -0.877791 | -2.207871 |
| 63 | 1 | 0 | 4.647947 | -3.151402 | -3.157368 |
| 64 | 1 | 0 | 4.883578 | -1.919017 | -4.405398 |
| 65 | 1 | 0 | 6.286103 | -2.763804 | -3.738195 |
| 66 | 1 | 0 | 6.344607 | 0.668261 | -2.063228 |
| 67 | 1 | 0 | 7.328446 | -0.433548 | -3.050595 |
| 68 | 1 | 0 | 5.919254 | 0.367921 | -3.758751 |
| 69 | 6 | 0 | 5.749649 | -2.308159 | 2.400997 |
| 70 | 6 | 0 | 6.674263 | -1.411440 | 3.217979 |
| 71 | 6 | 0 | 5.792117 | -3.770518 | 2.836013 |
| 72 | 1 | 0 | 4.722809 | -1.941057 | 2.485798 |
| 73 | 1 | 0 | 6.566415 | -0.368744 | 2.906854 |
| 74 | 1 | 0 | 6.413216 | -1.479793 | 4.277895 |
| 75 | 1 | 0 | 7.722724 | -1.712102 | 3.107646 |
| 76 | 1 | 0 | 5.135656 | -4.381124 | 2.209772 |
| 77 | 1 | 0 | 6.806601 | -4.181387 | 2.786240 |
| 78 | 1 | 0 | 5.452781 | -3.851075 | 3.872491 |
| 79 | 6 | 0 | 6.825026 | 2.288306 | 1.057445 |
| 80 | 6 | 0 | 7.540513 | 3.580877 | 1.433951 |
| 81 | 6 | 0 | 7.782789 | 1.187046 | 0.608590 |
| 82 | 1 | 0 | 6.249026 | 1.934391 | 1.915661 |
| 83 | 1 | 0 | 6.826330 | 4.373511 | 1.673900 |
| 84 | 1 | 0 | 8.158485 | 3.398991 | 2.317419 |
| 85 | 1 | 0 | 8.206763 | 3.932821 | 0.638943 |
| 86 | 1 | 0 | 7.238519 | 0.263621 | 0.388588 |
| 87 | 1 | 0 | 8.334484 | 1.487753 | -0.289293 |
| 88 | 1 | 0 | 8.507346 | 0.976463 | 1.400977 |
| 89 | 6 | 0 | 2.719026 | 1.973189 | -1.741791 |

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|---|---|---|---|---|---|
| 90 | 6 | 0 | 2.780723 | 1.653888 | -3.231291 |
| 91 | 6 | 0 | 1.699540 | 3.056660 | -1.408964 |
| 92 | 1 | 0 | 2.461190 | 1.057031 | -1.218822 |
| 93 | 1 | 0 | 3.567443 | 0.926283 | -3.451666 |
| 94 | 1 | 0 | 1.823849 | 1.214839 | -3.526048 |
| 95 | 1 | 0 | 2.941293 | 2.545402 | -3.847903 |
| 96 | 1 | 0 | 1.694454 | 3.271764 | -0.337251 |
| 97 | 1 | 0 | 1.912501 | 3.980551 | -1.960201 |
| 98 | 1 | 0 | 0.699871 | 2.708037 | -1.683370 |
| 99 | 6 | 0 | -5.406724 | 1.255251 | 2.427951 |
| 100 | 6 | 0 | -6.306500 | 0.094663 | 2.846297 |
| 101 | 6 | 0 | -5.305152 | 2.343738 | 3.490325 |
| 102 | 1 | 0 | -4.405128 | 0.877847 | 2.208399 |
| 103 | 1 | 0 | -6.344178 | -0.668525 | 2.063414 |
| 104 | 1 | 0 | -5.919316 | -0.368129 | 3.759046 |
| 105 | 1 | 0 | -7.328475 | 0.433095 | 3.050546 |
| 106 | 1 | 0 | -4.648342 | 3.151331 | 3.158114 |
| 107 | 1 | 0 | -6.286520 | 2.763432 | 3.738681 |
| 108 | 1 | 0 | -4.883964 | 1.918761 | 4.405963 |
| 109 | 6 | 0 | -5.749945 | 2.307773 | -2.400613 |
| 110 | 6 | 0 | -5.792694 | 3.770038 | -2.835922 |
| 111 | 6 | 0 | -6.674459 | 1.410719 | -3.217347 |
| 112 | 1 | 0 | -4.723051 | 1.940832 | -2.485432 |
| 113 | 1 | 0 | -5.136281 | 4.380890 | -2.209872 |
| 114 | 1 | 0 | -5.453465 | 3.850436 | -3.872449 |
| 115 | 1 | 0 | -6.807241 | 4.180749 | -2.786151 |
| 116 | 1 | 0 | -6.566463 | 0.368111 | -2.905980 |
| 117 | 1 | 0 | -7.722955 | 1.711259 | -3.107040 |
| 118 | 1 | 0 | -6.413460 | 1.478853 | -4.277287 |
| 119 | 6 | 0 | -2.719111 | -1.973196 | 1.741551 |
| 120 | 6 | 0 | -1.699630 | -3.056737 | 1.408922 |
| 121 | 6 | 0 | -2.780973 | -1.653820 | 3.231029 |
| 122 | 1 | 0 | -2.461144 | -1.057068 | 1.218576 |
| 123 | 1 | 0 | -1.694404 | -3.271908 | 0.337224 |
| 124 | 1 | 0 | -0.699976 | -2.708161 | 1.683443 |
| 125 | 1 | 0 | -1.912722 | -3.980584 | 1.960183 |
| 126 | 1 | 0 | -3.567672 | -0.926158 | 3.451288 |
| 127 | 1 | 0 | -2.941650 | -2.545293 | 3.847669 |
| 128 | 1 | 0 | -1.824105 | -1.214818 | 3.525872 |
| 129 | 6 | 0 | -6.824714 | -2.288240 | -1.058333 |
| 130 | 6 | 0 | -7.782859 | -1.187319 | -0.609464 |
| 131 | 6 | 0 | -7.539742 | -3.580922 | -1.435316 |
| 132 | 1 | 0 | -6.248608 | -1.933972 | -1.916338 |
| 133 | 1 | 0 | -7.238846 | -0.263811 | -0.389157 |

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|---|---|---|---|---|---|
| 134 | 1 | 0 | -8.507290 | -0.976744 | -1.401968 |
| 135 | 1 | 0 | -8.334692 | -1.488332 | 0.288232 |
| 136 | 1 | 0 | -6.825254 | -4.373259 | -1.675336 |
| 137 | 1 | 0 | -8.206027 | -3.933298 | -0.640531 |
| 138 | 1 | 0 | -8.157605 | -3.398994 | -2.318851 |
| 139 | 5 | 0 | -3.878750 | 0.900971 | -0.294905 |
| 140 | 5 | 0 | 3.878783 | -0.900823 | 0.295232 |

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**UM06-2X/6-31G***

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.264685 | -1.119224 | -1.399537 |
| 2 | 6 | 0 | -1.165283 | -0.519954 | -0.695560 |
| 3 | 6 | 0 | 0.136261 | -1.136310 | -0.836452 |
| 4 | 6 | 0 | 0.260679 | -2.298854 | -1.674077 |
| 5 | 6 | 0 | -0.826919 | -2.791504 | -2.401106 |
| 6 | 6 | 0 | -2.061951 | -2.199591 | -2.269066 |
| 7 | 6 | 0 | 1.299769 | -0.642530 | -0.153505 |
| 8 | 6 | 0 | 1.506551 | -2.988598 | -1.762224 |
| 9 | 1 | 0 | -0.684408 | -3.651832 | -3.049176 |
| 10 | 1 | 0 | -2.911744 | -2.591262 | -2.823167 |
| 11 | 6 | 0 | 2.588881 | -2.531464 | -1.094406 |
| 12 | 6 | 0 | 2.576651 | -1.323593 | -0.317360 |
| 13 | 1 | 0 | 1.552522 | -3.892568 | -2.364557 |
| 14 | 1 | 0 | 3.518500 | -3.096051 | -1.151908 |
| 15 | 6 | 0 | -2.589004 | 2.532432 | 1.092490 |
| 16 | 6 | 0 | -1.506693 | 2.989731 | 1.760115 |
| 17 | 6 | 0 | -0.260835 | 2.299726 | 1.672400 |
| 18 | 6 | 0 | -0.136477 | 1.136886 | 0.835159 |
| 19 | 6 | 0 | -1.299984 | 0.642987 | 0.152319 |
| 20 | 6 | 0 | -2.576939 | 1.324067 | 0.316053 |
| 21 | 1 | 0 | 0.684211 | 3.653058 | 3.047091 |
| 22 | 1 | 0 | -3.518574 | 3.097133 | 1.149683 |
| 23 | 1 | 0 | -1.552544 | 3.893993 | 2.362021 |
| 24 | 6 | 0 | 0.826654 | 2.792438 | 2.399388 |
| 25 | 6 | 0 | 1.164990 | 0.520386 | 0.694569 |
| 26 | 6 | 0 | 2.264277 | 1.119556 | 1.398755 |
| 27 | 6 | 0 | 2.061651 | 2.200175 | 2.267892 |
| 28 | 1 | 0 | 2.911366 | 2.591813 | 2.822133 |
| 29 | 15 | 0 | 4.019671 | 0.692261 | 1.264819 |
| 30 | 15 | 0 | -4.020099 | -0.692664 | -1.264807 |

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|---|---|---|---|---|---|
| 31 | 6 | 0 | 7.111653 | -2.468275 | -0.909357 |
| 32 | 6 | 0 | 7.208429 | -2.677571 | 0.426024 |
| 33 | 1 | 0 | 7.795591 | -2.707245 | -1.708493 |
| 34 | 1 | 0 | 7.989156 | -3.140160 | 1.009058 |
| 35 | 6 | 0 | 6.040811 | 3.364141 | -1.082592 |
| 36 | 6 | 0 | 4.928888 | 3.255865 | -1.852353 |
| 37 | 1 | 0 | 6.935928 | 3.948076 | -1.222113 |
| 38 | 1 | 0 | 4.672134 | 3.733652 | -2.784399 |
| 39 | 6 | 0 | -4.927721 | -3.255391 | 1.853799 |
| 40 | 6 | 0 | -6.039953 | -3.364104 | 1.084542 |
| 41 | 1 | 0 | -4.670506 | -3.732833 | 2.785894 |
| 42 | 1 | 0 | -6.934918 | -3.948135 | 1.224648 |
| 43 | 6 | 0 | -7.111828 | 2.467790 | 0.909833 |
| 44 | 6 | 0 | -7.209183 | 2.676909 | -0.425537 |
| 45 | 1 | 0 | -7.795497 | 2.706710 | 1.709216 |
| 46 | 1 | 0 | -7.990243 | 3.139259 | -1.008315 |
| 47 | 6 | 0 | 5.234453 | -1.670446 | 0.041003 |
| 48 | 6 | 0 | 4.638965 | 1.937867 | -0.069651 |
| 49 | 6 | 0 | -4.638752 | -1.937969 | 0.070505 |
| 50 | 6 | 0 | -5.234831 | 1.670282 | -0.041189 |
| 51 | 7 | 0 | 5.895820 | -1.854304 | -1.131488 |
| 52 | 7 | 0 | 6.049231 | -2.190151 | 0.994379 |
| 53 | 7 | 0 | 4.086955 | 2.367085 | -1.224363 |
| 54 | 7 | 0 | 5.843568 | 2.553484 | 0.014979 |
| 55 | 7 | 0 | -5.843291 | -2.553801 | -0.013400 |
| 56 | 7 | 0 | -4.086147 | -2.366788 | 1.225063 |
| 57 | 7 | 0 | -5.895800 | 1.854057 | 1.131536 |
| 58 | 7 | 0 | -6.050113 | 2.189650 | -0.994288 |
| 59 | 6 | 0 | 5.452689 | -1.317265 | -2.429917 |
| 60 | 6 | 0 | 5.478669 | -2.401915 | -3.499231 |
| 61 | 6 | 0 | 6.306775 | -0.103963 | -2.789203 |
| 62 | 1 | 0 | 4.419888 | -1.001172 | -2.259524 |
| 63 | 1 | 0 | 4.868969 | -3.258121 | -3.200011 |
| 64 | 1 | 0 | 5.072622 | -2.001068 | -4.431644 |
| 65 | 1 | 0 | 6.498437 | -2.746455 | -3.701792 |
| 66 | 1 | 0 | 6.231095 | 0.662883 | -2.010541 |
| 67 | 1 | 0 | 7.360336 | -0.383331 | -2.901469 |
| 68 | 1 | 0 | 5.969974 | 0.328178 | -3.736127 |
| 69 | 6 | 0 | 5.721105 | -2.278988 | 2.428570 |
| 70 | 6 | 0 | 6.627404 | -1.354830 | 3.234064 |
| 71 | 6 | 0 | 5.795109 | -3.730600 | 2.892091 |
| 72 | 1 | 0 | 4.686859 | -1.928545 | 2.495089 |
| 73 | 1 | 0 | 6.494083 | -0.317143 | 2.915812 |
| 74 | 1 | 0 | 6.374213 | -1.423336 | 4.295432 |

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| 75 | 1 | 0 | 7.680379 | -1.636177 | 3.117229 |
| 76 | 1 | 0 | 5.163517 | -4.370522 | 2.270750 |
| 77 | 1 | 0 | 6.821438 | -4.111250 | 2.860289 |
| 78 | 1 | 0 | 5.448127 | -3.799179 | 3.926209 |
| 79 | 6 | 0 | 6.854600 | 2.294791 | 1.061980 |
| 80 | 6 | 0 | 7.677560 | 3.545575 | 1.342832 |
| 81 | 6 | 0 | 7.718277 | 1.107971 | 0.642429 |
| 82 | 1 | 0 | 6.277552 | 2.029479 | 1.951414 |
| 83 | 1 | 0 | 7.036434 | 4.407910 | 1.543295 |
| 84 | 1 | 0 | 8.299259 | 3.368363 | 2.223735 |
| 85 | 1 | 0 | 8.350349 | 3.786068 | 0.513460 |
| 86 | 1 | 0 | 7.100890 | 0.217593 | 0.479161 |
| 87 | 1 | 0 | 8.256768 | 1.333963 | -0.284875 |
| 88 | 1 | 0 | 8.451922 | 0.881600 | 1.421902 |
| 89 | 6 | 0 | 2.759374 | 1.965408 | -1.740900 |
| 90 | 6 | 0 | 2.833252 | 1.679924 | -3.235923 |
| 91 | 6 | 0 | 1.716512 | 3.021110 | -1.394131 |
| 92 | 1 | 0 | 2.532314 | 1.033301 | -1.229599 |
| 93 | 1 | 0 | 3.641526 | 0.979370 | -3.467245 |
| 94 | 1 | 0 | 1.889061 | 1.224129 | -3.544854 |
| 95 | 1 | 0 | 2.973241 | 2.590602 | -3.828092 |
| 96 | 1 | 0 | 1.703852 | 3.221845 | -0.319095 |
| 97 | 1 | 0 | 1.916736 | 3.954545 | -1.933391 |
| 98 | 1 | 0 | 0.725432 | 2.656627 | -1.680533 |
| 99 | 6 | 0 | -5.451918 | 1.317491 | 2.429914 |
| 100 | 6 | 0 | -6.305821 | 0.104362 | 2.790202 |
| 101 | 6 | 0 | -5.477218 | 2.402573 | 3.498806 |
| 102 | 1 | 0 | -4.419239 | 1.001291 | 2.258997 |
| 103 | 1 | 0 | -6.230687 | -0.662778 | 2.011785 |
| 104 | 1 | 0 | -5.968396 | -0.327439 | 3.737059 |
| 105 | 1 | 0 | -7.359297 | 0.383812 | 2.903074 |
| 106 | 1 | 0 | -4.867613 | 3.258604 | 3.198893 |
| 107 | 1 | 0 | -6.496844 | 2.747282 | 3.701799 |
| 108 | 1 | 0 | -5.070677 | 2.002072 | 4.431153 |
| 109 | 6 | 0 | -5.722665 | 2.278080 | -2.428661 |
| 110 | 6 | 0 | -5.797260 | 3.729510 | -2.892654 |
| 111 | 6 | 0 | -6.629106 | 1.353399 | -3.233395 |
| 112 | 1 | 0 | -4.688360 | 1.927860 | -2.495499 |
| 113 | 1 | 0 | -5.165559 | 4.369823 | -2.271826 |
| 114 | 1 | 0 | -5.450762 | 3.797817 | -3.926952 |
| 115 | 1 | 0 | -6.823671 | 4.109907 | -2.860534 |
| 116 | 1 | 0 | -6.495377 | 0.315866 | -2.914811 |
| 117 | 1 | 0 | -7.682095 | 1.634544 | -3.116181 |
| 118 | 1 | 0 | -6.376409 | 1.421570 | -4.294901 |

| | | | | | |
|---|---|---|---|---|---|
| 119 | 6 | 0 | -2.758257 | -1.964875 | 1.740595 |
| 120 | 6 | 0 | -1.715514 | -3.020511 | 1.393244 |
| 121 | 6 | 0 | -2.831110 | -1.679151 | 3.235619 |
| 122 | 1 | 0 | -2.531685 | -1.032824 | 1.228954 |
| 123 | 1 | 0 | -1.703547 | -3.221374 | 0.318219 |
| 124 | 1 | 0 | -0.724279 | -2.655891 | 1.678935 |
| 125 | 1 | 0 | -1.915291 | -3.953900 | 1.932751 |
| 126 | 1 | 0 | -3.639374 | -0.978735 | 3.467416 |
| 127 | 1 | 0 | -2.970452 | -2.589756 | 3.828054 |
| 128 | 1 | 0 | -1.886794 | -1.223090 | 3.543775 |
| 129 | 6 | 0 | -6.854743 | -2.295720 | -1.060154 |
| 130 | 6 | 0 | -7.718482 | -1.108859 | -0.640856 |
| 131 | 6 | 0 | -7.677599 | -3.546765 | -1.340138 |
| 132 | 1 | 0 | -6.278036 | -2.030707 | -1.949897 |
| 133 | 1 | 0 | -7.101199 | -0.218313 | -0.478143 |
| 134 | 1 | 0 | -8.452371 | -0.882940 | -1.420230 |
| 135 | 1 | 0 | -8.256686 | -1.334542 | 0.286690 |
| 136 | 1 | 0 | -7.036409 | -4.409085 | -1.540464 |
| 137 | 1 | 0 | -8.350031 | -3.787003 | -0.510400 |
| 138 | 1 | 0 | -8.299665 | -3.370055 | -2.220882 |
| 139 | 5 | 0 | -3.880936 | 0.899369 | -0.263188 |
| 140 | 5 | 0 | 3.880626 | -0.899375 | 0.262612 |

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**BP86/6-31G(d)**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.332055 | -1.238378 | 1.216556 |
| 2 | 6 | 0 | 1.201928 | -0.588147 | 0.590796 |
| 3 | 6 | 0 | -0.103374 | -1.227600 | 0.721592 |
| 4 | 6 | 0 | -0.189283 | -2.488387 | 1.436786 |
| 5 | 6 | 0 | 0.932077 | -3.031707 | 2.098130 |
| 6 | 6 | 0 | 2.162359 | -2.401397 | 2.002184 |
| 7 | 6 | 0 | -1.307682 | -0.664410 | 0.146522 |
| 8 | 6 | 0 | -1.418627 | -3.214537 | 1.457858 |
| 9 | 1 | 0 | 0.816012 | -3.961972 | 2.667285 |
| 10 | 1 | 0 | 3.037163 | -2.824656 | 2.511819 |
| 11 | 6 | 0 | -2.540180 | -2.694759 | 0.871758 |
| 12 | 6 | 0 | -2.581079 | -1.386844 | 0.272394 |
| 13 | 1 | 0 | -1.433826 | -4.199444 | 1.941699 |
| 14 | 1 | 0 | -3.457863 | -3.295584 | 0.864900 |
| 15 | 6 | 0 | 2.540151 | 2.694788 | -0.871737 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 1.418600 | 3.214560 | -1.457846 |
| 17 | 6 | 0 | 0.189252 | 2.488415 | -1.436759 |
| 18 | 6 | 0 | 0.103340 | 1.227640 | -0.721543 |
| 19 | 6 | 0 | 1.307647 | 0.664455 | -0.146465 |
| 20 | 6 | 0 | 2.581046 | 1.386883 | -0.272348 |
| 21 | 1 | 0 | -0.816040 | 3.961983 | -2.667280 |
| 22 | 1 | 0 | 3.457836 | 3.295608 | -0.864895 |
| 23 | 1 | 0 | 1.433803 | 4.199455 | -1.941711 |
| 24 | 6 | 0 | -0.932108 | 3.031729 | -2.098110 |
| 25 | 6 | 0 | -1.201962 | 0.588188 | -0.590746 |
| 26 | 6 | 0 | -2.332088 | 1.238412 | -1.216514 |
| 27 | 6 | 0 | -2.162391 | 2.401422 | -2.002154 |
| 28 | 1 | 0 | -3.037195 | 2.824674 | -2.511797 |
| 29 | 15 | 0 | -4.090888 | 0.772192 | -1.073773 |
| 30 | 15 | 0 | 4.090854 | -0.772160 | 1.073818 |
| 31 | 6 | 0 | -7.069679 | -2.954635 | 0.556139 |
| 32 | 6 | 0 | -7.124054 | -2.909410 | -0.809520 |
| 33 | 1 | 0 | -7.747455 | -3.409823 | 1.273832 |
| 34 | 1 | 0 | -7.850981 | -3.330253 | -1.499721 |
| 35 | 6 | 0 | -6.082028 | 3.471744 | 1.322043 |
| 36 | 6 | 0 | -5.027431 | 3.239379 | 2.163442 |
| 37 | 1 | 0 | -6.950318 | 4.115581 | 1.438081 |
| 38 | 1 | 0 | -4.805515 | 3.651084 | 3.144714 |
| 39 | 6 | 0 | 5.027383 | -3.239392 | -2.163364 |
| 40 | 6 | 0 | 6.082077 | -3.471606 | -1.322045 |
| 41 | 1 | 0 | 4.805429 | -3.651162 | -3.144600 |
| 42 | 1 | 0 | 6.950430 | -4.115349 | -1.438132 |
| 43 | 6 | 0 | 7.069708 | 2.954507 | -0.556273 |
| 44 | 6 | 0 | 7.124114 | 2.909338 | 0.809387 |
| 45 | 1 | 0 | 7.747489 | 3.409630 | -1.274001 |
| 46 | 1 | 0 | 7.851080 | 3.330174 | 1.499552 |
| 47 | 6 | 0 | -5.243568 | -1.793361 | -0.164942 |
| 48 | 6 | 0 | -4.704863 | 1.980812 | 0.309877 |
| 49 | 6 | 0 | 4.704836 | -1.980781 | -0.309826 |
| 50 | 6 | 0 | 5.243562 | 1.793347 | 0.164904 |
| 51 | 7 | 0 | -5.918600 | -2.275887 | 0.941615 |
| 52 | 7 | 0 | -6.005513 | -2.206836 | -1.241444 |
| 53 | 7 | 0 | -4.197603 | 2.319600 | 1.537951 |
| 54 | 7 | 0 | -5.870862 | 2.699566 | 0.187360 |
| 55 | 7 | 0 | 5.870929 | -2.699394 | -0.187381 |
| 56 | 7 | 0 | 4.197506 | -2.319680 | -1.537839 |
| 57 | 7 | 0 | 5.918595 | 2.275785 | -0.941691 |
| 58 | 7 | 0 | 6.005560 | 2.206819 | 1.241368 |
| 59 | 6 | 0 | -5.560596 | -1.972056 | 2.349748 |

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|---|---|---|---|---|---|
| 60 | 6 | 0 | -5.458735 | -3.258636 | 3.181706 |
| 61 | 6 | 0 | -6.560226 | -0.964192 | 2.942392 |
| 62 | 1 | 0 | -4.563634 | -1.504287 | 2.278611 |
| 63 | 1 | 0 | -4.738986 | -3.965741 | 2.738236 |
| 64 | 1 | 0 | -5.112221 | -3.011112 | 4.199519 |
| 65 | 1 | 0 | -6.436260 | -3.764962 | 3.278848 |
| 66 | 1 | 0 | -6.597228 | -0.042325 | 2.337225 |
| 67 | 1 | 0 | -7.579013 | -1.388291 | 2.995858 |
| 68 | 1 | 0 | -6.256376 | -0.694142 | 3.968730 |
| 69 | 6 | 0 | -5.599252 | -2.078332 | -2.664765 |
| 70 | 6 | 0 | -6.629837 | -1.259950 | -3.453672 |
| 71 | 6 | 0 | -5.339953 | -3.467047 | -3.271478 |
| 72 | 1 | 0 | -4.646961 | -1.520805 | -2.620270 |
| 73 | 1 | 0 | -6.763133 | -0.262548 | -3.002915 |
| 74 | 1 | 0 | -6.278501 | -1.123581 | -4.490706 |
| 75 | 1 | 0 | -7.611508 | -1.766720 | -3.496621 |
| 76 | 1 | 0 | -4.591866 | -4.021670 | -2.680526 |
| 77 | 1 | 0 | -6.263422 | -4.071307 | -3.326041 |
| 78 | 1 | 0 | -4.953319 | -3.353118 | -4.298696 |
| 79 | 6 | 0 | -6.780160 | 2.697291 | -0.993000 |
| 80 | 6 | 0 | -6.896315 | 4.111896 | -1.579479 |
| 81 | 6 | 0 | -8.137670 | 2.084140 | -0.619026 |
| 82 | 1 | 0 | -6.266063 | 2.042934 | -1.719232 |
| 83 | 1 | 0 | -5.902853 | 4.520621 | -1.829198 |
| 84 | 1 | 0 | -7.496482 | 4.075553 | -2.504632 |
| 85 | 1 | 0 | -7.397977 | 4.809704 | -0.885119 |
| 86 | 1 | 0 | -8.016568 | 1.061070 | -0.224182 |
| 87 | 1 | 0 | -8.666991 | 2.690437 | 0.138181 |
| 88 | 1 | 0 | -8.780408 | 2.034900 | -1.514722 |
| 89 | 6 | 0 | -2.903018 | 1.845965 | 2.108506 |
| 90 | 6 | 0 | -3.091460 | 1.381297 | 3.559588 |
| 91 | 6 | 0 | -1.838805 | 2.944162 | 1.968472 |
| 92 | 1 | 0 | -2.621478 | 0.978248 | 1.493601 |
| 93 | 1 | 0 | -3.900918 | 0.636431 | 3.643149 |
| 94 | 1 | 0 | -2.155966 | 0.909395 | 3.903151 |
| 95 | 1 | 0 | -3.310750 | 2.219371 | 4.245950 |
| 96 | 1 | 0 | -1.725419 | 3.252752 | 0.916674 |
| 97 | 1 | 0 | -2.094847 | 3.829925 | 2.579130 |
| 98 | 1 | 0 | -0.866211 | 2.556134 | 2.314081 |
| 99 | 6 | 0 | 5.560554 | 1.971886 | -2.349801 |
| 100 | 6 | 0 | 6.560110 | 0.963916 | -2.942393 |
| 101 | 6 | 0 | 5.458767 | 3.258420 | -3.181841 |
| 102 | 1 | 0 | 4.563563 | 1.504187 | -2.278624 |
| 103 | 1 | 0 | 6.597053 | 0.042086 | -2.337167 |

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|---|---|---|---|---|---|
| 104 | 1 | 0 | 6.256231 | 0.693822 | -3.968711 |
| 105 | 1 | 0 | 7.578925 | 1.387942 | -2.995894 |
| 106 | 1 | 0 | 4.739078 | 3.965606 | -2.738402 |
| 107 | 1 | 0 | 6.436326 | 3.764670 | -3.279037 |
| 108 | 1 | 0 | 5.112215 | 3.010853 | -4.199630 |
| 109 | 6 | 0 | 5.599340 | 2.078367 | 2.664705 |
| 110 | 6 | 0 | 5.340119 | 3.467109 | 3.271390 |
| 111 | 6 | 0 | 6.629916 | 1.259961 | 3.453599 |
| 112 | 1 | 0 | 4.647025 | 1.520879 | 2.620254 |
| 113 | 1 | 0 | 4.592033 | 4.021746 | 2.680450 |
| 114 | 1 | 0 | 4.953517 | 3.353224 | 4.298625 |
| 115 | 1 | 0 | 6.263615 | 4.071333 | 3.325903 |
| 116 | 1 | 0 | 6.763160 | 0.262544 | 3.002861 |
| 117 | 1 | 0 | 7.611609 | 1.766693 | 3.496506 |
| 118 | 1 | 0 | 6.278606 | 1.123631 | 4.490646 |
| 119 | 6 | 0 | 2.902816 | -1.846216 | -2.108298 |
| 120 | 6 | 0 | 1.838756 | -2.944550 | -1.968176 |
| 121 | 6 | 0 | 3.091087 | -1.381534 | -3.559397 |
| 122 | 1 | 0 | 2.621213 | -0.978529 | -1.493377 |
| 123 | 1 | 0 | 1.725492 | -3.253152 | -0.916368 |
| 124 | 1 | 0 | 0.866085 | -2.556650 | -2.313711 |
| 125 | 1 | 0 | 2.094865 | -3.830282 | -2.578850 |
| 126 | 1 | 0 | 3.900449 | -0.636571 | -3.643031 |
| 127 | 1 | 0 | 3.310420 | -2.219586 | -4.245772 |
| 128 | 1 | 0 | 2.155508 | -0.909746 | -3.902889 |
| 129 | 6 | 0 | 6.780340 | -2.696954 | 0.992891 |
| 130 | 6 | 0 | 8.137741 | -2.083658 | 0.618759 |
| 131 | 6 | 0 | 6.896720 | -4.111519 | 1.579424 |
| 132 | 1 | 0 | 6.266234 | -2.042625 | 1.719142 |
| 133 | 1 | 0 | 8.016478 | -1.060620 | 0.223881 |
| 134 | 1 | 0 | 8.780559 | -2.034301 | 1.514391 |
| 135 | 1 | 0 | 8.667062 | -2.689925 | -0.138472 |
| 136 | 1 | 0 | 5.903331 | -4.520351 | 1.829256 |
| 137 | 1 | 0 | 7.398401 | -4.809299 | 0.885049 |
| 138 | 1 | 0 | 7.496970 | -4.075061 | 2.504519 |
| 139 | 5 | 0 | 3.933837 | 0.921540 | 0.221365 |
| 140 | 5 | 0 | -3.933869 | -0.921512 | -0.221329 |

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