# Higher Spin States in Some Low-Energy Bis(Tetramethyl-1,2-diaza-3,5-diborolyl) Sandwich Compounds of the First Row Transition Metals: Boraza Analogues of the Metallocenes

Jianlin Chen,[a*] Hao Feng,[a] Yaoming Xie,[b] R. Bruce King,[a,b*] Henry F. Schaefer[b]

[a]*School of Science, Research Center for Advanced Computation*

*Xihua University, Chengdu, China 610039*

[b]*Department of Chemistry and Center for Computational Chemistry*

*University of Georgia, Athens, Georgia 30602, USA*

E-mail: rbking@chem.uga.edu, chenjianlin2000@163.com

## Supporting Information.

**Tables S1 to S7.** Total energies ($E$ in hartree), relative energies ($\Delta E$ in kcal/mol), and numbers of imaginary vibrational frequencies (Nimg) for the $(Me_4B_2N_2CH)_2M$ structures.

**Tables S8 to S35:** Atomic coordinates of the optimized structures for the $(Me_4B_2N_2CH)_2M$ complexes.

**Table S1.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg) for the $(Me_4B_2N_2CH)_2Ti_2$ structures.

| | | **Ti-t-144($C_2$)** | | | **Ti-t-180($C_i$)** | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1564 | 0.77147 | 0.96500 | 0.25550 | 0.76922 | 0.96379 | 0.25498 |
| □△E | 0.0 | 0.0 | 0.0 | 1.4 | 0.8 | 0.3 |
| Nimg | none | none | none | 1（50i） | none | none |
| $\langle S^2 \rangle$ | | | | | | |
| | | **Ti-s-144($C_2$)** | | | **Ti-s-0($C_s$)** | |
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E-1564 | 0.75188 | 0.94956 | 0.23103 | 0.74602 | 0.94432 | 0.22572 |
| □△E | 12.3 | 9.7 | 15.3 | 16.0 | 13.0 | 18.7 |
| Nimg | none | none | none | none | none | none |

**Table S2.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2V_2$ structures.

| | | **V-q-180($C_{2h}$)** | | | **V-d-180($C_{2h}$)** | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1658 | 1.32504 | 1.54038 | 0.80300 | 1.27352 | 1.51714 | 0.76048 |
| □△E | 0.0 | 0.0 | 0.0 | 32.3 | 14.6 | 26.7 |
| Nimg | none | none | none | 2(84i,43i) | none | 2(50i,19i) |

**Table S3.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2Cr_2$ structures.

| | | **Cr-p-180($C_i$)** | | | **Cr-p-144($C_2$)** | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1759 | 0.77266 | 1.00702 | 0.25093 | 0.77163 | 1.00686 | 0.25056 |
| □△E | 0.0 | 0.0 | 0.0 | 0.6 | 1.4 | 0.2 |
| Nimg | none | none | none | none | none | none |
| | | **Cr-t-180($C_i$)** | | | **Cr-p-36($C_2$)** | |
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E-1759 | 0.76005 | 1.00905 | 0.23712 | 0.77140 | 1.00437 | 0.24783 |
| □△E | 7.9 | -1.3 | 8.7 | 0.8 | 1.7 | 1.9 |
| Nimg | none | none | none | none | none | none |
| | | **Cr-t-72($C_2$)** | | | | |
| | M06-L | BP86 | B3LYP* | | | |
| -E -1759 | 0.75351 | 0.00333 | 0.23057 | | | |
| □△E | 12.0 | 3.6 | 12.6 | | | |
| Nimg | none | none | none | | | |

**Table S4.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2Mn_2$ structures.

| | | **Mn-x-144($C_2$)** | | | **Mn-d-180($C_i$)** | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1865 | 1.30156 | 1.54743 | 0.77622 | 1.26715 | 1.55115 | 0.75317 |
| □△E | 0.0 | 0.0 | 0.0 | 21.6 | -2.3 | 14.5 |
| Nimg | none | none | none | none | none | none |
| | | **Mn-q-180($C_i$)** | | | **Mn-q-36($C_2$)** | |
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E-1865 | 1.27301 | 0.54220 | 0.75317 | 1.27133 | 0.53988 | 0.75036 |
| □△E | 17.9 | 5.6 | 14.5 | 18.9 | 7.1 | 16.2 |
| Nimg | none | none | none | none | none | none |
| | | **Mn-q-144($C_2$)** | | | | |
| | M06-L | BP86 | B3LYP* | | | |
| -E - 1865 | 1.26228 | 0.53304 | 0.74675 | | | |
| □△E | 24.6 | 11.4 | 18.5 | | | |
| Nimg | none | none | none | | | |

**Table S5.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2Fe_2$ structures.

| | | **Fe-s-180($C_2$)** | | | **Fe-s-72($C_2$)** | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1978 | 1.00577 | 1.31421 | 0.48220 | 1.00018 | 1.30947 | 0.47615 |
| □△E | 0.0 | 0.0 | 0.0 | 3.5 | 3.0 | 3.8 |
| Nimg | none | none | none | none | none | none |
| | | **Fe-t-180($C_i$)** | | | **Fe-t-36($C_2$)** | |
| | M06-L | BP86 | BLYP* | M06-L | BP86 | B3LYP* |
| -E- 1978 | 0.98484 | 1.28981 | 0.473553 | 0.98339 | 1.28877 | 0.47103 |
| □△E | 13.1 | 15.3 | 5.4 | 14.0 | 16.0 | 6.9 |
| Nimg | none | none | none | none | none | none |
| | | **Fe-t-144($C_2$)** | | | **Fe-p-180($C_i$)** | |
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -1978 | 0.97733 | 1.28355 | 0.46736 | 0.99074 | 1.27619 | 0.47364 |
| □△E | 17.8 | 16.2 | 9.3 | 9.4 | 23.8 | 5.3 |
| Nimg | none | none | none | 1(24i) | none | none |

**Table S6.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2Co_2$ structures.

| | **Co-d-180($C_i$)** | | | **Co-d-36($C_2$)** | | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -2097 | 1.05497 | 1.38390 | 0.53634 | 1.05219 | 1.38146 | 0.0.53253 |
| □△E | 0.0 | 0.0 | 0.0 | 1.7 | 1.5 | 2.4 |
| Nimg | none | none | none | none | none | none |
| | **Co-q-180($C_2$)** | | | **Co-q-36($C_2$)** | | |
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E- 2097 | 1.04105 | 1.36837 | 0.52948 | 1.03323 | 1.35314 | 0.52136 |
| □△E | 8.7 | 9.7 | 4.3 | 13.6 | 19.3 | 9.4 |
| Nimg | none | none | none | None | none | none |

**Table S7.** Total energies (*E* in hartree), relative energies (Δ*E* in kcal/mol), the number of imaginary vibrational frequencies (Nimg), spin expectation values ($\langle S^2 \rangle$) for the $(Me_4B_2N_2CH)_2Ni_2$ structures.

| | **Ni-s-180($C_i$)** | | | **Ni-t-180($C_2$)** | | |
|---|---|---|---|---|---|---|
| | M06-L | BP86 | B3LYP* | M06-L | BP86 | B3LYP* |
| -E -2223 | 0.59457 | 0.94788 | 0.07916 | 0.59273 | 0.93639 | 0.07477 |
| □△E | 0.0 | 0.0 | 0.0 | 1.2 | 7.2 | 2.7 |
| Nimg | none | none | none | none | none | 1(25i) |

**Table S8.** Atomic coordinates of the optimized structures for the **Ti-t-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 2.322581 | -0.376088 | 0.796889 | 6 | 2.384655 | -0.404427 | 0.671748 |
| 1 | 3.003329 | 0.296811 | 1.313465 | 1 | 3.104415 | 0.286161 | 1.114662 |
| 1 | -3.003329 | -0.296811 | 1.313465 | 1 | -3.104415 | -0.286161 | 1.114662 |
| 6 | -2.322581 | 0.376088 | 0.796889 | 6 | -2.384655 | 0.404427 | 0.671748 |
| 5 | 2.116950 | -0.421759 | -0.697048 | 5 | 2.144542 | -0.591849 | -0.810717 |
| 5 | -2.116950 | 0.421759 | -0.697048 | 5 | -2.144542 | 0.591849 | -0.810717 |
| 5 | -1.656642 | 1.582127 | 1.396608 | 5 | -1.719525 | 1.551422 | 1.392238 |
| 5 | 1.656642 | -1.582127 | 1.396608 | 5 | 1.719525 | -1.551422 | 1.392238 |
| 7 | 1.032442 | -1.425965 | -0.902891 | 7 | 1.026108 | -1.569719 | -0.904357 |
| 7 | 0.771299 | -2.111956 | 0.334936 | 7 | 0.759118 | -2.126336 | 0.413011 |
| 7 | -1.032442 | 1.425965 | -0.902891 | 7 | -1.026108 | 1.569719 | -0.904357 |
| 7 | -0.771299 | 2.111956 | 0.334936 | 7 | -0.759118 | 2.126336 | 0.413011 |
| 6 | -2.742420 | -0.331938 | -1.931065 | 6 | -2.773760 | -0.044707 | -2.123288 |
| 1 | -3.601540 | 0.222436 | -2.332271 | 1 | -3.455930 | 0.671577 | -2.611635 |
| 1 | -2.051787 | -0.471499 | -2.773956 | 1 | -2.028719 | -0.333889 | -2.881790 |
| 1 | -3.121885 | -1.321163 | -1.652140 | 1 | -3.369506 | -0.936402 | -1.884173 |
| 6 | -1.510105 | 2.167978 | 2.850078 | 6 | -1.756201 | 2.088827 | 2.883235 |
| 1 | -2.172238 | 1.670761 | 3.563283 | 1 | -2.384171 | 1.450563 | 3.518799 |
| 1 | -0.483878 | 2.051725 | 3.232568 | 1 | -0.758468 | 2.140922 | 3.349414 |
| 1 | -1.726009 | 3.243297 | 2.894909 | 1 | -2.176386 | 3.107738 | 2.926457 |
| 6 | 0.103533 | 3.262507 | 0.323409 | 6 | 0.000000 | 3.365640 | 0.511952 |
| 1 | -0.327561 | 4.108432 | -0.230106 | 1 | -0.536136 | 4.217583 | 0.062825 |
| 1 | 0.241886 | 3.567585 | 1.362831 | 1 | 0.137473 | 3.571933 | 1.578875 |
| 1 | 1.092049 | 3.027632 | -0.091829 | 1 | 0.994276 | 3.282359 | 0.053086 |
| 6 | -0.585877 | 2.044729 | -2.130940 | 6 | -0.565977 | 2.299972 | -2.077014 |
| 1 | -1.134579 | 2.972229 | -2.343686 | 1 | -1.062023 | 3.279288 | -2.171617 |
| 1 | 0.489437 | 2.257416 | -2.122782 | 1 | 0.522758 | 2.445269 | -2.080270 |
| 1 | -0.783911 | 1.338535 | -2.941191 | 1 | -0.831038 | 1.699052 | -2.953753 |
| 6 | 2.742420 | 0.331938 | -1.931065 | 6 | 2.773760 | 0.044707 | -2.123288 |
| 1 | 2.051787 | 0.471499 | -2.773956 | 1 | 2.028719 | 0.333889 | -2.881790 |
| 1 | 3.121885 | 1.321163 | -1.652140 | 1 | 3.369506 | 0.936402 | -1.884173 |
| 1 | 3.601540 | -0.222436 | -2.332271 | 1 | 3.455930 | -0.671577 | -2.611635 |
| 6 | 1.510105 | -2.167978 | 2.850078 | 6 | 1.756201 | -2.088827 | 2.883235 |
| 1 | 0.483878 | -2.051725 | 3.232568 | 1 | 0.758468 | -2.140922 | 3.349414 |
| 1 | 1.726009 | -3.243297 | 2.894909 | 1 | 2.176386 | -3.107738 | 2.926457 |
| 1 | 2.172238 | -1.670761 | 3.563283 | 1 | 2.384171 | -1.450563 | 3.518799 |
| 6 | -0.103533 | -3.262507 | 0.323409 | 6 | 0.000000 | -3.365640 | 0.511952 |
| 1 | 0.327561 | -4.108432 | -0.230106 | 1 | 0.536136 | -4.217583 | 0.062825 |
| 1 | -0.241886 | -3.567585 | 1.362831 | 1 | -0.137473 | -3.571933 | 1.578875 |
| 1 | -1.092049 | -3.027632 | -0.091829 | 1 | -0.994276 | -3.282359 | 0.053086 |
| 6 | 0.585877 | -2.044729 | -2.130940 | 6 | 0.565977 | -2.299972 | -2.077014 |
| 1 | 1.134579 | -2.972229 | -2.343686 | 1 | 1.062023 | -3.279288 | -2.171617 |
| 1 | -0.489437 | -2.257416 | -2.122782 | 1 | -0.522758 | -2.445269 | -2.080270 |
| 1 | 0.783911 | -1.338535 | -2.941191 | 1 | 0.831038 | -1.699052 | -2.953753 |
| 22 | 0.000000 | 0.000000 | 0.418247 | 22 | 0.000000 | 0.000000 | 0.301013 |

**Table S9.** Atomic coordinates of the optimized structures for the **Ti-t-180**complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -0.978718 | 1.440533 | -1.623969 | 6 | -1.031356 | 1.428276 | -1.631423 |
| 1 | -0.497687 | 2.322272 | -2.045209 | 1 | -0.602856 | 2.317081 | -2.098128 |
| 1 | 0.497687 | -2.322272 | 2.045209 | 1 | 0.602856 | -2.317081 | 2.098128 |
| 6 | 0.978718 | -1.440533 | 1.623969 | 6 | 1.031356 | -1.428276 | 1.631423 |
| 5 | -1.940922 | 1.463614 | -0.464981 | 5 | -2.034103 | 1.436458 | -0.493422 |
| 5 | 0.964231 | -0.057358 | 2.222035 | 5 | 1.090817 | -0.048533 | 2.259893 |
| 5 | 1.940922 | -1.463614 | 0.464981 | 5 | 2.034103 | -1.436458 | 0.493422 |
| 5 | -0.964231 | 0.057358 | -2.222035 | 5 | -1.090817 | 0.048533 | -2.259893 |
| 7 | -2.232721 | 0.033973 | -0.198721 | 7 | -2.275682 | 0.009272 | -0.182384 |
| 7 | -1.651659 | -0.804209 | -1.218852 | 7 | -1.714204 | -0.820793 | -1.232062 |
| 7 | 1.651659 | 0.804209 | 1.218852 | 7 | 1.714204 | 0.820793 | 1.232062 |
| 7 | 2.232721 | -0.033973 | 0.198721 | 7 | 2.275682 | -0.009272 | 0.182384 |
| 6 | 0.330635 | 0.608982 | 3.501005 | 6 | 0.580321 | 0.557099 | 3.635013 |
| 1 | 1.092563 | 0.851400 | 4.254399 | 1 | 1.431845 | 0.797225 | 4.294018 |
| 1 | -0.192851 | 1.550350 | 3.280476 | 1 | -0.000130 | 1.486513 | 3.520342 |
| 1 | -0.390478 | -0.054981 | 3.988052 | 1 | -0.049845 | -0.162450 | 4.175024 |
| 6 | 2.526276 | -2.567558 | -0.490573 | 6 | 2.699467 | -2.583804 | -0.377113 |
| 1 | 2.051613 | -3.538896 | -0.325408 | 1 | 2.262637 | -3.563395 | -0.140892 |
| 1 | 2.398472 | -2.323137 | -1.554543 | 1 | 2.597558 | -2.429228 | -1.463386 |
| 1 | 3.604430 | -2.708089 | -0.336338 | 1 | 3.780743 | -2.653051 | -0.170260 |
| 6 | 2.995695 | 0.597867 | -0.856018 | 6 | 3.236117 | 0.576473 | -0.741279 |
| 1 | 3.918153 | 1.059207 | -0.480371 | 1 | 4.165995 | 0.881610 | -0.234465 |
| 1 | 3.265156 | -0.183538 | -1.569915 | 1 | 3.485619 | -0.196289 | -1.476244 |
| 1 | 2.417414 | 1.363165 | -1.394220 | 1 | 2.821947 | 1.438534 | -1.282058 |
| 6 | 2.157849 | 2.148778 | 1.379446 | 6 | 2.218083 | 2.176735 | 1.395538 |
| 1 | 3.196922 | 2.157308 | 1.737534 | 1 | 3.271811 | 2.188767 | 1.719731 |
| 1 | 2.093948 | 2.733916 | 0.454850 | 1 | 2.116789 | 2.773543 | 0.479489 |
| 1 | 1.530982 | 2.637876 | 2.128306 | 1 | 1.614220 | 2.651838 | 2.176253 |
| 6 | -2.526276 | 2.567558 | 0.490573 | 6 | -2.699467 | 2.583804 | 0.377113 |
| 1 | -2.398472 | 2.323137 | 1.554543 | 1 | -2.597558 | 2.429228 | 1.463386 |
| 1 | -2.051613 | 3.538896 | 0.325408 | 1 | -2.262637 | 3.563395 | 0.140892 |
| 1 | -3.604430 | 2.708089 | 0.336338 | 1 | -3.780743 | 2.653051 | 0.170260 |
| 6 | -0.330635 | -0.608982 | -3.501005 | 6 | -0.580321 | -0.557099 | -3.635013 |
| 1 | 0.192851 | -1.550350 | -3.280476 | 1 | 0.000130 | -1.486513 | -3.520342 |
| 1 | -1.092563 | -0.851400 | -4.254399 | 1 | -1.431845 | -0.797225 | -4.294018 |
| 1 | 0.390478 | 0.054981 | -3.988052 | 1 | 0.049845 | 0.162450 | -4.175024 |
| 6 | -2.157849 | -2.148778 | -1.379446 | 6 | -2.218083 | -2.176735 | -1.395538 |
| 1 | -3.196922 | -2.157308 | -1.737534 | 1 | -3.271811 | -2.188767 | -1.719731 |
| 1 | -1.530982 | -2.637876 | -2.128306 | 1 | -1.614220 | -2.651838 | -2.176253 |
| 1 | -2.093948 | -2.733916 | -0.454850 | 1 | -2.116789 | -2.773543 | -0.479489 |
| 6 | -2.995695 | -0.597867 | 0.856018 | 6 | -3.236117 | -0.576473 | 0.741279 |
| 1 | -3.918153 | -1.059207 | 0.480371 | 1 | -4.165995 | -0.881610 | 0.234465 |
| 1 | -2.417414 | -1.363165 | 1.394220 | 1 | -2.821947 | -1.438534 | 1.282058 |
| 1 | -3.265156 | 0.183538 | 1.569915 | 1 | -3.485619 | 0.196289 | 1.476244 |
| 22 | 0.000000 | 0.000000 | 0.000000 | 22 | 0.000000 | 0.000000 | 0.000000 |

**Table S10.** Atomic coordinates of the optimized structures for the **Ti-s-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -2.105744 | -0.061381 | -0.703775 | 6 | -2.183388 | -0.127462 | -0.579151 |
| 1 | -2.612425 | 0.793996 | -1.148336 | 1 | -2.779907 | 0.695211 | -0.978355 |
| 1 | 2.612425 | -0.793996 | -1.148336 | 1 | 2.779907 | -0.695211 | -0.978355 |
| 6 | 2.105744 | 0.061381 | -0.703775 | 6 | 2.183388 | 0.127462 | -0.579151 |
| 5 | -2.380428 | -0.633378 | 0.642293 | 5 | -2.376540 | -0.788520 | 0.756827 |
| 5 | 2.380428 | 0.633378 | 0.642293 | 5 | 2.376540 | 0.788520 | 0.756827 |
| 5 | 1.100946 | 0.939068 | -1.464936 | 5 | 1.252004 | 1.002047 | -1.440821 |
| 5 | -1.100946 | -0.939068 | -1.464936 | 5 | -1.252004 | -1.002047 | -1.440821 |
| 7 | -1.324633 | -1.671915 | 0.838485 | 7 | -1.270347 | -1.774306 | 0.856796 |
| 7 | -0.578169 | -1.895240 | -0.379757 | 7 | -0.596156 | -1.929722 | -0.426458 |
| 7 | 1.324633 | 1.671915 | 0.838485 | 7 | 1.270347 | 1.774306 | 0.856796 |
| 7 | 0.578169 | 1.895240 | -0.379757 | 7 | 0.596156 | 1.929722 | -0.426458 |
| 6 | 3.244301 | 0.229394 | 1.895289 | 6 | 3.298876 | 0.510591 | 2.017384 |
| 1 | 3.854337 | 1.061474 | 2.269796 | 1 | 3.905106 | 1.394560 | 2.274995 |
| 1 | 2.617189 | -0.086385 | 2.745311 | 1 | 2.722088 | 0.253333 | 2.922931 |
| 1 | 3.922584 | -0.599400 | 1.677308 | 1 | 3.993226 | -0.318087 | 1.825519 |
| 6 | 0.877923 | 1.333733 | -2.971616 | 6 | 1.162452 | 1.287505 | -2.996799 |
| 1 | 1.169500 | 0.529797 | -3.653512 | 1 | 1.495767 | 0.412679 | -3.571775 |
| 1 | -0.165017 | 1.587700 | -3.206837 | 1 | 0.151528 | 1.540800 | -3.349593 |
| 1 | 1.486274 | 2.209772 | -3.240772 | 1 | 1.826435 | 2.123315 | -3.278520 |
| 6 | 0.000000 | 3.200800 | -0.600034 | 6 | 0.000000 | 3.221383 | -0.735578 |
| 1 | 0.774840 | 3.968664 | -0.734374 | 1 | 0.767686 | 4.007537 | -0.825976 |
| 1 | -0.585056 | 3.136294 | -1.519282 | 1 | -0.505557 | 3.115809 | -1.700816 |
| 1 | -0.674310 | 3.508295 | 0.207672 | 1 | -0.748283 | 3.529640 | 0.006956 |
| 6 | 0.964212 | 2.461882 | 1.993912 | 6 | 0.859913 | 2.628247 | 1.959984 |
| 1 | 1.224073 | 3.521501 | 1.868403 | 1 | 1.112411 | 3.685504 | 1.781989 |
| 1 | -0.112406 | 2.405980 | 2.220544 | 1 | -0.221512 | 2.562036 | 2.162624 |
| 1 | 1.517143 | 2.069664 | 2.850393 | 1 | 1.397878 | 2.291500 | 2.852972 |
| 6 | -3.244301 | -0.229394 | 1.895289 | 6 | -3.298876 | -0.510591 | 2.017384 |
| 1 | -2.617189 | 0.086385 | 2.745311 | 1 | -2.722088 | -0.253333 | 2.922931 |
| 1 | -3.922584 | 0.599400 | 1.677308 | 1 | -3.993226 | 0.318087 | 1.825519 |
| 1 | -3.854337 | -1.061474 | 2.269796 | 1 | -3.905106 | -1.394560 | 2.274995 |
| 6 | -0.877923 | -1.333733 | -2.971616 | 6 | -1.162452 | -1.287505 | -2.996799 |
| 1 | 0.165017 | -1.587700 | -3.206837 | 1 | -0.151528 | -1.540800 | -3.349593 |
| 1 | -1.486274 | -2.209772 | -3.240772 | 1 | -1.826435 | -2.123315 | -3.278520 |
| 1 | -1.169500 | -0.529797 | -3.653512 | 1 | -1.495767 | -0.412679 | -3.571775 |
| 6 | 0.000000 | -3.200800 | -0.600034 | 6 | 0.000000 | -3.221383 | -0.735578 |
| 1 | -0.774840 | -3.968664 | -0.734374 | 1 | -0.767686 | -4.007537 | -0.825976 |
| 1 | 0.585056 | -3.136294 | -1.519282 | 1 | 0.505557 | -3.115809 | -1.700816 |
| 1 | 0.674310 | -3.508295 | 0.207672 | 1 | 0.748283 | -3.529640 | 0.006956 |
| 6 | -0.964212 | -2.461882 | 1.993912 | 6 | -0.859913 | -2.628247 | 1.959984 |
| 1 | -1.224073 | -3.521501 | 1.868403 | 1 | -1.112411 | -3.685504 | 1.781989 |
| 1 | 0.112406 | -2.405980 | 2.220544 | 1 | 0.221512 | -2.562036 | 2.162624 |
| 1 | -1.517143 | -2.069664 | 2.850393 | 1 | -1.397878 | -2.291500 | 2.852972 |
| 22 | 0.000000 | 0.000000 | 0.262104 | 22 | 0.000000 | 0.000000 | 0.208147 |

**Table S11.** Atomic coordinates of the optimized structures for the **Ti-s-0** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -0.045458 | -1.662335 | 1.663093 | 6 | -0.030685 | -1.651733 | 1.734076 |
| 1 | -0.067642 | -2.740781 | 1.531755 | 1 | -0.032448 | -2.737458 | 1.634649 |
| 1 | -0.067642 | -2.740781 | -1.531755 | 1 | -0.032448 | -2.737458 | -1.634649 |
| 6 | -0.045458 | -1.662335 | -1.663093 | 6 | -0.030685 | -1.651733 | -1.734076 |
| 5 | -1.117961 | -0.832676 | 2.282586 | 5 | -1.136437 | -0.817836 | 2.322923 |
| 5 | 1.227852 | -0.812780 | -1.464776 | 5 | 1.238086 | -0.785464 | -1.626548 |
| 5 | -1.117961 | -0.832676 | -2.282586 | 5 | -1.136437 | -0.817836 | -2.322923 |
| 5 | 1.227852 | -0.812780 | 1.464776 | 5 | 1.238086 | -0.785464 | 1.626548 |
| 7 | -0.656006 | 0.574209 | 2.108629 | 7 | -0.690359 | 0.586223 | 2.138834 |
| 7 | 0.710153 | 0.623932 | 1.644424 | 7 | 0.705033 | 0.638883 | 1.727249 |
| 7 | 0.710153 | 0.623932 | -1.644424 | 7 | 0.705033 | 0.638883 | -1.727249 |
| 7 | -0.656006 | 0.574209 | -2.108629 | 7 | -0.690359 | 0.586223 | -2.138834 |
| 6 | 2.763208 | -1.114846 | -1.620179 | 6 | 2.784493 | -1.104275 | -1.757803 |
| 1 | 3.050752 | -1.132384 | -2.681504 | 1 | 3.097318 | -1.092625 | -2.816513 |
| 1 | 3.422868 | -0.388620 | -1.126745 | 1 | 3.441353 | -0.406097 | -1.217284 |
| 1 | 3.018508 | -2.097533 | -1.211919 | 1 | 3.000148 | -2.111309 | -1.375182 |
| 6 | -2.595584 | -1.064334 | -2.769195 | 6 | -2.603988 | -1.113529 | -2.843250 |
| 1 | -2.847571 | -2.126207 | -2.819798 | 1 | -2.812617 | -2.191204 | -2.845214 |
| 1 | -3.326848 | -0.599449 | -2.089286 | 1 | -3.377965 | -0.633533 | -2.219595 |
| 1 | -2.785809 | -0.631685 | -3.759831 | 1 | -2.753429 | -0.744187 | -3.871214 |
| 6 | -1.348956 | 1.831096 | -2.252511 | 6 | -1.395301 | 1.840045 | -2.335081 |
| 1 | -0.958863 | 2.432155 | -3.085061 | 1 | -1.008612 | 2.408250 | -3.195995 |
| 1 | -2.402189 | 1.614296 | -2.443993 | 1 | -2.447509 | 1.600669 | -2.523618 |
| 1 | -1.282819 | 2.452075 | -1.341274 | 1 | -1.345216 | 2.495201 | -1.447168 |
| 6 | 1.507772 | 1.769874 | -2.013457 | 6 | 1.490984 | 1.781891 | -2.168227 |
| 1 | 1.663901 | 1.821735 | -3.099932 | 1 | 1.576408 | 1.810177 | -3.266993 |
| 1 | 1.075943 | 2.719607 | -1.671572 | 1 | 1.080564 | 2.739902 | -1.818397 |
| 1 | 2.482275 | 1.648964 | -1.534709 | 1 | 2.495893 | 1.666188 | -1.748657 |
| 6 | -2.595584 | -1.064334 | 2.769195 | 6 | -2.603988 | -1.113529 | 2.843250 |
| 1 | -3.326848 | -0.599449 | 2.089286 | 1 | -3.377965 | -0.633533 | 2.219595 |
| 1 | -2.847571 | -2.126207 | 2.819798 | 1 | -2.812617 | -2.191204 | 2.845214 |
| 1 | -2.785809 | -0.631685 | 3.759831 | 1 | -2.753429 | -0.744187 | 3.871214 |
| 6 | 2.763208 | -1.114846 | 1.620179 | 6 | 2.784493 | -1.104275 | 1.757803 |
| 1 | 3.422868 | -0.388620 | 1.126745 | 1 | 3.441353 | -0.406097 | 1.217284 |
| 1 | 3.050752 | -1.132384 | 2.681504 | 1 | 3.097318 | -1.092625 | 2.816513 |
| 1 | 3.018508 | -2.097533 | 1.211919 | 1 | 3.000148 | -2.111309 | 1.375182 |
| 6 | 1.507772 | 1.769874 | 2.013457 | 6 | 1.490984 | 1.781891 | 2.168227 |
| 1 | 1.663901 | 1.821735 | 3.099932 | 1 | 1.576408 | 1.810177 | 3.266993 |
| 1 | 2.482275 | 1.648964 | 1.534709 | 1 | 2.495893 | 1.666188 | 1.748657 |
| 1 | 1.075943 | 2.719607 | 1.671572 | 1 | 1.080564 | 2.739902 | 1.818397 |
| 6 | -1.348956 | 1.831096 | 2.252511 | 6 | -1.395301 | 1.840045 | 2.335081 |
| 1 | -0.958863 | 2.432155 | 3.085061 | 1 | -1.008612 | 2.408250 | 3.195995 |
| 1 | -1.282819 | 2.452075 | 1.341274 | 1 | -1.345216 | 2.495201 | 1.447168 |
| 1 | -2.402189 | 1.614296 | 2.443993 | 1 | -2.447509 | 1.600669 | 2.523618 |
| 22 | -0.332444 | -0.153510 | 0.000000 | 22 | -0.272533 | -0.170691 | 0.000000 |

**Table S12.** Atomic coordinates of the optimized structures for the **V-q-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.631654 | 2.241391 | 0.000000 | 6 | 0.658557 | 2.292375 | 0.000000 |
| 1 | 1.656715 | 2.607988 | 0.000000 | 1 | 1.679610 | 2.678265 | 0.000000 |
| 1 | -1.656715 | -2.607988 | 0.000000 | 1 | -1.679610 | -2.678265 | 0.000000 |
| 6 | -0.631654 | -2.241391 | 0.000000 | 6 | -0.658557 | -2.292375 | 0.000000 |
| 5 | -0.214780 | 2.028749 | 1.225622 | 5 | -0.205086 | 2.105560 | 1.225129 |
| 5 | 0.214780 | -2.028749 | 1.225622 | 5 | 0.205086 | -2.105560 | 1.225129 |
| 5 | 0.214780 | -2.028749 | -1.225622 | 5 | 0.205086 | -2.105560 | -1.225129 |
| 5 | -0.214780 | 2.028749 | -1.225622 | 5 | -0.205086 | 2.105560 | -1.225129 |
| 7 | -1.468040 | 1.404775 | 0.720433 | 7 | -1.447619 | 1.451399 | 0.727555 |
| 7 | -1.468040 | 1.404775 | -0.720433 | 7 | -1.447619 | 1.451399 | -0.727555 |
| 7 | 1.468040 | -1.404775 | 0.720433 | 7 | 1.447619 | -1.451399 | 0.727555 |
| 7 | 1.468040 | -1.404775 | -0.720433 | 7 | 1.447619 | -1.451399 | -0.727555 |
| 6 | 0.000000 | -2.182507 | 2.777590 | 6 | 0.000000 | -2.369874 | 2.776415 |
| 1 | 0.539276 | -3.051806 | 3.176645 | 1 | 0.595397 | -3.238178 | 3.105539 |
| 1 | 0.350630 | -1.314193 | 3.352712 | 1 | 0.298032 | -1.522902 | 3.415165 |
| 1 | -1.056201 | -2.328120 | 3.024636 | 1 | -1.050287 | -2.600688 | 3.000569 |
| 6 | 0.000000 | -2.182507 | -2.777590 | 6 | 0.000000 | -2.369874 | -2.776415 |
| 1 | -1.056201 | -2.328120 | -3.024636 | 1 | -1.050287 | -2.600688 | -3.000569 |
| 1 | 0.350630 | -1.314193 | -3.352712 | 1 | 0.298032 | -1.522902 | -3.415165 |
| 1 | 0.539276 | -3.051806 | -3.176645 | 1 | 0.595397 | -3.238178 | -3.105539 |
| 6 | 2.679879 | -1.037594 | -1.418500 | 6 | 2.701367 | -1.221323 | -1.431209 |
| 1 | 3.481020 | -1.772700 | -1.265083 | 1 | 3.428358 | -2.028254 | -1.246175 |
| 1 | 2.438135 | -1.011006 | -2.483334 | 1 | 2.469715 | -1.209288 | -2.501595 |
| 1 | 3.042834 | -0.043685 | -1.130230 | 1 | 3.155390 | -0.256407 | -1.169758 |
| 6 | 2.679879 | -1.037594 | 1.418500 | 6 | 2.701367 | -1.221323 | 1.431209 |
| 1 | 3.481020 | -1.772700 | 1.265083 | 1 | 3.428358 | -2.028254 | 1.246175 |
| 1 | 3.042834 | -0.043685 | 1.130230 | 1 | 3.155390 | -0.256407 | 1.169758 |
| 1 | 2.438135 | -1.011006 | 2.483334 | 1 | 2.469715 | -1.209288 | 2.501595 |
| 6 | 0.000000 | 2.182507 | 2.777590 | 6 | 0.000000 | 2.369874 | 2.776415 |
| 1 | -0.350630 | 1.314193 | 3.352712 | 1 | -0.298032 | 1.522902 | 3.415165 |
| 1 | 1.056201 | 2.328120 | 3.024636 | 1 | 1.050287 | 2.600688 | 3.000569 |
| 1 | -0.539276 | 3.051806 | 3.176645 | 1 | -0.595397 | 3.238178 | 3.105539 |
| 6 | 0.000000 | 2.182507 | -2.777590 | 6 | 0.000000 | 2.369874 | -2.776415 |
| 1 | -0.350630 | 1.314193 | -3.352712 | 1 | -0.298032 | 1.522902 | -3.415165 |
| 1 | -0.539276 | 3.051806 | -3.176645 | 1 | -0.595397 | 3.238178 | -3.105539 |
| 1 | 1.056201 | 2.328120 | -3.024636 | 1 | 1.050287 | 2.600688 | -3.000569 |
| 6 | -2.679879 | 1.037594 | -1.418500 | 6 | -2.701367 | 1.221323 | -1.431209 |
| 1 | -3.481020 | 1.772700 | -1.265083 | 1 | -3.428358 | 2.028254 | -1.246175 |
| 1 | -2.438135 | 1.011006 | -2.483334 | 1 | -2.469715 | 1.209288 | -2.501595 |
| 1 | -3.042834 | 0.043685 | -1.130230 | 1 | -3.155390 | 0.256407 | -1.169758 |
| 6 | -2.679879 | 1.037594 | 1.418500 | 6 | -2.701367 | 1.221323 | 1.431209 |
| 1 | -3.481020 | 1.772700 | 1.265083 | 1 | -3.428358 | 2.028254 | 1.246175 |
| 1 | -3.042834 | 0.043685 | 1.130230 | 1 | -3.155390 | 0.256407 | 1.169758 |
| 1 | -2.438135 | 1.011006 | 2.483334 | 1 | -2.469715 | 1.209288 | 2.501595 |
| 23 | 0.000000 | 0.000000 | 0.000000 | 23 | 0.000000 | 0.000000 | 0.000000 |

**Table S13.** Atomic coordinates of the optimized structures for the **V-d-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.565178 | 2.318298 | 0.000000 | 6 | 0.595822 | 2.367786 | 0.000000 |
| 1 | 1.583609 | 2.704116 | 0.000000 | 1 | 1.610258 | 2.772826 | 0.000000 |
| 1 | -1.583609 | -2.704116 | 0.000000 | 1 | -1.610258 | -2.772826 | 0.000000 |
| 6 | -0.565178 | -2.318298 | 0.000000 | 6 | -0.595822 | -2.367786 | 0.000000 |
| 5 | -0.221804 | 1.981278 | 1.225958 | 5 | -0.211485 | 2.061491 | 1.229335 |
| 5 | 0.221804 | -1.981278 | 1.225958 | 5 | 0.211485 | -2.061491 | 1.229335 |
| 5 | 0.221804 | -1.981278 | -1.225958 | 5 | 0.211485 | -2.061491 | -1.229335 |
| 5 | -0.221804 | 1.981278 | -1.225958 | 5 | -0.211485 | 2.061491 | -1.229335 |
| 7 | -1.469367 | 1.298866 | 0.723717 | 7 | -1.443197 | 1.356569 | 0.731621 |
| 7 | -1.469367 | 1.298866 | -0.723717 | 7 | -1.443197 | 1.356569 | -0.731621 |
| 7 | 1.469367 | -1.298866 | 0.723717 | 7 | 1.443197 | -1.356569 | 0.731621 |
| 7 | 1.469367 | -1.298866 | -0.723717 | 7 | 1.443197 | -1.356569 | -0.731621 |
| 6 | 0.000000 | -2.086848 | 2.782808 | 6 | 0.000000 | -2.273910 | 2.789378 |
| 1 | 0.575885 | -2.914735 | 3.218247 | 1 | 0.633918 | -3.095423 | 3.163849 |
| 1 | 0.303471 | -1.184343 | 3.332485 | 1 | 0.241438 | -1.387289 | 3.398004 |
| 1 | -1.050562 | -2.274835 | 3.025846 | 1 | -1.040451 | -2.550984 | 3.007840 |
| 6 | 0.000000 | -2.086848 | -2.782808 | 6 | 0.000000 | -2.273910 | -2.789378 |
| 1 | -1.050562 | -2.274835 | -3.025846 | 1 | -1.040451 | -2.550984 | -3.007840 |
| 1 | 0.303471 | -1.184343 | -3.332485 | 1 | 0.241438 | -1.387289 | -3.398004 |
| 1 | 0.575885 | -2.914735 | -3.218247 | 1 | 0.633918 | -3.095423 | -3.163849 |
| 6 | 2.689282 | -0.955756 | -1.423945 | 6 | 2.695435 | -1.116423 | -1.438526 |
| 1 | 3.469354 | -1.714901 | -1.279215 | 1 | 3.421764 | -1.925749 | -1.262680 |
| 1 | 2.442175 | -0.915581 | -2.487154 | 1 | 2.457099 | -1.095701 | -2.507295 |
| 1 | 3.078547 | 0.025600 | -1.130252 | 1 | 3.148590 | -0.153435 | -1.170544 |
| 6 | 2.689282 | -0.955756 | 1.423945 | 6 | 2.695435 | -1.116423 | 1.438526 |
| 1 | 3.469354 | -1.714901 | 1.279215 | 1 | 3.421764 | -1.925749 | 1.262680 |
| 1 | 3.078547 | 0.025600 | 1.130252 | 1 | 3.148590 | -0.153435 | 1.170544 |
| 1 | 2.442175 | -0.915581 | 2.487154 | 1 | 2.457099 | -1.095701 | 2.507295 |
| 6 | 0.000000 | 2.086848 | 2.782808 | 6 | 0.000000 | 2.273910 | 2.789378 |
| 1 | -0.303471 | 1.184343 | 3.332485 | 1 | -0.241438 | 1.387289 | 3.398004 |
| 1 | 1.050562 | 2.274835 | 3.025846 | 1 | 1.040451 | 2.550984 | 3.007840 |
| 1 | -0.575885 | 2.914735 | 3.218247 | 1 | -0.633918 | 3.095423 | 3.163849 |
| 6 | 0.000000 | 2.086848 | -2.782808 | 6 | 0.000000 | 2.273910 | -2.789378 |
| 1 | -0.303471 | 1.184343 | -3.332485 | 1 | -0.241438 | 1.387289 | -3.398004 |
| 1 | -0.575885 | 2.914735 | -3.218247 | 1 | -0.633918 | 3.095423 | -3.163849 |
| 1 | 1.050562 | 2.274835 | -3.025846 | 1 | 1.040451 | 2.550984 | -3.007840 |
| 6 | -2.689282 | 0.955756 | -1.423945 | 6 | -2.695435 | 1.116423 | -1.438526 |
| 1 | -3.469354 | 1.714901 | -1.279215 | 1 | -3.421764 | 1.925749 | -1.262680 |
| 1 | -2.442175 | 0.915581 | -2.487154 | 1 | -2.457099 | 1.095701 | -2.507295 |
| 1 | -3.078547 | -0.025600 | -1.130252 | 1 | -3.148590 | 0.153435 | -1.170544 |
| 6 | -2.689282 | 0.955756 | 1.423945 | 6 | -2.695435 | 1.116423 | 1.438526 |
| 1 | -3.469354 | 1.714901 | 1.279215 | 1 | -3.421764 | 1.925749 | 1.262680 |
| 1 | -3.078547 | -0.025600 | 1.130252 | 1 | -3.148590 | 0.153435 | 1.170544 |
| 1 | -2.442175 | 0.915581 | 2.487154 | 1 | -2.457099 | 1.095701 | 2.507295 |
| 23 | 0.000000 | 0.000000 | 0.000000 | 23 | 0.000000 | 0.000000 | 0.000000 |

**Table S14.** Atomic coordinates of the optimized structures for the **Cr-p-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -1.330341 | 0.119205 | 1.833384 | 6 | -0.976125 | 1.444614 | -1.510161 |
| 1 | -0.953039 | 0.020297 | 2.849888 | 1 | -0.486536 | 2.331473 | -1.917102 |
| 1 | 0.953039 | -0.020297 | -2.849888 | 1 | 0.486536 | -2.331473 | 1.917102 |
| 6 | 1.330341 | -0.119205 | -1.833384 | 6 | 0.976125 | -1.444614 | 1.510161 |
| 5 | -2.017553 | -0.982920 | 1.038671 | 5 | -2.068375 | 1.454738 | -0.432508 |
| 5 | 1.505767 | -1.404240 | -1.078093 | 5 | 0.995784 | -0.079722 | 2.143947 |
| 5 | 2.017553 | 0.982920 | -1.038671 | 5 | 2.068375 | -1.454738 | 0.432508 |
| 5 | -1.505767 | 1.404240 | 1.078093 | 5 | -0.995784 | 0.079722 | -2.143947 |
| 7 | -2.430106 | -0.387123 | -0.236995 | 7 | -2.510160 | 0.071549 | -0.272964 |
| 7 | -1.893648 | 0.956201 | -0.298908 | 7 | -1.679854 | -0.782529 | -1.118386 |
| 7 | 1.893648 | -0.956201 | 0.298908 | 7 | 1.679854 | 0.782529 | 1.118386 |
| 7 | 2.430106 | 0.387123 | 0.236995 | 7 | 2.510160 | -0.071549 | 0.272964 |
| 6 | 1.226765 | -2.928392 | -1.349916 | 6 | 0.394815 | 0.551799 | 3.468661 |
| 1 | 2.159612 | -3.507333 | -1.379923 | 1 | 1.204484 | 0.812286 | 4.171418 |
| 1 | 0.605464 | -3.399103 | -0.574916 | 1 | -0.182467 | 1.475680 | 3.303179 |
| 1 | 0.722953 | -3.086075 | -2.307965 | 1 | -0.261129 | -0.161830 | 3.985201 |
| 6 | 2.273159 | 2.513773 | -1.307178 | 6 | 2.686564 | -2.618369 | -0.453278 |
| 1 | 1.925403 | 2.823915 | -2.296577 | 1 | 2.266759 | -3.596042 | -0.181122 |
| 1 | 1.767508 | 3.156276 | -0.572242 | 1 | 2.507396 | -2.472305 | -1.531319 |
| 1 | 3.338988 | 2.767704 | -1.244075 | 1 | 3.779097 | -2.682924 | -0.323806 |
| 6 | 2.670704 | 1.051028 | 1.498076 | 6 | 3.210218 | 0.551769 | -0.837076 |
| 1 | 3.484868 | 0.582609 | 2.065532 | 1 | 3.987281 | 1.253711 | -0.497872 |
| 1 | 2.966193 | 2.077531 | 1.270925 | 1 | 3.703856 | -0.250684 | -1.396389 |
| 1 | 1.776231 | 1.088831 | 2.143890 | 1 | 2.533894 | 1.086154 | -1.526872 |
| 6 | 2.365211 | -1.799480 | 1.378603 | 6 | 2.191734 | 2.124960 | 1.375726 |
| 1 | 3.448593 | -1.964443 | 1.310735 | 1 | 3.173308 | 2.083696 | 1.875149 |
| 1 | 2.130304 | -1.376553 | 2.361584 | 1 | 2.283125 | 2.713122 | 0.453523 |
| 1 | 1.857487 | -2.762974 | 1.293667 | 1 | 1.482590 | 2.633747 | 2.037215 |
| 6 | -2.273159 | -2.513773 | 1.307178 | 6 | -2.686564 | 2.618369 | 0.453278 |
| 1 | -1.767508 | -3.156276 | 0.572242 | 1 | -2.507396 | 2.472305 | 1.531319 |
| 1 | -1.925403 | -2.823915 | 2.296577 | 1 | -2.266759 | 3.596042 | 0.181122 |
| 1 | -3.338988 | -2.767704 | 1.244075 | 1 | -3.779097 | 2.682924 | 0.323806 |
| 6 | -1.226765 | 2.928392 | 1.349916 | 6 | -0.394815 | -0.551799 | -3.468661 |
| 1 | -0.605464 | 3.399103 | 0.574916 | 1 | 0.182467 | -1.475680 | -3.303179 |
| 1 | -2.159612 | 3.507333 | 1.379923 | 1 | -1.204484 | -0.812286 | -4.171418 |
| 1 | -0.722953 | 3.086075 | 2.307965 | 1 | 0.261129 | 0.161830 | -3.985201 |
| 6 | -2.365211 | 1.799480 | -1.378603 | 6 | -2.191734 | -2.124960 | -1.375726 |
| 1 | -3.448593 | 1.964443 | -1.310735 | 1 | -3.173308 | -2.083696 | -1.875149 |
| 1 | -1.857487 | 2.762974 | -1.293667 | 1 | -1.482590 | -2.633747 | -2.037215 |
| 1 | -2.130304 | 1.376553 | -2.361584 | 1 | -2.283125 | -2.713122 | -0.453523 |
| 6 | -2.670704 | -1.051028 | -1.498076 | 6 | -3.210218 | -0.551769 | 0.837076 |
| 1 | -3.484868 | -0.582609 | -2.065532 | 1 | -3.987281 | -1.253711 | 0.497872 |
| 1 | -1.776231 | -1.088831 | -2.143890 | 1 | -2.533894 | -1.086154 | 1.526872 |
| 1 | -2.966193 | -2.077531 | -1.270925 | 1 | -3.703856 | 0.250684 | 1.396389 |
| 24 | 0.000000 | 0.000000 | 0.000000 | 24 | 0.000000 | 0.000000 | 0.000000 |

**Table S15.** Atomic coordinates of the optimized structures for the **Cr-p-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 2.247760 | -0.274526 | 0.415868 | 6 | 2.281074 | -0.338238 | 0.511157 |
| 1 | 2.942027 | 0.512016 | 0.705663 | 1 | 2.998976 | 0.404658 | 0.863612 |
| 1 | -2.942027 | -0.512016 | 0.705663 | 1 | -2.998976 | -0.404658 | 0.863612 |
| 6 | -2.247760 | 0.274526 | 0.415868 | 6 | -2.281074 | 0.338238 | 0.511157 |
| 5 | 1.935299 | -0.691900 | -1.016857 | 5 | 2.042297 | -0.712279 | -0.956366 |
| 5 | -1.935299 | 0.691900 | -1.016857 | 5 | -2.042297 | 0.712279 | -0.956366 |
| 5 | -1.661969 | 1.310729 | 1.334575 | 5 | -1.651313 | 1.417051 | 1.352328 |
| 5 | 1.661969 | -1.310729 | 1.334575 | 5 | 1.651313 | -1.417051 | 1.352328 |
| 7 | 0.991488 | -1.798977 | -0.925951 | 7 | 1.053957 | -1.782474 | -0.954991 |
| 7 | 0.677499 | -2.037576 | 0.469275 | 7 | 0.656845 | -2.060228 | 0.425211 |
| 7 | -0.991488 | 1.798977 | -0.925951 | 7 | -1.053957 | 1.782474 | -0.954991 |
| 7 | -0.677499 | 2.037576 | 0.469275 | 7 | -0.656845 | 2.060228 | 0.425211 |
| 6 | -2.375469 | 0.153529 | -2.431267 | 6 | -2.649082 | 0.144160 | -2.309921 |
| 1 | -3.019751 | 0.879044 | -2.944079 | 1 | -3.414619 | 0.837017 | -2.696844 |
| 1 | -1.528090 | -0.028602 | -3.107658 | 1 | -1.911285 | 0.011831 | -3.116863 |
| 1 | -2.944834 | -0.778822 | -2.364919 | 1 | -3.151522 | -0.820516 | -2.152985 |
| 6 | -1.730620 | 1.642490 | 2.871046 | 6 | -1.746924 | 1.857197 | 2.872560 |
| 1 | -2.342006 | 0.918864 | 3.416640 | 1 | -2.346627 | 1.143179 | 3.452725 |
| 1 | -0.740677 | 1.653078 | 3.349060 | 1 | -0.768379 | 1.950933 | 3.370024 |
| 1 | -2.166135 | 2.634609 | 3.052115 | 1 | -2.239370 | 2.840697 | 2.960228 |
| 6 | 0.000000 | 3.275884 | 0.790265 | 6 | 0.000000 | 3.339680 | 0.670244 |
| 1 | -0.614401 | 4.148756 | 0.530849 | 1 | -0.660978 | 4.182973 | 0.411577 |
| 1 | 0.175928 | 3.284151 | 1.867850 | 1 | 0.231895 | 3.394881 | 1.739147 |
| 1 | 0.968978 | 3.360888 | 0.286284 | 1 | 0.939193 | 3.434957 | 0.110190 |
| 6 | -0.131560 | 2.402689 | -1.911846 | 6 | -0.274501 | 2.371192 | -2.027164 |
| 1 | -0.215425 | 3.497687 | -1.923657 | 1 | -0.352670 | 3.469543 | -2.045580 |
| 1 | 0.928768 | 2.138334 | -1.774425 | 1 | 0.792227 | 2.097550 | -1.985659 |
| 1 | -0.445428 | 2.031113 | -2.890000 | 1 | -0.685347 | 1.992098 | -2.969653 |
| 6 | 2.375469 | -0.153529 | -2.431267 | 6 | 2.649082 | -0.144160 | -2.309921 |
| 1 | 1.528090 | 0.028602 | -3.107658 | 1 | 1.911285 | -0.011831 | -3.116863 |
| 1 | 2.944834 | 0.778822 | -2.364919 | 1 | 3.151522 | 0.820516 | -2.152985 |
| 1 | 3.019751 | -0.879044 | -2.944079 | 1 | 3.414619 | -0.837017 | -2.696844 |
| 6 | 1.730620 | -1.642490 | 2.871046 | 6 | 1.746924 | -1.857197 | 2.872560 |
| 1 | 0.740677 | -1.653078 | 3.349060 | 1 | 0.768379 | -1.950933 | 3.370024 |
| 1 | 2.166135 | -2.634609 | 3.052115 | 1 | 2.239370 | -2.840697 | 2.960228 |
| 1 | 2.342006 | -0.918864 | 3.416640 | 1 | 2.346627 | -1.143179 | 3.452725 |
| 6 | 0.000000 | -3.275884 | 0.790265 | 6 | 0.000000 | -3.339680 | 0.670244 |
| 1 | 0.614401 | -4.148756 | 0.530849 | 1 | 0.660978 | -4.182973 | 0.411577 |
| 1 | -0.175928 | -3.284151 | 1.867850 | 1 | -0.231895 | -3.394881 | 1.739147 |
| 1 | -0.968978 | -3.360888 | 0.286284 | 1 | -0.939193 | -3.434957 | 0.110190 |
| 6 | 0.131560 | -2.402689 | -1.911846 | 6 | 0.274501 | -2.371192 | -2.027164 |
| 1 | 0.215425 | -3.497687 | -1.923657 | 1 | 0.352670 | -3.469543 | -2.045580 |
| 1 | -0.928768 | -2.138334 | -1.774425 | 1 | -0.792227 | -2.097550 | -1.985659 |
| 1 | 0.445428 | -2.031113 | -2.890000 | 1 | 0.685347 | -1.992098 | -2.969653 |
| 24 | 0.000000 | 0.000000 | 0.416668 | 24 | 0.000000 | 0.000000 | 0.457289 |

**Table S16.** Atomic coordinates of the optimized structures for the **Cr-t-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -0.864709 | 1.428821 | -1.566678 | 6 | -0.916396 | 1.427931 | -1.613027 |
| 1 | -0.335244 | 2.293953 | -1.963560 | 1 | -0.429535 | 2.304911 | -2.044407 |
| 1 | 0.335244 | -2.293953 | 1.963560 | 1 | 0.429535 | -2.304911 | 2.044407 |
| 6 | 0.864709 | -1.428821 | 1.566678 | 6 | 0.916396 | -1.427931 | 1.613027 |
| 5 | -1.728415 | 1.442636 | -0.341599 | 5 | -1.776150 | 1.436767 | -0.374550 |
| 5 | 0.788282 | -0.044281 | 2.136020 | 5 | 0.872056 | -0.042051 | 2.194283 |
| 5 | 1.728415 | -1.442636 | 0.341599 | 5 | 1.776150 | -1.436767 | 0.374550 |
| 5 | -0.788282 | 0.044281 | -2.136020 | 5 | -0.872056 | 0.042051 | -2.194283 |
| 7 | -2.052715 | -0.004346 | -0.080012 | 7 | -2.060974 | -0.012590 | -0.089995 |
| 7 | -1.500045 | -0.826279 | -1.134552 | 7 | -1.511224 | -0.837558 | -1.160257 |
| 7 | 1.500045 | 0.826279 | 1.134552 | 7 | 1.511224 | 0.837558 | 1.160257 |
| 7 | 2.052715 | 0.004346 | 0.080012 | 7 | 2.060974 | 0.012590 | 0.089995 |
| 6 | 0.110099 | 0.632180 | 3.385256 | 6 | 0.260736 | 0.601519 | 3.509708 |
| 1 | 0.837937 | 0.824771 | 4.184753 | 1 | 1.060496 | 0.890535 | 4.212151 |
| 1 | -0.361638 | 1.598687 | 3.159589 | 1 | -0.338586 | 1.507394 | 3.323688 |
| 1 | -0.662795 | -0.011540 | 3.817628 | 1 | -0.380889 | -0.117813 | 4.036674 |
| 6 | 2.237342 | -2.531254 | -0.675251 | 6 | 2.350667 | -2.567512 | -0.580958 |
| 1 | 1.652660 | -3.453734 | -0.598928 | 1 | 1.823179 | -3.518056 | -0.420224 |
| 1 | 2.194916 | -2.206133 | -1.724124 | 1 | 2.282085 | -2.328498 | -1.654247 |
| 1 | 3.282281 | -2.807882 | -0.481329 | 1 | 3.415932 | -2.756275 | -0.365549 |
| 6 | 2.954788 | 0.606023 | -0.877511 | 6 | 3.039313 | 0.591150 | -0.820686 |
| 1 | 3.903585 | 0.900071 | -0.410015 | 1 | 3.987269 | 0.813836 | -0.305431 |
| 1 | 3.165183 | -0.152767 | -1.634229 | 1 | 3.236005 | -0.158834 | -1.593929 |
| 1 | 2.512889 | 1.473571 | -1.380506 | 1 | 2.667265 | 1.499457 | -1.311235 |
| 6 | 1.867943 | 2.223797 | 1.199257 | 6 | 1.925186 | 2.229687 | 1.266224 |
| 1 | 2.927821 | 2.351622 | 1.455295 | 1 | 2.989755 | 2.315880 | 1.536294 |
| 1 | 1.652365 | 2.756676 | 0.266271 | 1 | 1.734654 | 2.791199 | 0.342934 |
| 1 | 1.266369 | 2.673159 | 1.992228 | 1 | 1.328898 | 2.678693 | 2.067419 |
| 6 | -2.237342 | 2.531254 | 0.675251 | 6 | -2.350667 | 2.567512 | 0.580958 |
| 1 | -2.194916 | 2.206133 | 1.724124 | 1 | -2.282085 | 2.328498 | 1.654247 |
| 1 | -1.652660 | 3.453734 | 0.598928 | 1 | -1.823179 | 3.518056 | 0.420224 |
| 1 | -3.282281 | 2.807882 | 0.481329 | 1 | -3.415932 | 2.756275 | 0.365549 |
| 6 | -0.110099 | -0.632180 | -3.385256 | 6 | -0.260736 | -0.601519 | -3.509708 |
| 1 | 0.361638 | -1.598687 | -3.159589 | 1 | 0.338586 | -1.507394 | -3.323688 |
| 1 | -0.837937 | -0.824771 | -4.184753 | 1 | -1.060496 | -0.890535 | -4.212151 |
| 1 | 0.662795 | 0.011540 | -3.817628 | 1 | 0.380889 | 0.117813 | -4.036674 |
| 6 | -1.867943 | -2.223797 | -1.199257 | 6 | -1.925186 | -2.229687 | -1.266224 |
| 1 | -2.927821 | -2.351622 | -1.455295 | 1 | -2.989755 | -2.315880 | -1.536294 |
| 1 | -1.266369 | -2.673159 | -1.992228 | 1 | -1.328898 | -2.678693 | -2.067419 |
| 1 | -1.652365 | -2.756676 | -0.266271 | 1 | -1.734654 | -2.791199 | -0.342934 |
| 6 | -2.954788 | -0.606023 | 0.877511 | 6 | -3.039313 | -0.591150 | 0.820686 |
| 1 | -3.903585 | -0.900071 | 0.410015 | 1 | -3.987269 | -0.813836 | 0.305431 |
| 1 | -2.512889 | -1.473571 | 1.380506 | 1 | -2.667265 | -1.499457 | 1.311235 |
| 1 | -3.165183 | 0.152767 | 1.634229 | 1 | -3.236005 | 0.158834 | 1.593929 |
| 24 | 0.000000 | 0.000000 | 0.000000 | 24 | 0.000000 | 0.000000 | 0.000000 |

**Table S17.** Atomic coordinates of the optimized structures for the **Cr-p-36** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -0.656189 | 1.776890 | 1.575834 | 6 | 1.709591 | -0.853054 | -1.556033 |
| 1 | -0.933032 | 1.683642 | 2.623084 | 1 | 1.577066 | -1.154730 | -2.595955 |
| 1 | 0.933032 | -1.683642 | 2.623084 | 1 | -1.577075 | 1.154735 | -2.595962 |
| 6 | 0.656189 | -1.776890 | 1.575834 | 6 | -1.709598 | 0.853057 | -1.556040 |
| 5 | -1.597829 | 1.706466 | 0.405773 | 5 | 1.592170 | -1.753587 | -0.353225 |
| 5 | 1.597829 | -1.706466 | 0.405773 | 5 | -1.592207 | 1.753594 | -0.353232 |
| 5 | -0.697499 | -2.246012 | 1.057231 | 5 | -2.393809 | -0.437746 | -1.088637 |
| 5 | 0.697499 | 2.246012 | 1.057231 | 5 | 2.393837 | 0.437728 | -1.088626 |
| 7 | -0.697499 | 1.719064 | -0.785851 | 7 | 1.713625 | -0.819204 | 0.813583 |
| 7 | 0.595956 | 2.253196 | -0.405914 | 7 | 2.407940 | 0.388723 | 0.371526 |
| 7 | 0.697499 | -1.719064 | -0.785851 | 7 | -1.713644 | 0.819209 | 0.813575 |
| 7 | -0.595956 | -2.253196 | -0.405914 | 7 | -2.407914 | -0.388742 | 0.371515 |
| 6 | 3.143113 | -1.485933 | 0.205900 | 6 | -1.281990 | 3.293762 | -0.135169 |
| 1 | 3.623024 | -2.374898 | -0.225286 | 1 | -2.186238 | 3.823419 | 0.210071 |
| 1 | 3.377053 | -0.655281 | -0.476483 | 1 | -0.498262 | 3.494053 | 0.613538 |
| 1 | 3.649584 | -1.275718 | 1.151586 | 1 | -0.970585 | 3.768401 | -1.075082 |
| 6 | -2.071079 | -2.588426 | 1.744961 | 6 | -2.971134 | -1.691011 | -1.870993 |
| 1 | -1.972500 | -2.707509 | 2.826970 | 1 | -2.905757 | -1.547232 | -2.957498 |
| 1 | -2.811223 | -1.791300 | 1.583394 | 1 | -2.429780 | -2.621138 | -1.632475 |
| 1 | -2.521131 | -3.508671 | 1.351495 | 1 | -4.030631 | -1.868688 | -1.624525 |
| 6 | -1.650460 | -2.146643 | -1.384030 | 6 | -2.574938 | -1.462746 | 1.331615 |
| 1 | -1.476410 | -2.782929 | -2.261620 | 1 | -3.240075 | -1.183427 | 2.163333 |
| 1 | -2.575623 | -2.474411 | -0.904849 | 1 | -3.035911 | -2.302174 | 0.799331 |
| 1 | -1.802829 | -1.110528 | -1.740894 | 1 | -1.618449 | -1.815585 | 1.760355 |
| 6 | 1.103974 | -1.948328 | -2.155805 | 6 | -1.988355 | 1.245635 | 2.180876 |
| 1 | 1.137621 | -3.021658 | -2.387245 | 1 | -3.064144 | 1.435261 | 2.329337 |
| 1 | 0.438333 | -1.457920 | -2.877509 | 1 | -1.656182 | 0.505878 | 2.922309 |
| 1 | 2.108448 | -1.536616 | -2.281122 | 1 | -1.444362 | 2.179891 | 2.358641 |
| 6 | -3.143113 | 1.485933 | 0.205900 | 6 | 1.281918 | -3.293748 | -0.135163 |
| 1 | -3.377053 | 0.655281 | -0.476483 | 1 | 0.498189 | -3.494024 | 0.613549 |
| 1 | -3.649584 | 1.275718 | 1.151586 | 1 | 0.970499 | -3.768379 | -1.075075 |
| 1 | -3.623024 | 2.374898 | -0.225286 | 1 | 2.186155 | -3.823426 | 0.210073 |
| 6 | 2.071079 | 2.588426 | 1.744961 | 6 | 2.971199 | 1.690977 | -1.870980 |
| 1 | 2.811223 | 1.791300 | 1.583394 | 1 | 2.429822 | 2.621104 | -1.632511 |
| 1 | 2.521131 | 3.508671 | 1.351495 | 1 | 4.030681 | 1.868671 | -1.624461 |
| 1 | 1.972500 | 2.707509 | 2.826970 | 1 | 2.905878 | 1.547175 | -2.957485 |
| 6 | 1.650460 | 2.146643 | -1.384030 | 6 | 2.574975 | 1.462728 | 1.331623 |
| 1 | 1.476410 | 2.782929 | -2.261620 | 1 | 3.240095 | 1.183397 | 2.163352 |
| 1 | 2.575623 | 2.474411 | -0.904849 | 1 | 3.035974 | 2.302144 | 0.799343 |
| 1 | 1.802829 | 1.110528 | -1.740894 | 1 | 1.618488 | 1.815591 | 1.760350 |
| 6 | -1.103974 | 1.948328 | -2.155805 | 6 | 1.988323 | -1.245640 | 2.180883 |
| 1 | -1.137621 | 3.021658 | -2.387245 | 1 | 3.064104 | -1.435324 | 2.329337 |
| 1 | -0.438333 | 1.457920 | -2.877509 | 1 | 1.656197 | -0.505862 | 2.922316 |
| 1 | -2.108448 | 1.536616 | -2.281122 | 1 | 1.444280 | -2.179867 | 2.358657 |
| 24 | 0.000000 | 0.000000 | 0.393720 | 24 | 0.000003 | 0.000022 | -0.338307 |

**Table S18.** Atomic coordinates of the optimized structures for the **Cr-t-72** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.479641 | 1.806934 | 1.442007 | 6 | 0.459664 | 1.877474 | 1.422899 |
| 1 | -0.034648 | 2.026226 | 2.375021 | 1 | -0.051936 | 2.131501 | 2.352343 |
| 1 | 0.034648 | -2.026226 | 2.375021 | 1 | 0.051936 | -2.131501 | 2.352343 |
| 6 | -0.479641 | -1.806934 | 1.442007 | 6 | -0.459664 | -1.877474 | 1.422899 |
| 5 | 0.000000 | 2.219260 | 0.072910 | 5 | 0.000000 | 2.279577 | 0.039788 |
| 5 | 0.000000 | -2.219260 | 0.072910 | 5 | 0.000000 | -2.279577 | 0.039788 |
| 5 | -1.746385 | -1.018811 | 1.340063 | 5 | -1.755724 | -1.123409 | 1.336731 |
| 5 | 1.746385 | 1.018811 | 1.340063 | 5 | 1.755724 | 1.123409 | 1.336731 |
| 7 | 0.921148 | 1.495720 | -0.879972 | 7 | 0.908669 | 1.525037 | -0.894049 |
| 7 | 1.917816 | 0.763518 | -0.128615 | 7 | 1.922041 | 0.811209 | -0.120752 |
| 7 | -0.921148 | -1.495720 | -0.879972 | 7 | -0.908669 | -1.525037 | -0.894049 |
| 7 | -1.917816 | -0.763518 | -0.128615 | 7 | -1.922041 | -0.811209 | -0.120752 |
| 6 | 1.133577 | -3.149579 | -0.504432 | 6 | 1.109907 | -3.263239 | -0.531399 |
| 1 | 0.761595 | -4.159357 | -0.724605 | 1 | 0.668876 | -4.236577 | -0.805455 |
| 1 | 1.586614 | -2.781051 | -1.437260 | 1 | 1.635542 | -2.890753 | -1.426111 |
| 1 | 1.947957 | -3.270889 | 0.217590 | 1 | 1.871904 | -3.467850 | 0.233413 |
| 6 | -2.731038 | -0.306508 | 2.335453 | 6 | -2.786751 | -0.539810 | 2.387357 |
| 1 | -2.373643 | -0.367839 | 3.366604 | 1 | -2.420222 | -0.681712 | 3.412551 |
| 1 | -2.858058 | 0.760657 | 2.103099 | 1 | -2.975386 | 0.537307 | 2.251594 |
| 1 | -3.734478 | -0.752115 | 2.313316 | 1 | -3.762514 | -1.049171 | 2.315530 |
| 6 | -2.986414 | -0.103196 | -0.842855 | 6 | -3.076412 | -0.248117 | -0.804500 |
| 1 | -3.677098 | -0.822203 | -1.303047 | 1 | -3.745054 | -1.032578 | -1.194116 |
| 1 | -3.538945 | 0.489542 | -0.110968 | 1 | -3.627522 | 0.339186 | -0.062509 |
| 1 | -2.615095 | 0.581421 | -1.616505 | 1 | -2.792762 | 0.425093 | -1.624620 |
| 6 | -1.104461 | -1.660531 | -2.303185 | 6 | -1.133364 | -1.743091 | -2.314861 |
| 1 | -1.959052 | -2.311179 | -2.530015 | 1 | -2.002603 | -2.396165 | -2.490289 |
| 1 | -1.238850 | -0.706514 | -2.828804 | 1 | -1.273422 | -0.806982 | -2.873714 |
| 1 | -0.200979 | -2.139628 | -2.688658 | 1 | -0.244492 | -2.249903 | -2.706335 |
| 6 | -1.133577 | 3.149579 | -0.504432 | 6 | -1.109907 | 3.263239 | -0.531399 |
| 1 | -1.586614 | 2.781051 | -1.437260 | 1 | -1.635542 | 2.890753 | -1.426111 |
| 1 | -1.947957 | 3.270889 | 0.217590 | 1 | -1.871904 | 3.467850 | 0.233413 |
| 1 | -0.761595 | 4.159357 | -0.724605 | 1 | -0.668876 | 4.236577 | -0.805455 |
| 6 | 2.731038 | 0.306508 | 2.335453 | 6 | 2.786751 | 0.539810 | 2.387357 |
| 1 | 2.858058 | -0.760657 | 2.103099 | 1 | 2.975386 | -0.537307 | 2.251594 |
| 1 | 3.734478 | 0.752115 | 2.313316 | 1 | 3.762514 | 1.049171 | 2.315530 |
| 1 | 2.373643 | 0.367839 | 3.366604 | 1 | 2.420222 | 0.681712 | 3.412551 |
| 6 | 2.986414 | 0.103196 | -0.842855 | 6 | 3.076412 | 0.248117 | -0.804500 |
| 1 | 3.677098 | 0.822203 | -1.303047 | 1 | 3.745054 | 1.032578 | -1.194116 |
| 1 | 3.538945 | -0.489542 | -0.110968 | 1 | 3.627522 | -0.339186 | -0.062509 |
| 1 | 2.615095 | -0.581421 | -1.616505 | 1 | 2.792762 | -0.425093 | -1.624620 |
| 6 | 1.104461 | 1.660531 | -2.303185 | 6 | 1.133364 | 1.743091 | -2.314861 |
| 1 | 1.959052 | 2.311179 | -2.530015 | 1 | 2.002603 | 2.396165 | -2.490289 |
| 1 | 1.238850 | 0.706514 | -2.828804 | 1 | 1.273422 | 0.806982 | -2.873714 |
| 1 | 0.200979 | 2.139628 | -2.688658 | 1 | 0.244492 | 2.249903 | -2.706335 |
| 24 | 0.000000 | 0.000000 | 0.174796 | 24 | 0.000000 | 0.000000 | 0.156813 |

**Table S19.** Atomic coordinates of the optimized structures for the **Mn-x-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 2.172261 | -0.280404 | 0.722179 | 6 | 2.149245 | -0.447693 | 0.624583 |
| 1 | 2.763700 | 0.485253 | 1.220260 | 1 | 2.806757 | 0.311721 | 1.052817 |
| 1 | -2.763700 | -0.485253 | 1.220260 | 1 | -2.806757 | -0.311721 | 1.052817 |
| 6 | -2.172261 | 0.280404 | 0.722179 | 6 | -2.149245 | 0.447693 | 0.624583 |
| 5 | 2.006142 | -0.435783 | -0.778095 | 5 | 1.964337 | -0.722797 | -0.866628 |
| 5 | -2.006142 | 0.435783 | -0.778095 | 5 | -1.964337 | 0.722797 | -0.866628 |
| 5 | -1.631028 | 1.552783 | 1.364282 | 5 | -1.607617 | 1.681158 | 1.360918 |
| 5 | 1.631028 | -1.552783 | 1.364282 | 5 | 1.607617 | -1.681158 | 1.360918 |
| 7 | 1.113149 | -1.592318 | -0.955841 | 7 | 1.041856 | -1.861303 | -0.945194 |
| 7 | 0.980766 | -2.296916 | 0.283860 | 7 | 0.901093 | -2.465049 | 0.354125 |
| 7 | -1.113149 | 1.592318 | -0.955841 | 7 | -1.041856 | 1.861303 | -0.945194 |
| 7 | -0.980766 | 2.296916 | 0.283860 | 7 | -0.901093 | 2.465049 | 0.354125 |
| 6 | -2.497357 | -0.380049 | -2.033192 | 6 | -2.524583 | 0.018745 | -2.176665 |
| 1 | -3.335275 | 0.127896 | -2.528700 | 1 | -3.282715 | 0.656312 | -2.661822 |
| 1 | -1.721941 | -0.506310 | -2.801579 | 1 | -1.754538 | -0.185714 | -2.937647 |
| 1 | -2.856312 | -1.378595 | -1.763362 | 1 | -3.017911 | -0.933787 | -1.939010 |
| 6 | -1.553089 | 2.088596 | 2.845067 | 6 | -1.642862 | 2.130933 | 2.885731 |
| 1 | -2.150137 | 1.482251 | 3.531502 | 1 | -2.188575 | 1.403565 | 3.501784 |
| 1 | -0.526134 | 2.089200 | 3.237058 | 1 | -0.641009 | 2.248094 | 3.329862 |
| 1 | -1.910599 | 3.122808 | 2.929650 | 1 | -2.153292 | 3.101202 | 3.001010 |
| 6 | 0.000000 | 3.352499 | 0.351199 | 6 | 0.000000 | 3.591087 | 0.507031 |
| 1 | -0.239933 | 4.189286 | -0.317321 | 1 | -0.307923 | 4.458109 | -0.097719 |
| 1 | 0.005919 | 3.728481 | 1.376162 | 1 | -0.028419 | 3.888004 | 1.560934 |
| 1 | 1.017454 | 3.002080 | 0.110056 | 1 | 1.043548 | 3.342347 | 0.250032 |
| 6 | -0.836453 | 2.326035 | -2.166674 | 6 | -0.723092 | 2.668314 | -2.108634 |
| 1 | -1.520175 | 3.177525 | -2.295344 | 1 | -1.380593 | 3.550663 | -2.192512 |
| 1 | 0.194338 | 2.699099 | -2.206196 | 1 | 0.322115 | 3.008709 | -2.110583 |
| 1 | -0.979593 | 1.643355 | -3.007470 | 1 | -0.876818 | 2.043648 | -2.995158 |
| 6 | 2.497357 | 0.380049 | -2.033192 | 6 | 2.524583 | -0.018745 | -2.176665 |
| 1 | 1.721941 | 0.506310 | -2.801579 | 1 | 1.754538 | 0.185714 | -2.937647 |
| 1 | 2.856312 | 1.378595 | -1.763362 | 1 | 3.017911 | 0.933787 | -1.939010 |
| 1 | 3.335275 | -0.127896 | -2.528700 | 1 | 3.282715 | -0.656312 | -2.661822 |
| 6 | 1.553089 | -2.088596 | 2.845067 | 6 | 1.642862 | -2.130933 | 2.885731 |
| 1 | 0.526134 | -2.089200 | 3.237058 | 1 | 0.641009 | -2.248094 | 3.329862 |
| 1 | 1.910599 | -3.122808 | 2.929650 | 1 | 2.153292 | -3.101202 | 3.001010 |
| 1 | 2.150137 | -1.482251 | 3.531502 | 1 | 2.188575 | -1.403565 | 3.501784 |
| 6 | 0.000000 | -3.352499 | 0.351199 | 6 | 0.000000 | -3.591087 | 0.507031 |
| 1 | 0.239933 | -4.189286 | -0.317321 | 1 | 0.307923 | -4.458109 | -0.097719 |
| 1 | -0.005919 | -3.728481 | 1.376162 | 1 | 0.028419 | -3.888004 | 1.560934 |
| 1 | -1.017454 | -3.002080 | 0.110056 | 1 | -1.043548 | -3.342347 | 0.250032 |
| 6 | 0.836453 | -2.326035 | -2.166674 | 6 | 0.723092 | -2.668314 | -2.108634 |
| 1 | 1.520175 | -3.177525 | -2.295344 | 1 | 1.380593 | -3.550663 | -2.192512 |
| 1 | -0.194338 | -2.699099 | -2.206196 | 1 | -0.322115 | -3.008709 | -2.110583 |
| 1 | 0.979593 | -1.643355 | -3.007470 | 1 | 0.876818 | -2.043648 | -2.995158 |
| 25 | 0.000000 | 0.000000 | 0.478140 | 25 | 0.000000 | 0.000000 | 0.440941 |

**Table S20.** Atomic coordinates of the optimized structures for the **Mn-d-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.104816 | 0.327622 | -1.861616 | 6 | 1.236736 | -0.242334 | 1.853952 |
| 1 | 0.735060 | 0.174714 | -2.874879 | 1 | 0.905107 | -0.142436 | 2.889264 |
| 1 | -0.735060 | -0.174714 | 2.874879 | 1 | -0.905107 | 0.142436 | -2.889264 |
| 6 | -1.104816 | -0.327622 | 1.861616 | 6 | -1.236736 | 0.242334 | -1.853952 |
| 5 | 1.907988 | -0.664028 | -1.077701 | 5 | 1.931986 | 0.831394 | 1.060182 |
| 5 | -0.979514 | -1.613356 | 1.073068 | 5 | -1.247132 | 1.534403 | -1.057476 |
| 5 | -1.907988 | 0.664028 | 1.077701 | 5 | -1.931986 | -0.831394 | -1.060182 |
| 5 | 0.979514 | 1.613356 | -1.073068 | 5 | 1.247132 | -1.534403 | 1.057476 |
| 7 | 2.012592 | -0.073544 | 0.291762 | 7 | 2.012539 | 0.278927 | -0.323979 |
| 7 | 1.522854 | 1.274301 | 0.282666 | 7 | 1.657649 | -1.123272 | -0.316540 |
| 7 | -1.522854 | -1.274301 | -0.282666 | 7 | -1.657649 | 1.123272 | 0.316540 |
| 7 | -2.012592 | 0.073544 | -0.291762 | 7 | -2.012539 | -0.278927 | 0.323979 |
| 6 | -0.448068 | -3.065239 | 1.371932 | 6 | -0.920688 | 3.050463 | -1.397487 |
| 1 | -1.259091 | -3.733418 | 1.690686 | 1 | -1.848446 | 3.626055 | -1.554306 |
| 1 | 0.032901 | -3.549689 | 0.511456 | 1 | -0.349881 | 3.572890 | -0.613550 |
| 1 | 0.283037 | -3.059861 | 2.187707 | 1 | -0.343670 | 3.125044 | -2.329995 |
| 6 | -2.435708 | 2.126537 | 1.311518 | 6 | -2.406278 | -2.314326 | -1.353615 |
| 1 | -2.078311 | 2.540249 | 2.259199 | 1 | -2.105566 | -2.635771 | -2.359890 |
| 1 | -2.127593 | 2.819869 | 0.516266 | 1 | -2.001658 | -3.045736 | -0.635418 |
| 1 | -3.532627 | 2.163637 | 1.341283 | 1 | -3.504950 | -2.395648 | -1.302688 |
| 6 | -2.696113 | 0.565580 | -1.468910 | 6 | -2.682985 | -0.837209 | 1.490217 |
| 1 | -3.660429 | 0.061988 | -1.616453 | 1 | -3.706113 | -0.442077 | 1.594943 |
| 1 | -2.882306 | 1.629151 | -1.306770 | 1 | -2.743235 | -1.919591 | 1.336691 |
| 1 | -2.084988 | 0.460370 | -2.371452 | 1 | -2.121991 | -0.653298 | 2.414275 |
| 6 | -1.729319 | -2.102650 | -1.451635 | 6 | -1.996721 | 1.947726 | 1.467915 |
| 1 | -2.790707 | -2.347205 | -1.588440 | 1 | -3.087690 | 2.046148 | 1.584365 |
| 1 | -1.337031 | -1.637735 | -2.362438 | 1 | -1.558663 | 1.562377 | 2.397016 |
| 1 | -1.181328 | -3.031814 | -1.281846 | 1 | -1.580400 | 2.943025 | 1.280470 |
| 6 | 2.435708 | -2.126537 | -1.311518 | 6 | 2.406278 | 2.314326 | 1.353615 |
| 1 | 2.127593 | -2.819869 | -0.516266 | 1 | 2.001658 | 3.045736 | 0.635418 |
| 1 | 2.078311 | -2.540249 | -2.259199 | 1 | 2.105566 | 2.635771 | 2.359890 |
| 1 | 3.532627 | -2.163637 | -1.341283 | 1 | 3.504950 | 2.395648 | 1.302688 |
| 6 | 0.448068 | 3.065239 | -1.371932 | 6 | 0.920688 | -3.050463 | 1.397487 |
| 1 | -0.032901 | 3.549689 | -0.511456 | 1 | 0.349881 | -3.572890 | 0.613550 |
| 1 | 1.259091 | 3.733418 | -1.690686 | 1 | 1.848446 | -3.626055 | 1.554306 |
| 1 | -0.283037 | 3.059861 | -2.187707 | 1 | 0.343670 | -3.125044 | 2.329995 |
| 6 | 1.729319 | 2.102650 | 1.451635 | 6 | 1.996721 | -1.947726 | -1.467915 |
| 1 | 2.790707 | 2.347205 | 1.588440 | 1 | 3.087690 | -2.046148 | -1.584365 |
| 1 | 1.181328 | 3.031814 | 1.281846 | 1 | 1.580400 | -2.943025 | -1.280470 |
| 1 | 1.337031 | 1.637735 | 2.362438 | 1 | 1.558663 | -1.562377 | -2.397016 |
| 6 | 2.696113 | -0.565580 | 1.468910 | 6 | 2.682985 | 0.837209 | -1.490217 |
| 1 | 3.660429 | -0.061988 | 1.616453 | 1 | 3.706113 | 0.442077 | -1.594943 |
| 1 | 2.084988 | -0.460370 | 2.371452 | 1 | 2.121991 | 0.653298 | -2.414275 |
| 1 | 2.882306 | -1.629151 | 1.306770 | 1 | 2.743235 | 1.919591 | -1.336691 |
| 25 | 0.000000 | 0.000000 | 0.000000 | 25 | 0.000000 | 0.000000 | 0.000000 |

**Table S21.** Atomic coordinates of the optimized structures for the **Mn-q-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.165688 | 0.197668 | -1.825806 | 6 | -1.263930 | 0.166726 | 1.797626 |
| 1 | 0.784011 | -0.030985 | -2.819490 | 1 | -0.927927 | -0.033547 | 2.816502 |
| 1 | -0.784011 | 0.030985 | 2.819490 | 1 | 0.927857 | 0.033579 | -2.816474 |
| 6 | -1.165688 | -0.197668 | 1.825806 | 6 | 1.263887 | -0.166706 | -1.797609 |
| 5 | 2.115236 | -0.690473 | -1.034375 | 5 | -2.220587 | -0.731294 | 0.999952 |
| 5 | -1.060339 | -1.530770 | 1.115380 | 5 | 1.196152 | -1.504103 | -1.086054 |
| 5 | -2.115236 | 0.690473 | 1.034375 | 5 | 2.220570 | 0.731301 | -0.999953 |
| 5 | 1.060339 | 1.530770 | -1.115380 | 5 | -1.196178 | 1.504115 | 1.086057 |
| 7 | 2.415055 | 0.019185 | 0.213448 | 7 | -2.469418 | -0.051747 | -0.267508 |
| 7 | 1.616548 | 1.228602 | 0.254869 | 7 | -1.673232 | 1.174745 | -0.306335 |
| 7 | -1.616548 | -1.228602 | -0.254869 | 7 | 1.673243 | -1.174749 | 0.306330 |
| 7 | -2.415055 | -0.019185 | -0.213448 | 7 | 2.469437 | 0.051739 | 0.267492 |
| 6 | -0.516894 | -2.968530 | 1.456288 | 6 | 0.737464 | -2.971721 | -1.480008 |
| 1 | -1.334237 | -3.650859 | 1.726644 | 1 | 1.614888 | -3.618539 | -1.649762 |
| 1 | 0.019943 | -3.448275 | 0.626683 | 1 | 0.120222 | -3.470721 | -0.716224 |
| 1 | 0.165668 | -2.948366 | 2.312124 | 1 | 0.163027 | -2.965026 | -2.416668 |
| 6 | -2.688125 | 2.137580 | 1.262190 | 6 | 2.849490 | 2.156382 | -1.298194 |
| 1 | -2.426640 | 2.538038 | 2.245510 | 1 | 2.609745 | 2.498042 | -2.313955 |
| 1 | -2.309095 | 2.848069 | 0.513869 | 1 | 2.485131 | 2.926304 | -0.597988 |
| 1 | -3.781712 | 2.166619 | 1.177773 | 1 | 3.947385 | 2.142758 | -1.205145 |
| 6 | -2.829928 | 0.526631 | -1.485627 | 6 | 2.953625 | 0.585745 | 1.528521 |
| 1 | -3.581512 | -0.101469 | -1.980872 | 1 | 3.702757 | -0.070640 | 1.997227 |
| 1 | -3.279080 | 1.502617 | -1.289749 | 1 | 3.436201 | 1.544368 | 1.307734 |
| 1 | -1.986157 | 0.671464 | -2.180042 | 1 | 2.143555 | 0.767692 | 2.254665 |
| 6 | -1.923762 | -2.183989 | -1.298698 | 6 | 2.031941 | -2.150988 | 1.328082 |
| 1 | -2.937889 | -2.586218 | -1.176423 | 1 | 3.067570 | -2.500137 | 1.187486 |
| 1 | -1.828133 | -1.745939 | -2.297728 | 1 | 1.920794 | -1.745092 | 2.341619 |
| 1 | -1.207719 | -3.004733 | -1.217082 | 1 | 1.355896 | -3.005901 | 1.224306 |
| 6 | 2.688125 | -2.137580 | -1.262190 | 6 | -2.849507 | -2.156378 | 1.298188 |
| 1 | 2.309095 | -2.848069 | -0.513869 | 1 | -2.485115 | -2.926302 | 0.598002 |
| 1 | 2.426640 | -2.538038 | -2.245510 | 1 | -2.609791 | -2.498023 | 2.313961 |
| 1 | 3.781712 | -2.166619 | -1.177773 | 1 | -3.947398 | -2.142766 | 1.205102 |
| 6 | 0.516894 | 2.968530 | -1.456288 | 6 | -0.737502 | 2.971738 | 1.480010 |
| 1 | -0.019943 | 3.448275 | -0.626683 | 1 | -0.120256 | 3.470741 | 0.716231 |
| 1 | 1.334237 | 3.650859 | -1.726644 | 1 | -1.614933 | 3.618549 | 1.649753 |
| 1 | -0.165668 | 2.948366 | -2.312124 | 1 | -0.163074 | 2.965050 | 2.416676 |
| 6 | 1.923762 | 2.183989 | 1.298698 | 6 | -2.031891 | 2.150966 | -1.328116 |
| 1 | 2.937889 | 2.586218 | 1.176423 | 1 | -3.067521 | 2.500121 | -1.187563 |
| 1 | 1.207719 | 3.004733 | 1.217082 | 1 | -1.355845 | 3.005878 | -1.224333 |
| 1 | 1.828133 | 1.745939 | 2.297728 | 1 | -1.920710 | 1.745050 | -2.341641 |
| 6 | 2.829928 | -0.526631 | 1.485627 | 6 | -2.953589 | -0.585760 | -1.528539 |
| 1 | 3.581512 | 0.101469 | 1.980872 | 1 | -3.702719 | 0.070620 | -1.997256 |
| 1 | 1.986157 | -0.671464 | 2.180042 | 1 | -2.143511 | -0.767706 | -2.254673 |
| 1 | 3.279080 | -1.502617 | 1.289749 | 1 | -3.436163 | -1.544384 | -1.307755 |
| 25 | 0.000000 | 0.000000 | 0.000000 | 25 | 0.000000 | 0.000000 | 0.000022 |

**Table S22.** Atomic coordinates of the optimized structures for the **Mn-q-36** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.062386 | 1.721045 | 1.583867 | 6 | 0.906062 | -1.465499 | 1.583074 |
| 1 | -0.218863 | 1.664095 | 2.632184 | 1 | 1.078428 | -1.267883 | 2.641349 |
| 1 | 0.218863 | -1.664095 | 2.632184 | 1 | -1.078428 | 1.267883 | 2.641349 |
| 6 | -0.062386 | -1.721045 | 1.583867 | 6 | -0.906062 | 1.465499 | 1.583074 |
| 5 | -0.877559 | 1.984928 | 0.420612 | 5 | 1.872660 | -1.154999 | 0.450837 |
| 5 | 0.877559 | -1.984928 | 0.420612 | 5 | -1.872660 | 1.154999 | 0.450837 |
| 5 | -1.493993 | -1.787656 | 1.063787 | 5 | 0.164203 | 2.417292 | 1.024999 |
| 5 | 1.493993 | 1.787656 | 1.063787 | 5 | -0.164203 | -2.417292 | 1.024999 |
| 7 | 0.000000 | 1.786136 | -0.783336 | 7 | 1.080299 | -1.487748 | -0.782739 |
| 7 | 1.398306 | 1.869609 | -0.394216 | 7 | 0.000000 | -2.411294 | -0.424047 |
| 7 | 0.000000 | -1.786136 | -0.783336 | 7 | -1.080299 | 1.487748 | -0.782739 |
| 7 | -1.398306 | -1.869609 | -0.394216 | 7 | 0.000000 | 2.411294 | -0.424047 |
| 6 | 2.400768 | -2.342269 | 0.240409 | 6 | -3.354887 | 0.594382 | 0.364398 |
| 1 | 2.535513 | -3.391632 | -0.056225 | 1 | -4.067201 | 1.412908 | 0.164148 |
| 1 | 2.909345 | -1.740719 | -0.527463 | 1 | -3.510411 | -0.159286 | -0.424258 |
| 1 | 2.956571 | -2.205314 | 1.172397 | 1 | -3.653752 | 0.139218 | 1.318376 |
| 6 | -2.903789 | -1.663949 | 1.746744 | 6 | 1.335306 | 3.233075 | 1.712832 |
| 1 | -2.856546 | -1.826360 | 2.826538 | 1 | 1.198161 | 3.287464 | 2.800940 |
| 1 | -3.321304 | -0.657795 | 1.599350 | 1 | 2.313061 | 2.754859 | 1.535998 |
| 1 | -3.640190 | -2.366294 | 1.336912 | 1 | 1.410276 | 4.264159 | 1.332479 |
| 6 | -2.360491 | -1.452571 | -1.384303 | 6 | 0.962078 | 2.743706 | -1.457616 |
| 1 | -2.415422 | -2.144909 | -2.234540 | 1 | 0.514899 | 3.330681 | -2.274575 |
| 1 | -3.340004 | -1.424830 | -0.902128 | 1 | 1.743834 | 3.353631 | -0.991381 |
| 1 | -2.148540 | -0.442823 | -1.781123 | 1 | 1.440827 | 1.849569 | -1.896817 |
| 6 | 0.308314 | -2.181556 | -2.140212 | 6 | -1.654248 | 1.670996 | -2.109345 |
| 1 | 0.004944 | -3.220495 | -2.327226 | 1 | -2.059955 | 2.689458 | -2.224592 |
| 1 | -0.174304 | -1.536106 | -2.884882 | 1 | -0.923769 | 1.488708 | -2.909635 |
| 1 | 1.390781 | -2.109894 | -2.271523 | 1 | -2.476538 | 0.956168 | -2.222762 |
| 6 | -2.400768 | 2.342269 | 0.240409 | 6 | 3.354887 | -0.594382 | 0.364398 |
| 1 | -2.909345 | 1.740719 | -0.527463 | 1 | 3.510411 | 0.159286 | -0.424258 |
| 1 | -2.956571 | 2.205314 | 1.172397 | 1 | 3.653752 | -0.139218 | 1.318376 |
| 1 | -2.535513 | 3.391632 | -0.056225 | 1 | 4.067201 | -1.412908 | 0.164148 |
| 6 | 2.903789 | 1.663949 | 1.746744 | 6 | -1.335306 | -3.233075 | 1.712832 |
| 1 | 3.321304 | 0.657795 | 1.599350 | 1 | -2.313061 | -2.754859 | 1.535998 |
| 1 | 3.640190 | 2.366294 | 1.336912 | 1 | -1.410276 | -4.264159 | 1.332479 |
| 1 | 2.856546 | 1.826360 | 2.826538 | 1 | -1.198161 | -3.287464 | 2.800940 |
| 6 | 2.360491 | 1.452571 | -1.384303 | 6 | -0.962078 | -2.743706 | -1.457616 |
| 1 | 2.415422 | 2.144909 | -2.234540 | 1 | -0.514899 | -3.330681 | -2.274575 |
| 1 | 3.340004 | 1.424830 | -0.902128 | 1 | -1.743834 | -3.353631 | -0.991381 |
| 1 | 2.148540 | 0.442823 | -1.781123 | 1 | -1.440827 | -1.849569 | -1.896817 |
| 6 | -0.308314 | 2.181556 | -2.140212 | 6 | 1.654248 | -1.670996 | -2.109345 |
| 1 | -0.004944 | 3.220495 | -2.327226 | 1 | 2.059955 | -2.689458 | -2.224592 |
| 1 | 0.174304 | 1.536106 | -2.884882 | 1 | 0.923769 | -1.488708 | -2.909635 |
| 1 | -1.390781 | 2.109894 | -2.271523 | 1 | 2.476538 | -0.956168 | -2.222762 |
| 25 | 0.000000 | 0.000000 | 0.316754 | 25 | 0.000000 | 0.000000 | 0.292720 |

**Table S23.** Atomic coordinates of the optimized structures for the **Mn-q-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 2.139740 | -0.075795 | 0.410555 | 6 | 2.244501 | -0.208689 | 0.519105 |
| 1 | 2.747704 | 0.785388 | 0.682630 | 1 | 2.931680 | 0.561893 | 0.871716 |
| 1 | -2.747704 | -0.785388 | 0.682630 | 1 | -2.931680 | -0.561893 | 0.871716 |
| 6 | -2.139740 | 0.075795 | 0.410555 | 6 | -2.244501 | 0.208689 | 0.519105 |
| 5 | 1.999861 | -0.642869 | -0.996916 | 5 | 2.012360 | -0.567147 | -0.950126 |
| 5 | -1.999861 | 0.642869 | -0.996916 | 5 | -2.012360 | 0.567147 | -0.950126 |
| 5 | -1.523391 | 1.064537 | 1.388801 | 5 | -1.632513 | 1.307267 | 1.350879 |
| 5 | 1.523391 | -1.064537 | 1.388801 | 5 | 1.632513 | -1.307267 | 1.350879 |
| 7 | 1.120311 | -1.805690 | -0.888544 | 7 | 1.022633 | -1.639395 | -0.955556 |
| 7 | 0.682595 | -1.930189 | 0.492948 | 7 | 0.677264 | -1.985722 | 0.419380 |
| 7 | -1.120311 | 1.805690 | -0.888544 | 7 | -1.022633 | 1.639395 | -0.955556 |
| 7 | -0.682595 | 1.930189 | 0.492948 | 7 | -0.677264 | 1.985722 | 0.419380 |
| 6 | -2.491514 | 0.173124 | -2.417459 | 6 | -2.614852 | -0.011812 | -2.299798 |
| 1 | -3.079228 | 0.949495 | -2.923091 | 1 | -3.410942 | 0.656122 | -2.668830 |
| 1 | -1.653116 | -0.056518 | -3.092224 | 1 | -1.884522 | -0.110362 | -3.117949 |
| 1 | -3.117348 | -0.722616 | -2.367152 | 1 | -3.080764 | -0.994791 | -2.143720 |
| 6 | -1.575323 | 1.321512 | 2.938769 | 6 | -1.675131 | 1.707284 | 2.886996 |
| 1 | -1.974931 | 0.454816 | 3.473969 | 1 | -2.265995 | 0.984001 | 3.464834 |
| 1 | -0.590932 | 1.538099 | 3.374577 | 1 | -0.679491 | 1.770243 | 3.355633 |
| 1 | -2.221931 | 2.173925 | 3.189250 | 1 | -2.148474 | 2.694486 | 3.021977 |
| 6 | 0.000000 | 3.151477 | 0.859742 | 6 | 0.000000 | 3.255447 | 0.646540 |
| 1 | -0.663557 | 4.020683 | 0.759015 | 1 | -0.640435 | 4.108982 | 0.369960 |
| 1 | 0.297799 | 3.058478 | 1.906034 | 1 | 0.219028 | 3.320584 | 1.717515 |
| 1 | 0.902214 | 3.318080 | 0.261533 | 1 | 0.948685 | 3.318937 | 0.099214 |
| 6 | -0.308153 | 2.448407 | -1.894261 | 6 | -0.356170 | 2.333542 | -2.039900 |
| 1 | -0.362943 | 3.543060 | -1.833963 | 1 | -0.593901 | 3.409148 | -2.054504 |
| 1 | 0.752129 | 2.153276 | -1.840348 | 1 | 0.737028 | 2.213169 | -2.014329 |
| 1 | -0.694728 | 2.143357 | -2.869292 | 1 | -0.723780 | 1.896652 | -2.975016 |
| 6 | 2.491514 | -0.173124 | -2.417459 | 6 | 2.614852 | 0.011812 | -2.299798 |
| 1 | 1.653116 | 0.056518 | -3.092224 | 1 | 1.884522 | 0.110362 | -3.117949 |
| 1 | 3.117348 | 0.722616 | -2.367152 | 1 | 3.080764 | 0.994791 | -2.143720 |
| 1 | 3.079228 | -0.949495 | -2.923091 | 1 | 3.410942 | -0.656122 | -2.668830 |
| 6 | 1.575323 | -1.321512 | 2.938769 | 6 | 1.675131 | -1.707284 | 2.886996 |
| 1 | 0.590932 | -1.538099 | 3.374577 | 1 | 0.679491 | -1.770243 | 3.355633 |
| 1 | 2.221931 | -2.173925 | 3.189250 | 1 | 2.148474 | -2.694486 | 3.021977 |
| 1 | 1.974931 | -0.454816 | 3.473969 | 1 | 2.265995 | -0.984001 | 3.464834 |
| 6 | 0.000000 | -3.151477 | 0.859742 | 6 | 0.000000 | -3.255447 | 0.646540 |
| 1 | 0.663557 | -4.020683 | 0.759015 | 1 | 0.640435 | -4.108982 | 0.369960 |
| 1 | -0.297799 | -3.058478 | 1.906034 | 1 | -0.219028 | -3.320584 | 1.717515 |
| 1 | -0.902214 | -3.318080 | 0.261533 | 1 | -0.948685 | -3.318937 | 0.099214 |
| 6 | 0.308153 | -2.448407 | -1.894261 | 6 | 0.356170 | -2.333542 | -2.039900 |
| 1 | 0.362943 | -3.543060 | -1.833963 | 1 | 0.593901 | -3.409148 | -2.054504 |
| 1 | -0.752129 | -2.153276 | -1.840348 | 1 | -0.737028 | -2.213169 | -2.014329 |
| 1 | 0.694728 | -2.143357 | -2.869292 | 1 | 0.723780 | -1.896652 | -2.975016 |
| 25 | 0.000000 | 0.000000 | 0.216378 | 25 | 0.000000 | 0.000000 | 0.443625 |

**Table S24.** Atomic coordinates of the optimized structures for the **Fe-s-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.622910 | -1.403028 | 0.000007 | 6 | -1.630445 | 1.481467 | 0.000012 |
| 1 | 1.525423 | -2.488326 | 0.000011 | 1 | -1.523483 | 2.568045 | 0.000019 |
| 1 | -1.525423 | 2.488326 | 0.000011 | 1 | 1.523483 | -2.568045 | 0.000019 |
| 6 | -1.622910 | 1.403028 | 0.000007 | 6 | 1.630445 | -1.481467 | 0.000012 |
| 5 | 1.695048 | -0.544136 | 1.232896 | 5 | -1.754646 | 0.621282 | 1.233499 |
| 5 | -1.695048 | 0.544136 | 1.232896 | 5 | 1.754646 | -0.621282 | 1.233499 |
| 5 | -1.695050 | 0.544146 | -1.232889 | 5 | 1.754643 | -0.621301 | -1.233489 |
| 5 | 1.695050 | -0.544146 | -1.232889 | 5 | -1.754643 | 0.621301 | -1.233489 |
| 7 | 1.622910 | 0.863020 | 0.718076 | 7 | -1.680087 | -0.783038 | 0.723447 |
| 7 | 1.622911 | 0.863014 | -0.718080 | 7 | -1.680083 | -0.783028 | -0.723456 |
| 7 | -1.622910 | -0.863020 | 0.718076 | 7 | 1.680087 | 0.783038 | 0.723447 |
| 7 | -1.622911 | -0.863014 | -0.718080 | 7 | 1.680083 | 0.783028 | -0.723456 |
| 6 | -1.750514 | 0.803257 | 2.783292 | 6 | 1.867946 | -0.911091 | 2.788499 |
| 1 | -2.783939 | 0.785055 | 3.153351 | 1 | 2.913024 | -0.811282 | 3.126524 |
| 1 | -1.192846 | 0.067982 | 3.378224 | 1 | 1.263855 | -0.236192 | 3.414546 |
| 1 | -1.352620 | 1.792244 | 3.035377 | 1 | 1.560637 | -1.941009 | 3.017859 |
| 6 | -1.750518 | 0.803277 | -2.783283 | 6 | 1.867945 | -0.911128 | -2.788485 |
| 1 | -1.352639 | 1.792273 | -3.035361 | 1 | 1.560655 | -1.941054 | -3.017833 |
| 1 | -1.192836 | 0.068015 | -3.378219 | 1 | 1.263840 | -0.236246 | -3.414537 |
| 1 | -2.783941 | 0.785060 | -3.153345 | 1 | 2.913020 | -0.811302 | -3.126513 |
| 6 | -1.672384 | -2.127681 | -1.418855 | 6 | 1.867946 | 2.038218 | -1.435784 |
| 1 | -2.644549 | -2.619352 | -1.287153 | 1 | 2.889366 | 2.426648 | -1.297777 |
| 1 | -1.535946 | -1.908786 | -2.479635 | 1 | 1.719252 | 1.826756 | -2.499560 |
| 1 | -0.870207 | -2.803413 | -1.103505 | 1 | 1.137974 | 2.797807 | -1.131607 |
| 6 | -1.672381 | -2.127693 | 1.418840 | 6 | 1.867945 | 2.038241 | 1.435754 |
| 1 | -2.644543 | -2.619367 | 1.287130 | 1 | 2.889357 | 2.426681 | 1.297726 |
| 1 | -0.870199 | -2.803418 | 1.103488 | 1 | 1.137958 | 2.797816 | 1.131578 |
| 1 | -1.535948 | -1.908805 | 2.479622 | 1 | 1.719270 | 1.826793 | 2.499536 |
| 6 | 1.750514 | -0.803257 | 2.783292 | 6 | -1.867946 | 0.911091 | 2.788499 |
| 1 | 1.192846 | -0.067982 | 3.378224 | 1 | -1.263855 | 0.236192 | 3.414546 |
| 1 | 1.352620 | -1.792244 | 3.035377 | 1 | -1.560637 | 1.941009 | 3.017859 |
| 1 | 2.783939 | -0.785055 | 3.153351 | 1 | -2.913024 | 0.811282 | 3.126524 |
| 6 | 1.750518 | -0.803277 | -2.783283 | 6 | -1.867945 | 0.911128 | -2.788485 |
| 1 | 1.192836 | -0.068015 | -3.378219 | 1 | -1.263840 | 0.236246 | -3.414537 |
| 1 | 2.783941 | -0.785060 | -3.153345 | 1 | -2.913020 | 0.811302 | -3.126513 |
| 1 | 1.352639 | -1.792273 | -3.035361 | 1 | -1.560655 | 1.941054 | -3.017833 |
| 6 | 1.672384 | 2.127681 | -1.418855 | 6 | -1.867946 | -2.038218 | -1.435784 |
| 1 | 2.644549 | 2.619352 | -1.287153 | 1 | -2.889366 | -2.426648 | -1.297777 |
| 1 | 1.535946 | 1.908786 | -2.479635 | 1 | -1.719252 | -1.826756 | -2.499560 |
| 1 | 0.870207 | 2.803413 | -1.103505 | 1 | -1.137974 | -2.797807 | -1.131607 |
| 6 | 1.672381 | 2.127693 | 1.418840 | 6 | -1.867945 | -2.038241 | 1.435754 |
| 1 | 2.644543 | 2.619367 | 1.287130 | 1 | -2.889357 | -2.426681 | 1.297726 |
| 1 | 0.870199 | 2.803418 | 1.103488 | 1 | -1.137958 | -2.797816 | 1.131578 |
| 1 | 1.535948 | 1.908805 | 2.479622 | 1 | -1.719270 | -1.826793 | 2.499536 |
| 26 | 0.000000 | 0.000000 | 0.000000 | 26 | 0.000000 | 0.000000 | 0.000006 |

**Table S25.** Atomic coordinates of the optimized structures for the **Fe-s-72** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.414261 | 1.678920 | 1.439442 | 6 | 0.378146 | 1.755346 | 1.407716 |
| 1 | -0.118502 | 1.877982 | 2.366027 | 1 | -0.160849 | 1.988657 | 2.326278 |
| 1 | 0.118502 | -1.877982 | 2.366027 | 1 | 0.160849 | -1.988657 | 2.326278 |
| 6 | -0.414261 | -1.678920 | 1.439442 | 6 | -0.378146 | -1.755346 | 1.407716 |
| 5 | 0.000000 | 2.174694 | 0.084380 | 5 | 0.000000 | 2.236801 | 0.030449 |
| 5 | 0.000000 | -2.174694 | 0.084380 | 5 | 0.000000 | -2.236801 | 0.030449 |
| 5 | -1.635660 | -0.805534 | 1.329472 | 5 | -1.637432 | -0.925487 | 1.337778 |
| 5 | 1.635660 | 0.805534 | 1.329472 | 5 | 1.637432 | 0.925487 | 1.337778 |
| 7 | 0.882386 | 1.437276 | -0.877371 | 7 | 0.882382 | 1.463947 | -0.895439 |
| 7 | 1.835174 | 0.638010 | -0.151661 | 7 | 1.840299 | 0.689032 | -0.129237 |
| 7 | -0.882386 | -1.437276 | -0.877371 | 7 | -0.882382 | -1.463947 | -0.895439 |
| 7 | -1.835174 | -0.638010 | -0.151661 | 7 | -1.840299 | -0.689032 | -0.129237 |
| 6 | 1.106682 | -3.146114 | -0.472094 | 6 | 1.082732 | -3.245579 | -0.542372 |
| 1 | 0.702110 | -4.150894 | -0.650885 | 1 | 0.616877 | -4.214159 | -0.789875 |
| 1 | 1.555772 | -2.823433 | -1.422792 | 1 | 1.592538 | -2.897422 | -1.455483 |
| 1 | 1.924835 | -3.266639 | 0.245424 | 1 | 1.857021 | -3.451970 | 0.209226 |
| 6 | -2.601439 | -0.064145 | 2.322166 | 6 | -2.625769 | -0.299387 | 2.404560 |
| 1 | -2.158829 | 0.005128 | 3.320075 | 1 | -2.151610 | -0.272309 | 3.395033 |
| 1 | -2.838401 | 0.961500 | 2.007634 | 1 | -2.944971 | 0.726970 | 2.166245 |
| 1 | -3.558223 | -0.591364 | 2.435062 | 1 | -3.538781 | -0.910927 | 2.502087 |
| 6 | -2.884601 | 0.038820 | -0.878829 | 6 | -2.967548 | -0.072524 | -0.810838 |
| 1 | -3.612218 | -0.672605 | -1.290306 | 1 | -3.686925 | -0.828003 | -1.165029 |
| 1 | -3.397540 | 0.686756 | -0.165531 | 1 | -3.470218 | 0.567627 | -0.078712 |
| 1 | -2.496873 | 0.668941 | -1.688766 | 1 | -2.654296 | 0.556489 | -1.654184 |
| 6 | -1.031173 | -1.574506 | -2.307512 | 6 | -1.089455 | -1.627841 | -2.325229 |
| 1 | -1.912326 | -2.175468 | -2.566786 | 1 | -1.999672 | -2.210861 | -2.536194 |
| 1 | -1.101567 | -0.606777 | -2.818723 | 1 | -1.150116 | -0.667660 | -2.855737 |
| 1 | -0.143619 | -2.095255 | -2.675564 | 1 | -0.231283 | -2.186316 | -2.714516 |
| 6 | -1.106682 | 3.146114 | -0.472094 | 6 | -1.082732 | 3.245579 | -0.542372 |
| 1 | -1.555772 | 2.823433 | -1.422792 | 1 | -1.592538 | 2.897422 | -1.455483 |
| 1 | -1.924835 | 3.266639 | 0.245424 | 1 | -1.857021 | 3.451970 | 0.209226 |
| 1 | -0.702110 | 4.150894 | -0.650885 | 1 | -0.616877 | 4.214159 | -0.789875 |
| 6 | 2.601439 | 0.064145 | 2.322166 | 6 | 2.625769 | 0.299387 | 2.404560 |
| 1 | 2.838401 | -0.961500 | 2.007634 | 1 | 2.944971 | -0.726970 | 2.166245 |
| 1 | 3.558223 | 0.591364 | 2.435062 | 1 | 3.538781 | 0.910927 | 2.502087 |
| 1 | 2.158829 | -0.005128 | 3.320075 | 1 | 2.151610 | 0.272309 | 3.395033 |
| 6 | 2.884601 | -0.038820 | -0.878829 | 6 | 2.967548 | 0.072524 | -0.810838 |
| 1 | 3.612218 | 0.672605 | -1.290306 | 1 | 3.686925 | 0.828003 | -1.165029 |
| 1 | 3.397540 | -0.686756 | -0.165531 | 1 | 3.470218 | -0.567627 | -0.078712 |
| 1 | 2.496873 | -0.668941 | -1.688766 | 1 | 2.654296 | -0.556489 | -1.654184 |
| 6 | 1.031173 | 1.574506 | -2.307512 | 6 | 1.089455 | 1.627841 | -2.325229 |
| 1 | 1.912326 | 2.175468 | -2.566786 | 1 | 1.999672 | 2.210861 | -2.536194 |
| 1 | 1.101567 | 0.606777 | -2.818723 | 1 | 1.150116 | 0.667660 | -2.855737 |
| 1 | 0.143619 | 2.095255 | -2.675564 | 1 | 0.231283 | 2.186316 | -2.714516 |
| 26 | 0.000000 | 0.000000 | 0.186158 | 26 | 0.000000 | 0.000000 | 0.167649 |

**Table S26.** Atomic coordinates of the optimized structures for the **Fe-t-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -1.009557 | -0.207167 | -1.852536 | 6 | 1.160375 | 0.191146 | -1.807653 |
| 1 | -0.582703 | 0.043843 | -2.822897 | 1 | 0.795519 | -0.002076 | -2.818053 |
| 1 | 0.582590 | -0.043700 | 2.822883 | 1 | -0.795503 | 0.002042 | 2.818054 |
| 6 | 1.009487 | 0.207256 | 1.852527 | 6 | -1.160366 | -0.191167 | 1.807655 |
| 26 | 0.000000 | 0.000000 | 0.000000 | 26 | -0.000002 | 0.000003 | -0.000004 |
| 5 | -1.946354 | 0.710629 | -1.069872 | 5 | 2.082823 | -0.755168 | -1.021200 |
| 5 | 0.973018 | 1.550199 | 1.164209 | 5 | -1.165020 | -1.527962 | 1.098467 |
| 5 | 1.946331 | -0.710577 | 1.069967 | 5 | -2.082821 | 0.755156 | 1.021222 |
| 5 | -0.973071 | -1.550154 | -1.164300 | 5 | 1.165030 | 1.527952 | -1.098485 |
| 7 | -2.303153 | -0.015891 | 0.154888 | 7 | 2.361156 | -0.091363 | 0.247311 |
| 7 | -1.560439 | -1.256798 | 0.182206 | 7 | 1.630828 | 1.171853 | 0.281060 |
| 7 | 1.560454 | 1.256765 | -0.182255 | 7 | -1.630831 | -1.171846 | -0.281070 |
| 7 | 2.303177 | 0.015864 | -0.154828 | 7 | -2.361159 | 0.091370 | -0.247299 |
| 6 | 0.407261 | 2.984201 | 1.480830 | 6 | -0.739333 | -3.008503 | 1.474459 |
| 1 | 1.212049 | 3.708124 | 1.666704 | 1 | -1.628402 | -3.644901 | 1.621184 |
| 1 | -0.197669 | 3.398546 | 0.662439 | 1 | -0.120906 | -3.501089 | 0.707531 |
| 1 | -0.223573 | 2.980126 | 2.375366 | 1 | -0.175058 | -3.028579 | 2.417059 |
| 6 | 2.500736 | -2.153551 | 1.352685 | 6 | -2.666904 | 2.194654 | 1.338769 |
| 1 | 1.801495 | -2.735598 | 1.962841 | 1 | -2.334680 | 2.556671 | 2.321003 |
| 1 | 2.716906 | -2.741168 | 0.451861 | 1 | -2.367929 | 2.946466 | 0.590361 |
| 1 | 3.435374 | -2.104192 | 1.925516 | 1 | -3.769030 | 2.183803 | 1.350683 |
| 6 | 2.802881 | -0.480533 | -1.416549 | 6 | -2.909960 | 0.613213 | -1.485750 |
| 1 | 3.606477 | 0.150310 | -1.817345 | 1 | -3.707101 | -0.029966 | -1.889594 |
| 1 | 3.211873 | -1.476208 | -1.234002 | 1 | -3.350233 | 1.588939 | -1.252056 |
| 1 | 2.011054 | -0.570133 | -2.175858 | 1 | -2.144407 | 0.760136 | -2.264077 |
| 6 | 1.879354 | 2.203126 | -1.230192 | 6 | -1.976645 | -2.108742 | -1.342451 |
| 1 | 2.910282 | 2.567267 | -1.131561 | 1 | -3.021189 | -2.445803 | -1.245406 |
| 1 | 1.740759 | 1.774727 | -2.228081 | 1 | -1.824592 | -1.674287 | -2.338236 |
| 1 | 1.197440 | 3.049036 | -1.123359 | 1 | -1.317309 | -2.977076 | -1.243279 |
| 6 | -2.500761 | 2.153632 | -1.352443 | 6 | 2.666904 | -2.194672 | -1.338723 |
| 1 | -2.716590 | 2.741263 | -0.451546 | 1 | 2.367897 | -2.946476 | -0.590320 |
| 1 | -1.801684 | 2.735631 | -1.962829 | 1 | 2.334707 | -2.556691 | -2.320966 |
| 1 | -3.435599 | 2.104333 | -1.924954 | 1 | 3.769031 | -2.183832 | -1.350602 |
| 6 | -0.407308 | -2.984133 | -1.481018 | 6 | 0.739356 | 3.008490 | -1.474503 |
| 1 | 0.197804 | -3.398430 | -0.662736 | 1 | 0.120927 | 3.501092 | -0.707587 |
| 1 | -1.212091 | -3.708106 | -1.666723 | 1 | 1.628429 | 3.644879 | -1.621233 |
| 1 | 0.223355 | -2.980035 | -2.375674 | 1 | 0.175086 | 3.028555 | -2.417107 |
| 6 | -1.879291 | -2.203219 | 1.230103 | 6 | 1.976638 | 2.108763 | 1.342430 |
| 1 | -2.910238 | -2.567321 | 1.131523 | 1 | 3.021186 | 2.445814 | 1.245392 |
| 1 | -1.197414 | -3.049144 | 1.123159 | 1 | 1.317311 | 2.977102 | 1.243236 |
| 1 | -1.740609 | -1.774891 | 2.228010 | 1 | 1.824570 | 1.674325 | 2.338220 |
| 6 | -2.802824 | 0.480424 | 1.416654 | 6 | 2.909940 | -0.613194 | 1.485775 |
| 1 | -3.606397 | -0.150456 | 1.817437 | 1 | 3.707075 | 0.029989 | 1.889623 |
| 1 | -2.010974 | 0.569991 | 2.175942 | 1 | 2.144377 | -0.760108 | 2.264093 |
| 1 | -3.211839 | 1.476102 | 1.234176 | 1 | 3.350217 | -1.588921 | 1.252097 |

**Table S27.** Atomic coordinates of the optimized structures for the **Fe-t-36** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.018087 | -1.269970 | 1.601648 | 6 | 0.843138 | -1.432269 | 1.597862 |
| 1 | 1.104797 | -1.065491 | 2.666290 | 1 | 0.953182 | -1.262227 | 2.669245 |
| 1 | -1.104797 | 1.065491 | 2.666290 | 1 | -0.953182 | 1.262227 | 2.669245 |
| 6 | -1.018087 | 1.269970 | 1.601648 | 6 | -0.843138 | 1.432269 | 1.597862 |
| 5 | 1.987659 | -0.829630 | 0.517680 | 5 | 1.886802 | -1.136840 | 0.532392 |
| 5 | -1.987659 | 0.829630 | 0.517680 | 5 | -1.886802 | 1.136840 | 0.532392 |
| 5 | 0.000000 | 2.226716 | 0.978661 | 5 | 0.238643 | 2.319705 | 0.955118 |
| 5 | 0.000000 | -2.226716 | 0.978661 | 5 | -0.238643 | -2.319705 | 0.955118 |
| 7 | 1.297343 | -1.217374 | -0.743425 | 7 | 1.160121 | -1.400965 | -0.742552 |
| 7 | 0.224921 | -2.152815 | -0.464081 | 7 | 0.000000 | -2.251071 | -0.479254 |
| 7 | -1.297343 | 1.217374 | -0.743425 | 7 | -1.160121 | 1.400965 | -0.742552 |
| 7 | -0.224921 | 2.152815 | -0.464081 | 7 | 0.000000 | 2.251071 | -0.479254 |
| 6 | -3.364326 | 0.069281 | 0.469002 | 6 | -3.382774 | 0.611861 | 0.549949 |
| 1 | -4.201534 | 0.753086 | 0.273536 | 1 | -4.087760 | 1.439473 | 0.361506 |
| 1 | -3.405861 | -0.702014 | -0.313485 | 1 | -3.596088 | -0.163911 | -0.202571 |
| 1 | -3.578480 | -0.429872 | 1.418497 | 1 | -3.636499 | 0.194681 | 1.533843 |
| 6 | 1.150111 | 3.105662 | 1.586113 | 6 | 1.463740 | 3.129971 | 1.548948 |
| 1 | 1.529685 | 2.666125 | 2.513899 | 1 | 1.467109 | 3.098814 | 2.646422 |
| 1 | 2.009512 | 3.249686 | 0.919336 | 1 | 2.429632 | 2.722209 | 1.209346 |
| 1 | 0.782824 | 4.106359 | 1.846667 | 1 | 1.439848 | 4.189983 | 1.248091 |
| 6 | 0.628285 | 2.524282 | -1.564622 | 6 | 0.851695 | 2.623283 | -1.591493 |
| 1 | 0.099966 | 3.120644 | -2.320089 | 1 | 0.333043 | 3.264352 | -2.321341 |
| 1 | 1.438937 | 3.132577 | -1.158702 | 1 | 1.689856 | 3.193804 | -1.176461 |
| 1 | 1.075793 | 1.649505 | -2.063767 | 1 | 1.263366 | 1.750262 | -2.125867 |
| 6 | -1.853311 | 1.242694 | -2.076919 | 6 | -1.767657 | 1.519346 | -2.059591 |
| 1 | -2.293251 | 2.222328 | -2.309160 | 1 | -2.144035 | 2.540529 | -2.236203 |
| 1 | -1.111152 | 1.001224 | -2.848567 | 1 | -1.071396 | 1.255408 | -2.867701 |
| 1 | -2.647603 | 0.493600 | -2.116332 | 1 | -2.617671 | 0.829259 | -2.096899 |
| 6 | 3.364326 | -0.069281 | 0.469002 | 6 | 3.382774 | -0.611861 | 0.549949 |
| 1 | 3.405861 | 0.702014 | -0.313485 | 1 | 3.596088 | 0.163911 | -0.202571 |
| 1 | 3.578480 | 0.429872 | 1.418497 | 1 | 3.636499 | -0.194681 | 1.533843 |
| 1 | 4.201534 | -0.753086 | 0.273536 | 1 | 4.087760 | -1.439473 | 0.361506 |
| 6 | -1.150111 | -3.105662 | 1.586113 | 6 | -1.463740 | -3.129971 | 1.548948 |
| 1 | -2.009512 | -3.249686 | 0.919336 | 1 | -2.429632 | -2.722209 | 1.209346 |
| 1 | -0.782824 | -4.106359 | 1.846667 | 1 | -1.439848 | -4.189983 | 1.248091 |
| 1 | -1.529685 | -2.666125 | 2.513899 | 1 | -1.467109 | -3.098814 | 2.646422 |
| 6 | -0.628285 | -2.524282 | -1.564622 | 6 | -0.851695 | -2.623283 | -1.591493 |
| 1 | -0.099966 | -3.120644 | -2.320089 | 1 | -0.333043 | -3.264352 | -2.321341 |
| 1 | -1.438937 | -3.132577 | -1.158702 | 1 | -1.689856 | -3.193804 | -1.176461 |
| 1 | -1.075793 | -1.649505 | -2.063767 | 1 | -1.263366 | -1.750262 | -2.125867 |
| 6 | 1.853311 | -1.242694 | -2.076919 | 6 | 1.767657 | -1.519346 | -2.059591 |
| 1 | 2.293251 | -2.222328 | -2.309160 | 1 | 2.144035 | -2.540529 | -2.236203 |
| 1 | 1.111152 | -1.001224 | -2.848567 | 1 | 1.071396 | -1.255408 | -2.867701 |
| 1 | 2.647603 | -0.493600 | -2.116332 | 1 | 2.617671 | -0.829259 | -2.096899 |
| 26 | 0.000000 | 0.000000 | 0.336260 | 26 | 0.000000 | 0.000000 | 0.323049 |

**Table S28.** Atomic coordinates of the optimized structures for the **Fe-t-144** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.000000 | 2.096528 | 0.292316 | 6 | 0.000000 | 2.146238 | 0.368875 |
| 1 | -0.884867 | 2.703390 | 0.480175 | 1 | -0.873718 | 2.753490 | 0.612252 |
| 1 | 0.884867 | -2.703390 | 0.480175 | 1 | 0.873718 | -2.753490 | 0.612252 |
| 6 | 0.000000 | -2.096528 | 0.292316 | 6 | 0.000000 | -2.146238 | 0.368875 |
| 5 | 0.619931 | 1.858028 | -1.081875 | 5 | 0.595917 | 1.991186 | -1.037313 |
| 5 | -0.619931 | -1.858028 | -1.081875 | 5 | -0.595917 | -1.991186 | -1.037313 |
| 5 | -0.963503 | -1.575975 | 1.345518 | 5 | -1.019689 | -1.621516 | 1.362977 |
| 5 | 0.963503 | 1.575975 | 1.345518 | 5 | 1.019689 | 1.621516 | 1.362977 |
| 7 | 1.767523 | 0.985318 | -0.856031 | 7 | 1.748940 | 1.114379 | -0.890265 |
| 7 | 1.881910 | 0.702796 | 0.563085 | 7 | 1.886683 | 0.743466 | 0.519943 |
| 7 | -1.767523 | -0.985318 | -0.856031 | 7 | -1.748940 | -1.114379 | -0.890265 |
| 7 | -1.881910 | -0.702796 | 0.563085 | 7 | -1.886683 | -0.743466 | 0.519943 |
| 6 | -0.217931 | -2.259810 | -2.550211 | 6 | -0.143320 | -2.517790 | -2.464069 |
| 1 | -1.019807 | -2.809581 | -3.059028 | 1 | -0.934247 | -3.120027 | -2.939806 |
| 1 | -0.006510 | -1.381564 | -3.177265 | 1 | 0.088708 | -1.696682 | -3.162059 |
| 1 | 0.672637 | -2.894553 | -2.577517 | 1 | 0.749521 | -3.153583 | -2.393876 |
| 6 | -1.117127 | -1.711871 | 2.903957 | 6 | -1.249495 | -1.765859 | 2.923978 |
| 1 | -0.196711 | -2.081028 | 3.367009 | 1 | -0.383793 | -2.240014 | 3.406323 |
| 1 | -1.366074 | -0.763409 | 3.398083 | 1 | -1.424517 | -0.804291 | 3.431096 |
| 1 | -1.911766 | -2.420901 | 3.172738 | 1 | -2.124883 | -2.403048 | 3.135982 |
| 6 | -3.073094 | -0.022699 | 1.016684 | 6 | -3.138369 | -0.120055 | 0.924680 |
| 1 | -3.966105 | -0.649527 | 0.888547 | 1 | -3.987594 | -0.810630 | 0.794584 |
| 1 | -2.943008 | 0.183771 | 2.080979 | 1 | -3.051200 | 0.128814 | 1.987379 |
| 1 | -3.226700 | 0.930903 | 0.501262 | 1 | -3.336543 | 0.806363 | 0.370938 |
| 6 | -2.554791 | -0.198345 | -1.772987 | 6 | -2.552602 | -0.420896 | -1.879346 |
| 1 | -3.631337 | -0.379216 | -1.655024 | 1 | -3.629687 | -0.601767 | -1.739752 |
| 1 | -2.367011 | 0.880739 | -1.675767 | 1 | -2.376319 | 0.666017 | -1.890582 |
| 1 | -2.268628 | -0.500199 | -2.782987 | 1 | -2.268386 | -0.822149 | -2.858646 |
| 6 | 0.217931 | 2.259810 | -2.550211 | 6 | 0.143320 | 2.517790 | -2.464069 |
| 1 | 0.006510 | 1.381564 | -3.177265 | 1 | -0.088708 | 1.696682 | -3.162059 |
| 1 | -0.672637 | 2.894553 | -2.577517 | 1 | -0.749521 | 3.153583 | -2.393876 |
| 1 | 1.019807 | 2.809581 | -3.059028 | 1 | 0.934247 | 3.120027 | -2.939806 |
| 6 | 1.117127 | 1.711871 | 2.903957 | 6 | 1.249495 | 1.765859 | 2.923978 |
| 1 | 1.366074 | 0.763409 | 3.398083 | 1 | 1.424517 | 0.804291 | 3.431096 |
| 1 | 1.911766 | 2.420901 | 3.172738 | 1 | 2.124883 | 2.403048 | 3.135982 |
| 1 | 0.196711 | 2.081028 | 3.367009 | 1 | 0.383793 | 2.240014 | 3.406323 |
| 6 | 3.073094 | 0.022699 | 1.016684 | 6 | 3.138369 | 0.120055 | 0.924680 |
| 1 | 3.966105 | 0.649527 | 0.888547 | 1 | 3.987594 | 0.810630 | 0.794584 |
| 1 | 2.943008 | -0.183771 | 2.080979 | 1 | 3.051200 | -0.128814 | 1.987379 |
| 1 | 3.226700 | -0.930903 | 0.501262 | 1 | 3.336543 | -0.806363 | 0.370938 |
| 6 | 2.554791 | 0.198345 | -1.772987 | 6 | 2.552602 | 0.420896 | -1.879346 |
| 1 | 3.631337 | 0.379216 | -1.655024 | 1 | 3.629687 | 0.601767 | -1.739752 |
| 1 | 2.367011 | -0.880739 | -1.675767 | 1 | 2.376319 | -0.666017 | -1.890582 |
| 1 | 2.268628 | 0.500199 | -2.782987 | 1 | 2.268386 | 0.822149 | -2.858646 |
| 26 | 0.000000 | 0.000000 | 0.187128 | 26 | 0.000000 | 0.000000 | 0.228107 |

**Table S29.** Atomic coordinates of the optimized structures for the **Fe-p-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -1.064084 | 0.004358 | -1.839151 | 6 | 1.194221 | 0.006209 | -1.773168 |
| 1 | -0.534053 | -0.013865 | -2.789723 | 1 | 0.717197 | 0.028798 | -2.754678 |
| 1 | 0.534053 | 0.013865 | 2.789723 | 1 | -0.717190 | -0.028828 | 2.754675 |
| 6 | 1.064084 | -0.004358 | 1.839151 | 6 | -1.194217 | -0.006227 | 1.773167 |
| 26 | 0.000000 | 0.000000 | 0.000000 | 26 | -0.000001 | 0.000007 | -0.000003 |
| 5 | -1.605959 | 1.249079 | -1.146114 | 5 | 1.760470 | -1.241627 | -1.082620 |
| 5 | 1.615748 | 1.214128 | 1.107103 | 5 | -1.762441 | -1.221842 | 1.034853 |
| 5 | 1.605959 | -1.249079 | 1.146114 | 5 | -1.760479 | 1.241615 | 1.082642 |
| 5 | -1.615748 | -1.214128 | -1.107103 | 5 | 1.762455 | 1.221831 | -1.034874 |
| 7 | -2.273160 | 0.754291 | 0.066320 | 7 | 2.374241 | -0.753497 | 0.152312 |
| 7 | -2.249104 | -0.671884 | 0.106269 | 7 | 2.338558 | 0.683356 | 0.203312 |
| 7 | 2.249104 | 0.671884 | -0.106269 | 7 | -2.338554 | -0.683350 | -0.203322 |
| 7 | 2.273160 | -0.754291 | -0.066320 | 7 | -2.374248 | 0.753502 | -0.152298 |
| 6 | 1.587265 | 2.764600 | 1.380996 | 6 | -1.798235 | -2.774923 | 1.362867 |
| 1 | 2.513833 | 3.102732 | 1.862813 | 1 | -2.815140 | -3.089668 | 1.651239 |
| 1 | 1.468803 | 3.371249 | 0.473669 | 1 | -1.497463 | -3.410863 | 0.515362 |
| 1 | 0.769942 | 3.036954 | 2.057355 | 1 | -1.138893 | -3.017039 | 2.207588 |
| 6 | 1.519572 | -2.791999 | 1.450484 | 6 | -1.736734 | 2.788831 | 1.442441 |
| 1 | 0.682585 | -3.020055 | 2.119113 | 1 | -1.125289 | 2.977420 | 2.335338 |
| 1 | 1.393126 | -3.414603 | 0.555226 | 1 | -1.337744 | 3.419548 | 0.631972 |
| 1 | 2.425746 | -3.151799 | 1.954513 | 1 | -2.751528 | 3.159233 | 1.662867 |
| 6 | 2.744791 | -1.465573 | -1.228679 | 6 | -2.901153 | 1.483975 | -1.289240 |
| 1 | 3.789987 | -1.227752 | -1.462758 | 1 | -3.958142 | 1.244353 | -1.483249 |
| 1 | 2.682104 | -2.531670 | -1.003375 | 1 | -2.834566 | 2.549919 | -1.047437 |
| 1 | 2.134025 | -1.270458 | -2.122714 | 1 | -2.326263 | 1.305065 | -2.212048 |
| 6 | 2.933666 | 1.344934 | -1.179653 | 6 | -3.137973 | -1.363559 | -1.203742 |
| 1 | 4.018777 | 1.175682 | -1.147935 | 1 | -4.217921 | -1.196927 | -1.052052 |
| 1 | 2.562616 | 1.048557 | -2.169381 | 1 | -2.877004 | -1.063748 | -2.228753 |
| 1 | 2.753501 | 2.414992 | -1.058665 | 1 | -2.942018 | -2.436440 | -1.104077 |
| 6 | -1.519572 | 2.791999 | -1.450484 | 6 | 1.736709 | -2.788849 | -1.442389 |
| 1 | -1.393126 | 3.414603 | -0.555226 | 1 | 1.337688 | -3.419542 | -0.631916 |
| 1 | -0.682585 | 3.020055 | -2.119113 | 1 | 1.125280 | -2.977447 | -2.335296 |
| 1 | -2.425746 | 3.151799 | -1.954513 | 1 | 2.751500 | -3.159274 | -1.662784 |
| 6 | -1.587265 | -2.764600 | -1.380996 | 6 | 1.798266 | 2.774905 | -1.362917 |
| 1 | -1.468803 | -3.371249 | -0.473669 | 1 | 1.497506 | 3.410866 | -0.515423 |
| 1 | -2.513833 | -3.102732 | -1.862813 | 1 | 2.815173 | 3.089632 | -1.651299 |
| 1 | -0.769942 | -3.036954 | -2.057355 | 1 | 1.138923 | 3.017013 | -2.207640 |
| 6 | -2.933666 | -1.344934 | 1.179653 | 6 | 3.137986 | 1.363574 | 1.203720 |
| 1 | -4.018777 | -1.175682 | 1.147935 | 1 | 4.217931 | 1.196929 | 1.052031 |
| 1 | -2.753501 | -2.414992 | 1.058665 | 1 | 2.942041 | 2.436455 | 1.104036 |
| 1 | -2.562616 | -1.048557 | 2.169381 | 1 | 2.877014 | 1.063783 | 2.228736 |
| 6 | -2.744791 | 1.465573 | 1.228679 | 6 | 2.901135 | -1.483955 | 1.289268 |
| 1 | -3.789987 | 1.227752 | 1.462758 | 1 | 3.958126 | -1.244342 | 1.483276 |
| 1 | -2.134025 | 1.270458 | 2.122714 | 1 | 2.326245 | -1.305022 | 2.212072 |
| 1 | -2.682104 | 2.531670 | 1.003375 | 1 | 2.834537 | -2.549903 | 1.047485 |

**Table S30.** Atomic coordinates of the optimized structures for the **Co-d-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -0.961163 | 0.304509 | 1.871593 | 6 | 1.095832 | -0.281002 | 1.849254 |
| 1 | -0.522670 | 0.051018 | 2.835938 | 1 | 0.708964 | -0.068255 | 2.847475 |
| 1 | 0.522670 | -0.051018 | -2.835938 | 1 | -0.708963 | 0.068259 | -2.847476 |
| 6 | 0.961163 | -0.304509 | -1.871593 | 6 | -1.095831 | 0.281004 | -1.849254 |
| 5 | -1.885834 | -0.604230 | 1.073525 | 5 | 2.016597 | 0.648569 | 1.051674 |
| 5 | 0.820532 | -1.616978 | -1.157392 | 5 | -0.997659 | 1.597089 | -1.125424 |
| 5 | 1.885834 | 0.604230 | -1.073525 | 5 | -2.016596 | -0.648568 | -1.051675 |
| 5 | -0.820532 | 1.616978 | 1.157392 | 5 | 0.997659 | -1.597088 | 1.125425 |
| 7 | -2.202173 | 0.123301 | -0.170238 | 7 | 2.268686 | -0.027657 | -0.223095 |
| 7 | -1.420391 | 1.341735 | -0.192866 | 7 | 1.494077 | -1.264480 | -0.254012 |
| 7 | 1.420391 | -1.341735 | 0.192866 | 7 | -1.494077 | 1.264479 | 0.254012 |
| 7 | 2.202173 | -0.123301 | 0.170238 | 7 | -2.268685 | 0.027656 | 0.223095 |
| 6 | 0.143576 | -3.008893 | -1.437438 | 6 | -0.445409 | 3.043222 | -1.468288 |
| 1 | 0.888860 | -3.793914 | -1.622036 | 1 | -1.275067 | 3.759753 | -1.589771 |
| 1 | -0.477008 | -3.361811 | -0.602313 | 1 | 0.220856 | 3.457375 | -0.695204 |
| 1 | -0.498937 | -2.972784 | -2.322896 | 1 | 0.110760 | 3.037310 | -2.415850 |
| 6 | 2.475469 | 2.037369 | -1.338926 | 6 | -2.635294 | -2.075650 | -1.360218 |
| 1 | 1.809136 | 2.631362 | -1.974284 | 1 | -2.214097 | -2.503130 | -2.280337 |
| 1 | 2.672074 | 2.623155 | -0.432162 | 1 | -2.476768 | -2.804947 | -0.550140 |
| 1 | 3.427656 | 1.969388 | -1.880259 | 1 | -3.725039 | -2.002377 | -1.511005 |
| 6 | 2.774205 | 0.331064 | 1.415267 | 6 | -2.861290 | -0.455321 | 1.456908 |
| 1 | 3.574616 | -0.333062 | 1.766674 | 1 | -3.643180 | 0.222712 | 1.832785 |
| 1 | 3.208573 | 1.315186 | 1.227686 | 1 | -3.332026 | -1.417803 | 1.228209 |
| 1 | 2.021879 | 0.437147 | 2.210353 | 1 | -2.114599 | -0.616912 | 2.249366 |
| 6 | 1.655586 | -2.275593 | 1.272995 | 6 | -1.777093 | 2.208798 | 1.326644 |
| 1 | 2.668835 | -2.693171 | 1.214612 | 1 | -2.801793 | 2.603941 | 1.239504 |
| 1 | 1.507850 | -1.815354 | 2.254981 | 1 | -1.641456 | 1.757502 | 2.316765 |
| 1 | 0.935669 | -3.088780 | 1.162145 | 1 | -1.071294 | 3.039565 | 1.226810 |
| 6 | -2.475469 | -2.037369 | 1.338926 | 6 | 2.635295 | 2.075651 | 1.360214 |
| 1 | -2.672074 | -2.623155 | 0.432162 | 1 | 2.476761 | 2.804948 | 0.550138 |
| 1 | -1.809136 | -2.631362 | 1.974284 | 1 | 2.214106 | 2.503129 | 2.280337 |
| 1 | -3.427656 | -1.969388 | 1.880259 | 1 | 3.725041 | 2.002380 | 1.510991 |
| 6 | -0.143576 | 3.008893 | 1.437438 | 6 | 0.445408 | -3.043220 | 1.468291 |
| 1 | 0.477008 | 3.361811 | 0.602313 | 1 | -0.220858 | -3.457373 | 0.695208 |
| 1 | -0.888860 | 3.793914 | 1.622036 | 1 | 1.275067 | -3.759751 | 1.589774 |
| 1 | 0.498937 | 2.972784 | 2.322896 | 1 | -0.110760 | -3.037307 | 2.415854 |
| 6 | -1.655586 | 2.275593 | -1.272995 | 6 | 1.777092 | -2.208800 | -1.326642 |
| 1 | -2.668835 | 2.693171 | -1.214612 | 1 | 2.801793 | -2.603943 | -1.239501 |
| 1 | -0.935669 | 3.088780 | -1.162145 | 1 | 1.071294 | -3.039567 | -1.226806 |
| 1 | -1.507850 | 1.815354 | -2.254981 | 1 | 1.641456 | -1.757506 | -2.316763 |
| 6 | -2.774205 | -0.331064 | -1.415267 | 6 | 2.861289 | 0.455319 | -1.456910 |
| 1 | -3.574616 | 0.333062 | -1.766674 | 1 | 3.643177 | -0.222715 | -1.832788 |
| 1 | -2.021879 | -0.437147 | -2.210353 | 1 | 2.114596 | 0.616911 | -2.249366 |
| 1 | -3.208573 | -1.315186 | -1.227686 | 1 | 3.332026 | 1.417801 | -1.228212 |
| 27 | 0.000000 | 0.000000 | 0.000000 | 27 | 0.000000 | 0.000000 | 0.000000 |

**Table S31.** Atomic coordinates of the optimized structures for the **Co-d-36** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | -1.154379 | 1.140486 | 1.554001 | 6 | 1.123785 | -1.227479 | 1.534847 |
| 1 | -1.343737 | 0.808037 | 2.571911 | 1 | 1.360839 | -0.921619 | 2.553779 |
| 1 | 1.343737 | -0.808037 | 2.571911 | 1 | -1.360839 | 0.921619 | 2.553779 |
| 6 | 1.154379 | -1.140486 | 1.554001 | 6 | -1.123785 | 1.227479 | 1.534847 |
| 5 | -1.991342 | 0.804956 | 0.347984 | 5 | 1.965863 | -0.961572 | 0.309771 |
| 5 | 1.991342 | -0.804956 | 0.347984 | 5 | -1.965863 | 0.961572 | 0.309771 |
| 5 | 0.000000 | -2.046335 | 1.136162 | 5 | 0.030578 | 2.160913 | 1.146029 |
| 5 | 0.000000 | 2.046335 | 1.136162 | 5 | -0.030578 | -2.160913 | 1.146029 |
| 7 | -1.159675 | 1.277208 | -0.800546 | 7 | 1.074317 | -1.375488 | -0.816664 |
| 7 | -0.085118 | 2.135273 | -0.331716 | 7 | 0.000000 | -2.232687 | -0.314467 |
| 7 | 1.159675 | -1.277208 | -0.800546 | 7 | -1.074317 | 1.375488 | -0.816664 |
| 7 | 0.085118 | -2.135273 | -0.331716 | 7 | 0.000000 | 2.232687 | -0.314467 |
| 6 | 3.344013 | -0.047586 | 0.079242 | 6 | -3.391307 | 0.320594 | 0.040861 |
| 1 | 4.157200 | -0.743975 | -0.165487 | 1 | -4.131658 | 1.103333 | -0.196205 |
| 1 | 3.289949 | 0.666435 | -0.755431 | 1 | -3.413470 | -0.398122 | -0.794382 |
| 1 | 3.665023 | 0.514454 | 0.961242 | 1 | -3.756631 | -0.202191 | 0.935162 |
| 6 | -1.144831 | -2.773235 | 1.927304 | 6 | 1.128124 | 2.929482 | 1.990313 |
| 1 | -1.420954 | -2.202337 | 2.819711 | 1 | 1.138733 | 2.579293 | 3.030995 |
| 1 | -2.063469 | -2.932150 | 1.348428 | 1 | 2.148217 | 2.813482 | 1.592146 |
| 1 | -0.817757 | -3.759293 | 2.280567 | 1 | 0.913806 | 4.010987 | 2.015917 |
| 6 | -0.869645 | -2.595201 | -1.307540 | 6 | 0.954293 | 2.776877 | -1.259233 |
| 1 | -0.425968 | -3.298483 | -2.024730 | 1 | 0.486335 | 3.479231 | -1.966773 |
| 1 | -1.661132 | -3.116634 | -0.765561 | 1 | 1.698903 | 3.330464 | -0.677295 |
| 1 | -1.333446 | -1.769211 | -1.871216 | 1 | 1.482362 | 1.998806 | -1.835399 |
| 6 | 1.546850 | -1.394357 | -2.187583 | 6 | -1.460565 | 1.542309 | -2.209615 |
| 1 | 1.945438 | -2.393849 | -2.407123 | 1 | -1.865955 | 2.550679 | -2.392718 |
| 1 | 0.718532 | -1.189056 | -2.876258 | 1 | -0.624316 | 1.366653 | -2.899826 |
| 1 | 2.338436 | -0.663471 | -2.369922 | 1 | -2.248329 | 0.812173 | -2.424503 |
| 6 | -3.344013 | 0.047586 | 0.079242 | 6 | 3.391307 | -0.320594 | 0.040861 |
| 1 | -3.289949 | -0.666435 | -0.755431 | 1 | 3.413470 | 0.398122 | -0.794382 |
| 1 | -3.665023 | -0.514454 | 0.961242 | 1 | 3.756631 | 0.202191 | 0.935162 |
| 1 | -4.157200 | 0.743975 | -0.165487 | 1 | 4.131658 | -1.103333 | -0.196205 |
| 6 | 1.144831 | 2.773235 | 1.927304 | 6 | -1.128124 | -2.929482 | 1.990313 |
| 1 | 2.063469 | 2.932150 | 1.348428 | 1 | -2.148217 | -2.813482 | 1.592146 |
| 1 | 0.817757 | 3.759293 | 2.280567 | 1 | -0.913806 | -4.010987 | 2.015917 |
| 1 | 1.420954 | 2.202337 | 2.819711 | 1 | -1.138733 | -2.579293 | 3.030995 |
| 6 | 0.869645 | 2.595201 | -1.307540 | 6 | -0.954293 | -2.776877 | -1.259233 |
| 1 | 0.425968 | 3.298483 | -2.024730 | 1 | -0.486335 | -3.479231 | -1.966773 |
| 1 | 1.661132 | 3.116634 | -0.765561 | 1 | -1.698903 | -3.330464 | -0.677295 |
| 1 | 1.333446 | 1.769211 | -1.871216 | 1 | -1.482362 | -1.998806 | -1.835399 |
| 6 | -1.546850 | 1.394357 | -2.187583 | 6 | 1.460565 | -1.542309 | -2.209615 |
| 1 | -1.945438 | 2.393849 | -2.407123 | 1 | 1.865955 | -2.550679 | -2.392718 |
| 1 | -0.718532 | 1.189056 | -2.876258 | 1 | 0.624316 | -1.366653 | -2.899826 |
| 1 | -2.338436 | 0.663471 | -2.369922 | 1 | 2.248329 | -0.812173 | -2.424503 |
| 27 | 0.000000 | 0.000000 | 0.249365 | 27 | 0.000000 | 0.000000 | 0.230739 |

**Table S32.** Atomic coordinates of the optimized structures for the **Co-q-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.001261 | 0.008196 | 1.845875 | 6 | 1.134818 | -0.052420 | 1.801934 |
| 1 | 0.480550 | 0.014687 | 2.801589 | 1 | 0.668468 | -0.084819 | 2.787635 |
| 1 | -0.480550 | 0.008235 | -2.801616 | 1 | -0.668468 | -0.084820 | -2.787635 |
| 6 | -1.001261 | 0.003945 | -1.845889 | 6 | -1.134818 | -0.052420 | -1.801934 |
| 5 | 1.547590 | 1.230857 | 1.122390 | 5 | 1.694152 | 1.196505 | 1.124788 |
| 5 | -1.547591 | 1.228268 | -1.125222 | 5 | -1.694150 | 1.196507 | -1.124789 |
| 5 | -1.532523 | -1.228408 | -1.127017 | 5 | -1.668949 | -1.258857 | -1.026614 |
| 5 | 1.532524 | -1.225809 | 1.129843 | 5 | 1.668947 | -1.258858 | 1.026615 |
| 7 | 2.167040 | 0.705684 | -0.108638 | 7 | 2.224911 | 0.729204 | -0.167514 |
| 7 | 2.169453 | -0.716856 | -0.098863 | 7 | 2.249051 | -0.704323 | -0.203358 |
| 7 | -2.167041 | 0.705932 | 0.107012 | 7 | -2.224910 | 0.729206 | 0.167514 |
| 7 | -2.169453 | -0.716627 | 0.100514 | 7 | -2.249052 | -0.704320 | 0.203358 |
| 6 | -1.517666 | 2.775741 | -1.410857 | 6 | -1.750019 | 2.729240 | -1.532244 |
| 1 | -2.466409 | 3.124567 | -1.838808 | 1 | -2.779287 | 3.027132 | -1.793553 |
| 1 | -1.339904 | 3.383404 | -0.513742 | 1 | -1.417229 | 3.409753 | -0.732464 |
| 1 | -0.736822 | 3.034797 | -2.133595 | 1 | -1.126721 | 2.927068 | -2.414886 |
| 6 | -1.474653 | -2.774695 | -1.415791 | 6 | -1.651309 | -2.823183 | -1.297350 |
| 1 | -0.673621 | -3.019600 | -2.121347 | 1 | -1.045828 | -3.064203 | -2.181753 |
| 1 | -1.309688 | -3.384555 | -0.517875 | 1 | -1.250622 | -3.408287 | -0.454406 |
| 1 | -2.407897 | -3.133949 | -1.868308 | 1 | -2.668565 | -3.201332 | -1.491835 |
| 6 | -2.706558 | -1.415761 | 1.240758 | 6 | -2.763491 | -1.372882 | 1.383614 |
| 1 | -3.773020 | -1.202450 | 1.389305 | 1 | -3.823903 | -1.136737 | 1.563381 |
| 1 | -2.597967 | -2.484052 | 1.044729 | 1 | -2.681204 | -2.450138 | 1.205752 |
| 1 | -2.167594 | -1.183915 | 2.169382 | 1 | -2.187295 | -1.129784 | 2.289554 |
| 6 | -2.770657 | 1.397656 | 1.217300 | 6 | -2.977599 | 1.466249 | 1.164477 |
| 1 | -3.851524 | 1.213280 | 1.278971 | 1 | -4.063086 | 1.295422 | 1.068863 |
| 1 | -2.312107 | 1.130949 | 2.178188 | 1 | -2.670268 | 1.219553 | 2.190220 |
| 1 | -2.616822 | 2.466067 | 1.054485 | 1 | -2.784286 | 2.531156 | 0.997852 |
| 6 | 1.517664 | 2.778983 | 1.404460 | 6 | 1.750023 | 2.729239 | 1.532243 |
| 1 | 1.339901 | 3.384579 | 0.505948 | 1 | 1.417234 | 3.409753 | 0.732463 |
| 1 | 0.736819 | 3.039704 | 2.126599 | 1 | 1.126725 | 2.927068 | 2.414885 |
| 1 | 2.466406 | 3.128795 | 1.831607 | 1 | 2.779291 | 3.027129 | 1.793553 |
| 6 | 1.474655 | -2.771426 | 1.422178 | 6 | 1.651304 | -2.823184 | 1.297351 |
| 1 | 1.309692 | -3.383353 | 0.525669 | 1 | 1.250617 | -3.408287 | 0.454406 |
| 1 | 2.407899 | -3.129637 | 1.875522 | 1 | 2.668559 | -3.201334 | 1.491836 |
| 1 | 0.673623 | -3.014706 | 2.128295 | 1 | 1.045823 | -3.064203 | 2.181754 |
| 6 | 2.706559 | -1.418614 | -1.237495 | 6 | 2.763489 | -1.372886 | -1.383613 |
| 1 | 3.773020 | -1.205643 | -1.386534 | 1 | 3.823901 | -1.136743 | -1.563381 |
| 1 | 2.597969 | -2.486450 | -1.039005 | 1 | 2.681200 | -2.450142 | -1.205751 |
| 1 | 2.167593 | -1.188907 | -2.166649 | 1 | 2.187293 | -1.129787 | -2.289553 |
| 6 | 2.770657 | 1.394850 | -1.220515 | 6 | 2.977602 | 1.466245 | -1.164477 |
| 1 | 3.851524 | 1.210335 | -1.281759 | 1 | 4.063089 | 1.295417 | -1.068862 |
| 1 | 2.312109 | 1.125930 | -2.180787 | 1 | 2.670272 | 1.219549 | -2.190220 |
| 1 | 2.616820 | 2.463633 | -1.060162 | 1 | 2.784290 | 2.531152 | -0.997852 |
| 27 | 0.000000 | 0.012723 | 0.000000 | 27 | 0.000000 | 0.038578 | 0.000000 |

**Table S33.** Atomic coordinates of the optimized structures for the **Co-q-36** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.985728 | -1.584252 | 1.599094 | 6 | 0.710764 | -1.739576 | 1.613441 |
| 1 | 1.160147 | -1.529812 | 2.669705 | 1 | 0.745870 | -1.749688 | 2.702840 |
| 1 | -1.160147 | 1.529812 | 2.669705 | 1 | -0.745870 | 1.749688 | 2.702840 |
| 6 | -0.985728 | 1.584252 | 1.599094 | 6 | -0.710764 | 1.739576 | 1.613441 |
| 5 | 1.948580 | -1.142060 | 0.515261 | 5 | 1.863130 | -1.385490 | 0.689689 |
| 5 | -1.948580 | 1.142060 | 0.515261 | 5 | -1.863130 | 1.385490 | 0.689689 |
| 5 | 0.177754 | 2.288932 | 0.931719 | 5 | 0.393892 | 2.345644 | 0.753347 |
| 5 | -0.177754 | -2.288932 | 0.931719 | 5 | -0.393892 | -2.345644 | 0.753347 |
| 7 | 1.212384 | -1.336280 | -0.762669 | 7 | 1.290272 | -1.435147 | -0.682227 |
| 7 | 0.000000 | -2.047480 | -0.513851 | 7 | 0.000000 | -2.072294 | -0.637618 |
| 7 | -1.212384 | 1.336280 | -0.762669 | 7 | -1.290272 | 1.435147 | -0.682227 |
| 7 | 0.000000 | 2.047480 | -0.513851 | 7 | 0.000000 | 2.072294 | -0.637618 |
| 6 | -3.404206 | 0.544196 | 0.481322 | 6 | -3.377887 | 0.979518 | 0.922485 |
| 1 | -4.140176 | 1.297198 | 0.168866 | 1 | -4.054602 | 1.798233 | 0.624394 |
| 1 | -3.511229 | -0.297505 | -0.218052 | 1 | -3.688548 | 0.088062 | 0.354175 |
| 1 | -3.717917 | 0.185656 | 1.465521 | 1 | -3.569778 | 0.775713 | 1.984243 |
| 6 | 1.454154 | 3.056338 | 1.437622 | 6 | 1.760111 | 3.079561 | 1.089644 |
| 1 | 1.464631 | 3.148268 | 2.526623 | 1 | 1.953620 | 3.067760 | 2.170454 |
| 1 | 2.386103 | 2.548011 | 1.154424 | 1 | 2.636000 | 2.627075 | 0.597372 |
| 1 | 1.518450 | 4.072083 | 1.025765 | 1 | 1.730533 | 4.136655 | 0.777092 |
| 6 | 0.892926 | 2.294175 | -1.616847 | 6 | 0.732625 | 2.259383 | -1.873866 |
| 1 | 0.446351 | 2.950321 | -2.375670 | 1 | 0.204685 | 2.923072 | -2.576356 |
| 1 | 1.776215 | 2.792935 | -1.212959 | 1 | 1.686873 | 2.730856 | -1.616015 |
| 1 | 1.220844 | 1.367450 | -2.111707 | 1 | 0.948681 | 1.308632 | -2.388571 |
| 6 | -1.732820 | 1.344347 | -2.106436 | 6 | -2.035068 | 1.498817 | -1.927689 |
| 1 | -2.001883 | 2.358396 | -2.435916 | 1 | -2.299861 | 2.536688 | -2.193623 |
| 1 | -1.029652 | 0.922638 | -2.838449 | 1 | -1.489194 | 1.053764 | -2.772245 |
| 1 | -2.639965 | 0.735417 | -2.111845 | 1 | -2.963402 | 0.935314 | -1.785017 |
| 6 | 3.404206 | -0.544196 | 0.481322 | 6 | 3.377887 | -0.979518 | 0.922485 |
| 1 | 3.511229 | 0.297505 | -0.218052 | 1 | 3.688548 | -0.088062 | 0.354175 |
| 1 | 3.717917 | -0.185656 | 1.465521 | 1 | 3.569778 | -0.775713 | 1.984243 |
| 1 | 4.140176 | -1.297198 | 0.168866 | 1 | 4.054602 | -1.798233 | 0.624394 |
| 6 | -1.454154 | -3.056338 | 1.437622 | 6 | -1.760111 | -3.079561 | 1.089644 |
| 1 | -2.386103 | -2.548011 | 1.154424 | 1 | -2.636000 | -2.627075 | 0.597372 |
| 1 | -1.518450 | -4.072083 | 1.025765 | 1 | -1.730533 | -4.136655 | 0.777092 |
| 1 | -1.464631 | -3.148268 | 2.526623 | 1 | -1.953620 | -3.067760 | 2.170454 |
| 6 | -0.892926 | -2.294175 | -1.616847 | 6 | -0.732625 | -2.259383 | -1.873866 |
| 1 | -0.446351 | -2.950321 | -2.375670 | 1 | -0.204685 | -2.923072 | -2.576356 |
| 1 | -1.776215 | -2.792935 | -1.212959 | 1 | -1.686873 | -2.730856 | -1.616015 |
| 1 | -1.220844 | -1.367450 | -2.111707 | 1 | -0.948681 | -1.308632 | -2.388571 |
| 6 | 1.732820 | -1.344347 | -2.106436 | 6 | 2.035068 | -1.498817 | -1.927689 |
| 1 | 2.001883 | -2.358396 | -2.435916 | 1 | 2.299861 | -2.536688 | -2.193623 |
| 1 | 1.029652 | -0.922638 | -2.838449 | 1 | 1.489194 | -1.053764 | -2.772245 |
| 1 | 2.639965 | -0.735417 | -2.111845 | 1 | 2.963402 | -0.935314 | -1.785017 |
| 27 | 0.000000 | 0.000000 | 0.535252 | 27 | 0.000000 | 0.000000 | 0.533400 |

**Table S34.** Atomic coordinates of the optimized structures for the **Ni-s-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 1.016579 | -0.241430 | 1.803994 | 6 | 1.097712 | -0.206926 | 1.807426 |
| 1 | 0.597368 | 0.079105 | 2.756569 | 1 | 0.707046 | 0.096524 | 2.780457 |
| 1 | -0.597368 | -0.079105 | -2.756569 | 1 | -0.707046 | -0.096524 | -2.780457 |
| 6 | -1.016579 | 0.241430 | -1.803994 | 6 | -1.097712 | 0.206926 | -1.807426 |
| 5 | 2.055084 | 0.543792 | 0.995877 | 5 | 2.211050 | 0.532563 | 1.033726 |
| 5 | -0.829637 | 1.577755 | -1.142873 | 5 | -0.922314 | 1.554471 | -1.155541 |
| 5 | -2.055084 | -0.543792 | -0.995877 | 5 | -2.211050 | -0.532563 | -1.033726 |
| 5 | 0.829637 | -1.577755 | 1.142873 | 5 | 0.922314 | -1.554471 | 1.155541 |
| 7 | 2.437192 | -0.285524 | -0.163388 | 7 | 2.518043 | -0.265813 | -0.152942 |
| 7 | 1.429262 | -1.330162 | -0.218049 | 7 | 1.471474 | -1.293483 | -0.224424 |
| 7 | -1.429262 | 1.330162 | 0.218049 | 7 | -1.471474 | 1.293483 | 0.224424 |
| 7 | -2.437192 | 0.285524 | 0.163388 | 7 | -2.518043 | 0.265813 | 0.152942 |
| 6 | -0.123868 | 2.943212 | -1.464117 | 6 | -0.266407 | 2.940370 | -1.547672 |
| 1 | -0.857531 | 3.745001 | -1.622432 | 1 | -1.045446 | 3.708124 | -1.691904 |
| 1 | 0.534634 | 3.287192 | -0.654915 | 1 | 0.424758 | 3.333381 | -0.785503 |
| 1 | 0.483216 | 2.885411 | -2.372577 | 1 | 0.288327 | 2.864699 | -2.492844 |
| 6 | -2.726462 | -1.947034 | -1.219842 | 6 | -2.968868 | -1.892302 | -1.325867 |
| 1 | -2.295108 | -2.486963 | -2.068168 | 1 | -2.753780 | -2.273057 | -2.333320 |
| 1 | -2.650347 | -2.600212 | -0.340113 | 1 | -2.676249 | -2.677232 | -0.608515 |
| 1 | -3.800198 | -1.840549 | -1.421602 | 1 | -4.061120 | -1.780276 | -1.236833 |
| 6 | -2.849956 | -0.244321 | 1.446925 | 6 | -3.012725 | -0.249397 | 1.421437 |
| 1 | -3.431568 | 0.484553 | 2.024630 | 1 | -3.569325 | 0.512147 | 1.987413 |
| 1 | -3.497808 | -1.100584 | 1.247469 | 1 | -3.710572 | -1.060881 | 1.185039 |
| 1 | -2.002998 | -0.588558 | 2.065002 | 1 | -2.214419 | -0.656015 | 2.066122 |
| 6 | -1.569433 | 2.309924 | 1.277279 | 6 | -1.652694 | 2.311887 | 1.253681 |
| 1 | -2.515979 | 2.853979 | 1.167490 | 1 | -2.604099 | 2.844652 | 1.097222 |
| 1 | -1.534199 | 1.846566 | 2.267820 | 1 | -1.642308 | 1.877836 | 2.260603 |
| 1 | -0.739972 | 3.015412 | 1.195944 | 1 | -0.826121 | 3.025393 | 1.176485 |
| 6 | 2.726462 | 1.947034 | 1.219842 | 6 | 2.968868 | 1.892302 | 1.325867 |
| 1 | 2.650347 | 2.600212 | 0.340113 | 1 | 2.676249 | 2.677232 | 0.608515 |
| 1 | 2.295108 | 2.486963 | 2.068168 | 1 | 2.753780 | 2.273057 | 2.333320 |
| 1 | 3.800198 | 1.840549 | 1.421602 | 1 | 4.061120 | 1.780276 | 1.236833 |
| 6 | 0.123868 | -2.943212 | 1.464117 | 6 | 0.266407 | -2.940370 | 1.547672 |
| 1 | -0.534634 | -3.287192 | 0.654915 | 1 | -0.424758 | -3.333381 | 0.785503 |
| 1 | 0.857531 | -3.745001 | 1.622432 | 1 | 1.045446 | -3.708124 | 1.691904 |
| 1 | -0.483216 | -2.885411 | 2.372577 | 1 | -0.288327 | -2.864699 | 2.492844 |
| 6 | 1.569433 | -2.309924 | -1.277279 | 6 | 1.652694 | -2.311887 | -1.253681 |
| 1 | 2.515979 | -2.853979 | -1.167490 | 1 | 2.604099 | -2.844652 | -1.097222 |
| 1 | 0.739972 | -3.015412 | -1.195944 | 1 | 0.826121 | -3.025393 | -1.176485 |
| 1 | 1.534199 | -1.846566 | -2.267820 | 1 | 1.642308 | -1.877836 | -2.260603 |
| 6 | 2.849956 | 0.244321 | -1.446925 | 6 | 3.012725 | 0.249397 | -1.421437 |
| 1 | 3.431568 | -0.484553 | -2.024630 | 1 | 3.569325 | -0.512147 | -1.987413 |
| 1 | 2.002998 | 0.588558 | -2.065002 | 1 | 2.214419 | 0.656015 | -2.066122 |
| 1 | 3.497808 | 1.100584 | -1.247469 | 1 | 3.710572 | 1.060881 | -1.185039 |
| 28 | 0.000000 | 0.000000 | 0.000000 | 28 | 0.000000 | 0.000000 | 0.000000 |

**Table S35.** Atomic coordinates of the optimized structures for the **Ni-t-180** complexes.

| | M06-L | | | | B3LYP* | | |
|---|---|---|---|---|---|---|---|
| | X | Y | Z | | X | Y | Z |
| 6 | 0.000000 | 2.143836 | 0.000086 | 6 | 0.000000 | 2.188000 | 0.000110 |
| 1 | -0.909249 | 2.741929 | 0.000140 | 1 | -0.904426 | 2.798355 | 0.000182 |
| 1 | 0.909249 | -2.741929 | 0.000140 | 1 | 0.904426 | -2.798355 | 0.000182 |
| 6 | 0.000000 | -2.143836 | 0.000086 | 6 | 0.000000 | -2.188000 | 0.000110 |
| 5 | 0.765549 | 1.709252 | -1.228341 | 5 | 0.792616 | 1.785448 | -1.229666 |
| 5 | -0.765549 | -1.709252 | -1.228341 | 5 | -0.792616 | -1.785448 | -1.229666 |
| 5 | -0.765653 | -1.709179 | 1.228426 | 5 | -0.792754 | -1.785357 | 1.229773 |
| 5 | 0.765653 | 1.709179 | 1.228426 | 5 | 0.792754 | 1.785357 | 1.229773 |
| 7 | 1.871143 | 0.862092 | -0.714879 | 7 | 1.882814 | 0.922200 | -0.719298 |
| 7 | 1.871222 | 0.862077 | 0.714824 | 7 | 1.882913 | 0.922179 | 0.719225 |
| 7 | -1.871143 | -0.862092 | -0.714879 | 7 | -1.882814 | -0.922200 | -0.719298 |
| 7 | -1.871222 | -0.862077 | 0.714824 | 7 | -1.882913 | -0.922179 | 0.719225 |
| 6 | -0.586619 | -1.910188 | -2.778889 | 6 | -0.634802 | -2.058086 | -2.785126 |
| 1 | -1.241656 | -2.706573 | -3.155295 | 1 | -1.409222 | -2.758696 | -3.139505 |
| 1 | -0.816582 | -1.014115 | -3.370252 | 1 | -0.721171 | -1.150985 | -3.404019 |
| 1 | 0.436805 | -2.208691 | -3.029237 | 1 | 0.337015 | -2.519342 | -3.008043 |
| 6 | -0.586836 | -1.910020 | 2.779000 | 6 | -0.635082 | -2.057867 | 2.785270 |
| 1 | 0.436594 | -2.208422 | 3.029445 | 1 | 0.336711 | -2.519115 | 3.008309 |
| 1 | -0.816921 | -1.013938 | 3.370301 | 1 | -0.721491 | -1.150714 | 3.404080 |
| 1 | -1.241833 | -2.706445 | 3.155388 | 1 | -1.409540 | -2.758438 | 3.139642 |
| 6 | -2.888917 | -0.114357 | 1.409417 | 6 | -2.964578 | -0.264591 | 1.427843 |
| 1 | -3.892981 | -0.517070 | 1.221703 | 1 | -3.934451 | -0.753534 | 1.241678 |
| 1 | -2.680374 | -0.202475 | 2.477339 | 1 | -2.742782 | -0.342447 | 2.497159 |
| 1 | -2.878386 | 0.951339 | 1.147099 | 1 | -3.044721 | 0.801217 | 1.172174 |
| 6 | -2.888862 | -0.114532 | -1.409606 | 6 | -2.964508 | -0.264839 | -1.428081 |
| 1 | -3.892888 | -0.517414 | -1.222038 | 1 | -3.934306 | -0.753990 | -1.242066 |
| 1 | -2.878546 | 0.951161 | -1.147272 | 1 | -3.044918 | 0.800950 | -1.172420 |
| 1 | -2.680153 | -0.202599 | -2.477499 | 1 | -2.742531 | -0.342641 | -2.497364 |
| 6 | 0.586619 | 1.910188 | -2.778889 | 6 | 0.634802 | 2.058086 | -2.785126 |
| 1 | 0.816582 | 1.014115 | -3.370252 | 1 | 0.721171 | 1.150985 | -3.404019 |
| 1 | -0.436805 | 2.208691 | -3.029237 | 1 | -0.337015 | 2.519342 | -3.008043 |
| 1 | 1.241656 | 2.706573 | -3.155295 | 1 | 1.409222 | 2.758696 | -3.139505 |
| 6 | 0.586836 | 1.910020 | 2.779000 | 6 | 0.635082 | 2.057867 | 2.785270 |
| 1 | 0.816921 | 1.013938 | 3.370301 | 1 | 0.721491 | 1.150714 | 3.404080 |
| 1 | 1.241833 | 2.706445 | 3.155388 | 1 | 1.409540 | 2.758438 | 3.139642 |
| 1 | -0.436594 | 2.208422 | 3.029445 | 1 | -0.336711 | 2.519115 | 3.008309 |
| 6 | 2.888917 | 0.114357 | 1.409417 | 6 | 2.964578 | 0.264591 | 1.427843 |
| 1 | 3.892981 | 0.517070 | 1.221703 | 1 | 3.934451 | 0.753534 | 1.241678 |
| 1 | 2.680374 | 0.202475 | 2.477339 | 1 | 2.742782 | 0.342447 | 2.497159 |
| 1 | 2.878386 | -0.951339 | 1.147099 | 1 | 3.044721 | -0.801217 | 1.172174 |
| 6 | 2.888862 | 0.114532 | -1.409606 | 6 | 2.964508 | 0.264839 | -1.428081 |
| 1 | 3.892888 | 0.517414 | -1.222038 | 1 | 3.934306 | 0.753990 | -1.242066 |
| 1 | 2.878546 | -0.951161 | -1.147272 | 1 | 3.044918 | -0.800950 | -1.172420 |
| 1 | 2.680153 | 0.202599 | -2.477499 | 1 | 2.742531 | 0.342641 | -2.497364 |
| 28 | 0.000000 | 0.000000 | 0.000006 | 28 | 0.000000 | 0.000000 | 0.000005 |