

# Influence of Bridging Group and Substitution Effect of Bis(1,2,4-Triazine) N-Donor Extractants on Their Interactions with Neptunium (V) Cation

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Supporting Information:

## SI\_Geometry Structures of Main Complexes

In the gas phase: (Standard orientation)

| [NpO <sub>2</sub> (H <sub>2</sub> O) <sub>5</sub> ] <sup>+</sup> |                         |           |           |
|------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                                    | Coordinates (Angstroms) |           |           |
|                                                                  | X                       | Y         | Z         |
| 93                                                               | 0.005722                | 0.037727  | 0.003178  |
| 8                                                                | 0.102728                | 0.095050  | 1.786956  |
| 8                                                                | -0.096374               | 0.071934  | -1.781166 |
| 8                                                                | -0.298943               | 2.578245  | 0.010621  |
| 1                                                                | -0.309125               | 3.158743  | -0.767091 |
| 1                                                                | -0.303626               | 3.145476  | 0.798139  |
| 8                                                                | 1.560584                | -2.014869 | -0.137293 |
| 1                                                                | 2.503844                | -1.799689 | -0.050001 |
| 1                                                                | 1.469286                | -2.528399 | -0.957295 |
| 8                                                                | -2.607626               | 0.242433  | -0.072731 |
| 1                                                                | -2.955851               | 0.558769  | -0.923356 |
| 1                                                                | -3.121267               | 0.690167  | 0.619681  |
| 8                                                                | 2.515825                | 0.719059  | 0.023807  |
| 1                                                                | 2.962506                | 1.163362  | -0.715413 |
| 1                                                                | 2.863857                | 1.113852  | 0.840602  |
| 8                                                                | -1.225581               | -2.217945 | 0.145363  |
| 1                                                                | -2.187190               | -2.085156 | 0.092147  |
| 1                                                                | -1.059497               | -2.716968 | 0.962539  |

| NpO <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> NO <sub>3</sub> |                         |           |           |
|------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                                    | Coordinates (Angstroms) |           |           |
|                                                                  | X                       | Y         | Z         |
| 93                                                               | -0.305564               | -0.001607 | 0.002214  |
| 8                                                                | -0.346249               | 0.322174  | -1.771037 |
| 8                                                                | -0.348013               | -0.326415 | 1.774512  |
| 8                                                                | -0.093318               | 2.740291  | -0.153045 |
| 1                                                                | -0.032999               | 2.634930  | -1.120119 |
| 1                                                                | 0.834463                | 2.806035  | 0.139801  |
| 8                                                                | -0.106589               | -2.732885 | 0.120892  |
| 1                                                                | -0.041353               | -2.658981 | 1.090463  |
| 1                                                                | 0.818991                | -2.804405 | -0.177595 |
| 8                                                                | -2.435064               | -1.443887 | -0.500303 |
| 1                                                                | -1.994148               | -2.313010 | -0.551031 |
| 1                                                                | -2.672463               | -1.210208 | -1.412814 |
| 8                                                                | -2.416711               | 1.464412  | 0.505797  |
| 1                                                                | -2.643555               | 1.251479  | 1.426046  |
| 1                                                                | -1.964181               | 2.328972  | 0.532444  |
| 7                                                                | 2.692227                | -0.002407 | 0.001537  |
| 8                                                                | 3.904797                | -0.002464 | -0.001029 |
| 8                                                                | 2.000096                | 1.069437  | 0.145631  |
| 8                                                                | 1.999446                | -1.074228 | -0.139401 |

| [NpO <sub>2</sub> (H <sub>2</sub> O) <sub>6</sub> ] <sup>+</sup> |                         |           |           |
|------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                                    | Coordinates (Angstroms) |           |           |
|                                                                  | X                       | Y         | Z         |
| 93                                                               | -0.234561               | -0.030110 | 0.053952  |
| 8                                                                | 0.229597                | -0.002720 | -1.674364 |
| 8                                                                | -0.736819               | -0.033715 | 1.771345  |
| 8                                                                | -0.662506               | 2.583512  | -0.203308 |
| 1                                                                | -0.931562               | 2.815055  | -1.109066 |
| 1                                                                | -1.325020               | 2.987030  | 0.383182  |
| 8                                                                | -1.117236               | -2.428547 | -0.191558 |
| 1                                                                | -1.240667               | -2.921738 | 0.636735  |
| 1                                                                | -0.568980               | -2.994536 | -0.761328 |
| 8                                                                | 1.796268                | 1.607655  | 0.590280  |
| 1                                                                | 2.047570                | 1.692875  | 1.526080  |
| 1                                                                | 1.381659                | 2.457484  | 0.346775  |
| 8                                                                | -2.704534               | 0.224868  | -0.623796 |
| 1                                                                | -3.366877               | -0.023847 | 0.042473  |
| 1                                                                | -2.975284               | -0.209518 | -1.450169 |
| 8                                                                | 3.647172                | -0.244487 | -0.708470 |
| 1                                                                | 3.659524                | -0.362998 | -1.672117 |
| 1                                                                | 3.274406                | 0.643480  | -0.555748 |
| 8                                                                | 1.715317                | -1.501614 | 0.550602  |
| 1                                                                | 2.532749                | -1.179381 | 0.060434  |
| 1                                                                | 1.988598                | -1.743300 | 1.449364  |

| NpO <sub>2</sub> (H <sub>2</sub> O) <sub>5</sub> NO <sub>3</sub> |                         |           |           |
|------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                                    | Coordinates (Angstroms) |           |           |
|                                                                  | X                       | Y         | Z         |
| 93                                                               | 0.412240                | 0.034210  | -0.006805 |
| 8                                                                | 0.728306                | -0.236571 | 1.753374  |
| 8                                                                | 0.144392                | 0.344967  | -1.750110 |
| 8                                                                | -0.637443               | 2.334265  | 0.717562  |
| 1                                                                | -1.560869               | 2.459663  | 0.337564  |
| 1                                                                | -0.751309               | 2.241225  | 1.677396  |
| 8                                                                | 2.975214                | -0.352107 | -0.455776 |
| 1                                                                | 3.439240                | 0.048813  | 0.297149  |
| 1                                                                | 2.977345                | -1.315789 | -0.299068 |
| 8                                                                | -3.101001               | 2.332553  | -0.287428 |
| 1                                                                | -3.088201               | 1.350697  | -0.336654 |
| 1                                                                | -3.814495               | 2.540626  | 0.335549  |
| 8                                                                | 1.903410                | 2.226047  | -0.179060 |
| 1                                                                | 1.974210                | 2.281682  | -1.147101 |
| 1                                                                | 1.142188                | 2.794041  | 0.057763  |
| 8                                                                | 1.488547                | -2.550193 | 0.177387  |
| 1                                                                | 0.761958                | -3.058545 | -0.224767 |
| 1                                                                | 1.233832                | -2.457828 | 1.113730  |
| 7                                                                | -2.251309               | -1.406938 | -0.040151 |
| 8                                                                | -2.159377               | -0.143907 | 0.201989  |
| 8                                                                | -1.132563               | -2.020118 | -0.108684 |
| 8                                                                | -3.321118               | -1.962130 | -0.181462 |

| [NpO <sub>2</sub> (BTP)] <sup>+</sup> |                         |           |           |
|---------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                         | Coordinates (Angstroms) |           |           |
|                                       | X                       | Y         | Z         |
| 6                                     | -1.201997               | 3.400393  | -0.000694 |
| 6                                     | -1.156707               | 2.002377  | -0.000181 |
| 6                                     | 1.156689                | 2.002259  | 0.000035  |
| 6                                     | 1.202097                | 3.400290  | 0.000413  |
| 6                                     | 0.000085                | 4.105121  | -0.000185 |
| 1                                     | -2.162199               | 3.902484  | -0.001374 |
| 1                                     | 2.162342                | 3.902294  | 0.001105  |
| 1                                     | 0.000130                | 5.190356  | -0.000245 |
| 6                                     | -2.397918               | 1.192068  | 0.002148  |
| 6                                     | -4.646588               | 1.005075  | 0.002600  |
| 6                                     | -4.495333               | -0.394488 | 0.012152  |
| 1                                     | -5.630503               | 1.467928  | -0.001333 |
| 1                                     | -5.340674               | -1.074481 | 0.017252  |
| 6                                     | 2.397891                | 1.191929  | -0.002152 |
| 6                                     | 4.646595                | 1.005110  | -0.002298 |
| 6                                     | 4.495446                | -0.394455 | -0.012534 |
| 1                                     | 5.630467                | 1.468049  | 0.002124  |
| 1                                     | 5.340832                | -1.074393 | -0.017922 |
| 7                                     | -0.000037               | 1.314846  | -0.000054 |
| 7                                     | -2.236800               | -0.138197 | 0.008794  |
| 7                                     | -3.287781               | -0.949212 | 0.013278  |
| 7                                     | -3.590063               | 1.806122  | -0.002679 |
| 7                                     | 2.236877                | -0.138361 | -0.009230 |
| 7                                     | 3.287942                | -0.949269 | -0.013925 |
| 7                                     | 3.589998                | 1.806056  | 0.003120  |
| 93                                    | -0.000030               | -1.317851 | 0.000087  |
| 8                                     | -0.062782               | -1.349193 | -1.772457 |
| 8                                     | 0.062771                | -1.348312 | 1.772630  |

| [NpO <sub>2</sub> (C2-BTP)] <sup>+</sup> |                         |           |           |
|------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                            | Coordinates (Angstroms) |           |           |
|                                          | X                       | Y         | Z         |
| 6                                        | -1.200727               | 3.436385  | -0.066905 |
| 6                                        | -1.156509               | 2.038972  | -0.063597 |
| 6                                        | 1.156595                | 2.038979  | 0.062729  |
| 6                                        | 1.200846                | 3.436379  | 0.065771  |
| 6                                        | 0.000064                | 4.140226  | -0.000654 |
| 1                                        | -2.159935               | 3.937102  | -0.120966 |
| 1                                        | 2.160055                | 3.937097  | 0.119803  |
| 1                                        | 0.000080                | 5.225618  | -0.000752 |
| 6                                        | -2.392357               | 1.222654  | -0.128841 |
| 6                                        | -4.657721               | 1.040869  | -0.257547 |
| 6                                        | -4.499167               | -0.384284 | -0.238736 |
| 6                                        | 2.392390                | 1.222579  | 0.128373  |
| 6                                        | 4.657700                | 1.040708  | 0.257787  |
| 6                                        | 4.499103                | -0.384431 | 0.238891  |
| 7                                        | 0.000048                | 1.354021  | -0.000400 |
| 7                                        | -2.226051               | -0.099729 | -0.113273 |
| 7                                        | -3.279555               | -0.910009 | -0.169584 |
| 7                                        | -3.585638               | 1.825634  | -0.201899 |
| 7                                        | 2.226010                | -0.099803 | 0.113067  |
| 7                                        | 3.279484                | -0.910116 | 0.169606  |
| 7                                        | 3.585673                | 1.825517  | 0.201704  |
| 6                                        | -6.000297               | 1.716502  | -0.299439 |
| 6                                        | -6.521596               | 2.036181  | 1.119991  |
| 1                                        | -6.725188               | 1.092866  | -0.830681 |
| 1                                        | -5.884625               | 2.649354  | -0.859816 |
| 1                                        | -7.487013               | 2.545563  | 1.050757  |
| 1                                        | -6.660443               | 1.129192  | 1.718007  |
| 1                                        | -5.823735               | 2.692333  | 1.649047  |
| 6                                        | -5.671820               | -1.332516 | -0.307792 |
| 6                                        | -5.316666               | -2.817443 | -0.204289 |
| 1                                        | -6.205580               | -1.141363 | -1.250045 |
| 1                                        | -6.380761               | -1.058410 | 0.485269  |
| 1                                        | -6.231330               | -3.414508 | -0.261561 |
| 1                                        | -4.653529               | -3.127926 | -1.016662 |
| 1                                        | -4.818295               | -3.044904 | 0.742820  |
| 6                                        | 6.000294                | 1.716263  | 0.300448  |
| 6                                        | 6.522136                | 2.036447  | -1.118656 |
| 1                                        | 6.724940                | 1.092405  | 0.831758  |
| 1                                        | 5.884435                | 2.648911  | 0.861133  |
| 1                                        | 7.487455                | 2.545943  | -1.048878 |
| 1                                        | 6.661364                | 1.129657  | -1.716890 |
| 1                                        | 5.824394                | 2.692651  | -1.647806 |
| 6                                        | 5.671751                | -1.332669 | 0.307951  |
| 6                                        | 5.316709                | -2.817540 | 0.203205  |
| 1                                        | 6.204957                | -1.142172 | 1.250659  |
| 1                                        | 6.381132                | -1.057974 | -0.484503 |
| 1                                        | 6.231390                | -3.414602 | 0.260243  |
| 1                                        | 4.653388                | -3.128696 | 1.015166  |
| 1                                        | 4.818591                | -3.044287 | -0.744212 |
| 93                                       | -0.000051               | -1.268852 | 0.000102  |
| 8                                        | -0.039125               | -1.309575 | 1.776310  |
| 8                                        | 0.038974                | -1.311027 | -1.776073 |

| [NpO <sub>2</sub> (BTPen)] <sup>+</sup> |                         |           |           |
|-----------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                           | Coordinates (Angstroms) |           |           |
|                                         | X                       | Y         | Z         |
| 6                                       | 3.482593                | 2.255771  | 0.001900  |
| 6                                       | 2.829500                | 3.470542  | 0.003072  |
| 6                                       | 1.418908                | 3.510050  | 0.001796  |
| 6                                       | 0.726018                | 2.267602  | -0.000423 |
| 6                                       | 2.713802                | 1.075183  | -0.002075 |
| 6                                       | 0.681883                | 4.740507  | 0.001384  |
| 6                                       | -0.724874               | 2.267764  | 0.001272  |
| 6                                       | -1.417471               | 3.510351  | -0.001550 |
| 6                                       | -0.680174               | 4.740647  | -0.001357 |
| 6                                       | -2.828067               | 3.471143  | -0.003370 |
| 1                                       | -3.390628               | 4.400331  | -0.005708 |
| 6                                       | -3.481389               | 2.256509  | -0.002348 |
| 6                                       | -2.712887               | 1.075706  | 0.002225  |
| 1                                       | 1.234683                | 5.675208  | 0.002495  |
| 1                                       | 4.563200                | 2.183637  | 0.003508  |
| 1                                       | 3.392247                | 4.399619  | 0.004996  |
| 1                                       | -1.232785               | 5.675460  | -0.002759 |
| 1                                       | -4.562004               | 2.184605  | -0.004528 |
| 7                                       | -2.577742               | -1.325142 | 0.008092  |
| 6                                       | -3.378631               | -0.249942 | 0.003997  |
| 6                                       | -5.241986               | -1.524015 | 0.003423  |
| 6                                       | -4.418218               | -2.663045 | 0.010294  |
| 7                                       | -3.093324               | -2.548363 | 0.011047  |
| 1                                       | -6.326202               | -1.608124 | 0.000104  |
| 1                                       | -4.815903               | -3.672507 | 0.013744  |
| 7                                       | 2.577133                | -1.325316 | -0.008007 |
| 6                                       | 3.378883                | -0.250772 | -0.004223 |
| 6                                       | 5.241211                | -1.526250 | -0.004690 |
| 6                                       | 4.416554                | -2.664656 | -0.011198 |
| 7                                       | 3.091748                | -2.548953 | -0.011286 |
| 1                                       | 6.325362                | -1.611214 | -0.001922 |
| 1                                       | 4.813472                | -3.674419 | -0.014846 |
| 7                                       | -4.719605               | -0.305542 | 0.000091  |
| 7                                       | 4.719794                | -0.307359 | -0.001014 |
| 7                                       | -1.374960               | 1.082064  | 0.005334  |
| 7                                       | 1.375891                | 1.081807  | -0.004351 |
| 93                                      | -0.000229               | -1.144507 | 0.000155  |
| 8                                       | -0.063767               | -1.168715 | -1.781368 |
| 8                                       | 0.062935                | -1.170578 | 1.781669  |

| [NpO <sub>2</sub> (BTBP)] <sup>+</sup> |                         |           |           |
|----------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                          | Coordinates (Angstroms) |           |           |
|                                        | X                       | Y         | Z         |
| 6                                      | -0.745278               | 2.517675  | 0.035850  |
| 6                                      | -2.719031               | 1.288667  | 0.034319  |
| 6                                      | -3.505764               | 2.437834  | 0.131484  |
| 6                                      | -2.863352               | 3.669988  | 0.198904  |
| 6                                      | -1.475041               | 3.712383  | 0.152956  |
| 6                                      | 0.745330                | 2.517695  | -0.036078 |
| 6                                      | 2.719066                | 1.288646  | -0.035076 |
| 6                                      | 3.505815                | 2.437826  | -0.131898 |
| 6                                      | 2.863419                | 3.670019  | -0.198810 |
| 6                                      | 1.475116                | 3.712441  | -0.152688 |
| 1                                      | -4.584472               | 2.346425  | 0.159747  |
| 1                                      | -3.436599               | 4.587115  | 0.288980  |
| 1                                      | -0.972607               | 4.668390  | 0.219907  |
| 1                                      | 4.584523                | 2.346425  | -0.160214 |
| 1                                      | 3.436683                | 4.587166  | -0.288589 |
| 1                                      | 0.972714                | 4.668499  | -0.219135 |
| 7                                      | 1.370699                | 1.324972  | 0.009406  |
| 7                                      | -1.370674               | 1.324977  | -0.010256 |
| 7                                      | 2.557876                | -1.110850 | 0.065632  |
| 6                                      | 3.367581                | -0.046020 | 0.021013  |
| 6                                      | 5.217512                | -1.339136 | 0.074949  |
| 6                                      | 4.381524                | -2.468987 | 0.125875  |
| 7                                      | 3.058915                | -2.340063 | 0.117091  |
| 1                                      | 6.300781                | -1.434852 | 0.076825  |
| 1                                      | 4.768757                | -3.481536 | 0.170644  |
| 7                                      | 4.708349                | -0.116948 | 0.020754  |
| 7                                      | -3.059084               | -2.340111 | -0.116412 |
| 6                                      | -4.381697               | -2.468928 | -0.125702 |
| 6                                      | -5.217611               | -1.338985 | -0.075746 |
| 6                                      | -3.367583               | -0.045994 | -0.021656 |
| 7                                      | -2.557935               | -1.110923 | -0.065362 |
| 1                                      | -6.300888               | -1.434596 | -0.078041 |
| 1                                      | -4.768988               | -3.481471 | -0.170090 |
| 7                                      | -4.708353               | -0.116818 | -0.021955 |
| 93                                     | 0.000014                | -0.907107 | 0.000194  |
| 8                                      | 0.116819                | -0.931438 | -1.779071 |
| 8                                      | -0.116797               | -0.928691 | 1.779504  |

| [NpO <sub>2</sub> (C2-BTBP)] <sup>+</sup> |                         |           |           |
|-------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                    | Coordinates (Angstroms) |           |           |
| Number                                    | X                       | Y         | Z         |
| 6                                         | 0.666102                | 3.060099  | -0.033004 |
| 6                                         | 2.670941                | 1.879549  | -0.037782 |
| 6                                         | 3.427902                | 3.051446  | -0.095946 |
| 6                                         | 2.755624                | 4.268061  | -0.134892 |
| 6                                         | 1.365840                | 4.275288  | -0.105176 |
| 6                                         | -0.825028               | 3.017967  | 0.012521  |
| 6                                         | -2.760688               | 1.726958  | -0.013761 |
| 6                                         | -3.582212               | 2.853444  | 0.062436  |
| 6                                         | -2.979137               | 4.104795  | 0.129144  |
| 6                                         | -1.591921               | 4.190550  | 0.105974  |
| 1                                         | 4.508544                | 2.985608  | -0.115815 |
| 1                                         | 3.306342                | 5.201722  | -0.190627 |
| 1                                         | 0.840477                | 5.220236  | -0.147634 |
| 1                                         | -4.657580               | 2.727481  | 0.074125  |
| 1                                         | -3.581519               | 5.004893  | 0.200491  |
| 1                                         | -1.120653               | 5.162555  | 0.169001  |
| 7                                         | -1.413693               | 1.806475  | -0.036745 |
| 7                                         | 1.321827                | 1.882655  | -0.008033 |
| 7                                         | -2.525135               | -0.661438 | -0.097328 |
| 6                                         | -3.364780               | 0.371017  | -0.069065 |
| 6                                         | -5.201346               | -0.975628 | -0.129957 |
| 6                                         | -4.313961               | -2.099548 | -0.149159 |
| 7                                         | -2.997453               | -1.904492 | -0.137787 |
| 7                                         | -4.700669               | 0.253099  | -0.087969 |
| 7                                         | 3.113270                | -1.733817 | 0.034254  |
| 6                                         | 4.440807                | -1.855629 | 0.030913  |
| 6                                         | 5.260575                | -0.685595 | 0.000214  |
| 6                                         | 3.351627                | 0.559439  | -0.010592 |
| 7                                         | 2.571366                | -0.521292 | 0.012393  |
| 7                                         | 4.690087                | 0.516490  | -0.016271 |
| 6                                         | 4.973999                | -3.264860 | 0.016972  |
| 6                                         | 5.184554                | -3.795341 | -1.416313 |
| 1                                         | 4.246316                | -3.897473 | 0.534386  |
| 1                                         | 5.911712                | -3.317987 | 0.579159  |
| 1                                         | 5.549917                | -4.826119 | -1.382062 |
| 1                                         | 4.242708                | -3.783811 | -1.973888 |
| 1                                         | 5.915506                | -3.196375 | -1.970662 |
| 6                                         | 6.764920                | -0.727993 | 0.032336  |
| 6                                         | 7.306226                | -0.668376 | 1.477478  |
| 1                                         | 7.132121                | 0.137510  | -0.527756 |
| 1                                         | 7.132327                | -1.628926 | -0.467548 |
| 1                                         | 8.400077                | -0.670728 | 1.463546  |
| 1                                         | 6.970971                | 0.245340  | 1.978021  |
| 1                                         | 6.973102                | -1.525986 | 2.071897  |
| 6                                         | -4.771845               | -3.534426 | -0.147441 |
| 6                                         | -4.953718               | -4.089048 | 1.281397  |
| 1                                         | -4.012659               | -4.124333 | -0.669957 |
| 1                                         | -5.707216               | -3.631108 | -0.707938 |
| 1                                         | -5.267752               | -5.136132 | 1.235966  |
| 1                                         | -4.012597               | -4.037047 | 1.837635  |
| 1                                         | -5.713078               | -3.534656 | 1.843765  |
| 6                                         | -6.699809               | -1.146925 | -0.172042 |
| 6                                         | -7.504100               | 0.150466  | -0.083522 |
| 1                                         | -6.989114               | -1.832210 | 0.636338  |
| 1                                         | -6.949113               | -1.682841 | -1.099881 |
| 1                                         | -8.573280               | -0.077516 | -0.121448 |
| 1                                         | -7.300819               | 0.683355  | 0.850263  |
| 1                                         | -7.267613               | 0.823497  | -0.912600 |
| 93                                        | 0.017142                | -0.388219 | -0.037857 |
| 8                                         | 0.123027                | -0.398255 | -1.820360 |
| 8                                         | -0.087020               | -0.432074 | 1.744353  |

| [NpO <sub>2</sub> (C2-BTPhen)] <sup>+</sup> |                         |           |           |
|---------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                      | Coordinates (Angstroms) |           |           |
| Number                                      | X                       | Y         | Z         |
| 6                                           | 3.475851                | 2.843599  | -0.046728 |
| 6                                           | 2.822297                | 4.052805  | 0.060032  |
| 6                                           | 1.412568                | 4.086937  | 0.127747  |
| 6                                           | 0.723859                | 2.843946  | 0.081701  |
| 6                                           | 2.711140                | 1.660208  | -0.084339 |
| 6                                           | 0.672522                | 5.310290  | 0.239276  |
| 6                                           | -0.724746               | 2.835604  | 0.144707  |
| 6                                           | -1.420922               | 4.070150  | 0.257245  |
| 6                                           | -0.688331               | 5.302172  | 0.302665  |
| 6                                           | -2.830385               | 4.019291  | 0.318601  |
| 1                                           | -3.396504               | 4.942369  | 0.405613  |
| 6                                           | -3.476822               | 2.802570  | 0.267595  |
| 6                                           | -2.705067               | 1.628748  | 0.152789  |
| 1                                           | 1.221755                | 6.246599  | 0.272836  |
| 1                                           | 4.555112                | 2.774410  | -0.103195 |
| 1                                           | 3.382959                | 4.982747  | 0.092059  |
| 1                                           | -1.243215               | 6.231839  | 0.388023  |
| 1                                           | -4.555726               | 2.720599  | 0.312377  |
| 7                                           | -2.557325               | -0.761027 | -0.018313 |
| 6                                           | -3.361537               | 0.299381  | 0.092680  |
| 6                                           | -5.241444               | -0.987983 | 0.103148  |
| 6                                           | -4.399051               | -2.134755 | -0.018978 |
| 7                                           | -3.074886               | -1.981964 | -0.075829 |
| 7                                           | 2.577699                | -0.732355 | -0.236565 |
| 6                                           | 3.375626                | 0.338675  | -0.200339 |
| 6                                           | 5.266859                | -0.925479 | -0.373459 |
| 6                                           | 4.431569                | -2.084677 | -0.385891 |
| 7                                           | 3.104996                | -1.944834 | -0.330261 |
| 7                                           | -4.696685               | 0.225708  | 0.153496  |
| 7                                           | 4.709838                | 0.281110  | -0.275236 |
| 7                                           | -1.369119               | 1.647373  | 0.092814  |
| 7                                           | 1.375201                | 1.662751  | -0.020192 |
| 6                                           | -6.744605               | -1.063796 | 0.131298  |
| 6                                           | -7.347525               | -0.943657 | -1.285438 |
| 1                                           | -7.105734               | -0.236354 | 0.749853  |
| 1                                           | -7.071532               | -1.997107 | 0.598740  |
| 1                                           | -8.439576               | -0.969915 | -1.226529 |
| 1                                           | -7.051255               | 0.000853  | -1.752249 |
| 1                                           | -7.023574               | -1.763364 | -1.935848 |
| 6                                           | -4.901253               | -3.554995 | -0.049095 |
| 6                                           | -5.051033               | -4.151672 | 1.365735  |
| 1                                           | -4.178894               | -4.147931 | -0.618290 |
| 1                                           | -5.856794               | -3.604445 | -0.580924 |
| 1                                           | -5.395043               | -5.188171 | 1.298468  |
| 1                                           | -4.091134               | -4.142625 | 1.891689  |
| 1                                           | -5.775401               | -3.594204 | 1.969872  |
| 6                                           | 6.770290                | -0.973208 | -0.449814 |
| 6                                           | 7.422625                | -1.242288 | 0.922896  |
| 1                                           | 7.105266                | -0.003359 | -0.828729 |
| 1                                           | 7.088123                | -1.736638 | -1.167698 |
| 1                                           | 8.511933                | -1.228837 | 0.822425  |
| 1                                           | 7.137122                | -0.472620 | 1.647076  |
| 1                                           | 7.133534                | -2.217545 | 1.327509  |
| 6                                           | 4.925351                | -3.508987 | -0.448399 |
| 6                                           | 4.737586                | -4.254235 | 0.888378  |
| 1                                           | 5.976154                | -3.534606 | -0.747257 |
| 1                                           | 4.353671                | -4.024892 | -1.228169 |
| 1                                           | 5.076090                | -5.289827 | 0.787961  |
| 1                                           | 5.311137                | -3.786495 | 1.695717  |
| 1                                           | 3.683014                | -4.263077 | 1.179821  |
| 93                                          | 0.009355                | -0.565699 | -0.118697 |
| 8                                           | -0.014039               | -0.461707 | -1.900321 |
| 8                                           | 0.033786                | -0.722865 | 1.659590  |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTP)] <sup>+</sup> |                         |           |           |
|----------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                                   | Coordinates (Angstroms) |           |           |
| Number                                                   | X                       | Y         | Z         |
| 6                                                        | -1.202669               | 3.370261  | -0.048417 |
| 6                                                        | -1.158831               | 1.973074  | -0.037226 |
| 6                                                        | 1.158996                | 1.973363  | -0.037629 |
| 6                                                        | 1.202564                | 3.370543  | -0.049088 |
| 6                                                        | -0.000136               | 4.074064  | -0.055247 |
| 1                                                        | -2.163203               | 3.871143  | -0.051242 |
| 1                                                        | 2.162997                | 3.871621  | -0.052819 |
| 1                                                        | -0.000271               | 5.159457  | -0.064643 |
| 6                                                        | -2.396511               | 1.156027  | -0.027157 |
| 6                                                        | -4.669410               | 0.963985  | -0.005464 |
| 6                                                        | -4.503615               | -0.457732 | 0.011956  |
| 6                                                        | 2.396670                | 1.156430  | -0.025533 |
| 6                                                        | 4.669517                | 0.963932  | -0.005891 |
| 6                                                        | 4.503385                | -0.457569 | 0.020867  |
| 7                                                        | 0.000168                | 1.288619  | -0.033311 |
| 7                                                        | -2.224432               | -0.168583 | -0.027592 |
| 7                                                        | -3.274598               | -0.976052 | -0.006116 |
| 7                                                        | -3.591557               | 1.749175  | -0.016487 |
| 7                                                        | 2.224289                | -0.168140 | -0.019553 |
| 7                                                        | 3.274284                | -0.975753 | 0.003908  |
| 7                                                        | 3.591848                | 1.749347  | -0.021310 |
| 6                                                        | 6.030579                | 1.643468  | 0.024460  |
| 6                                                        | 5.661009                | -1.449857 | 0.029659  |
| 6                                                        | 7.145644                | 0.620559  | -0.296556 |
| 6                                                        | 6.964214                | -0.716843 | 0.425232  |
| 6                                                        | 6.217140                | 2.234712  | 1.447928  |
| 1                                                        | 7.171908                | 2.769203  | 1.495215  |
| 1                                                        | 5.414915                | 2.942007  | 1.680364  |
| 1                                                        | 6.223174                | 1.461206  | 2.222848  |
| 6                                                        | 6.072076                | 2.794113  | -1.004317 |
| 1                                                        | 7.065321                | 3.255188  | -0.989536 |
| 1                                                        | 5.886179                | 2.428322  | -2.020392 |
| 1                                                        | 5.331853                | 3.564781  | -0.775651 |
| 6                                                        | 5.777157                | -2.056972 | -1.392814 |
| 1                                                        | 6.582101                | -2.799704 | -1.408239 |
| 1                                                        | 4.844922                | -2.555773 | -1.676552 |
| 1                                                        | 5.999641                | -1.300965 | -2.153072 |
| 6                                                        | 5.386609                | -2.586443 | 1.037970  |
| 1                                                        | 5.238404                | -2.195237 | 2.050816  |
| 1                                                        | 4.502228                | -3.165971 | 0.761745  |
| 1                                                        | 6.246959                | -3.263836 | 1.060903  |
| 1                                                        | 7.179779                | 0.455363  | -1.380929 |
| 1                                                        | 8.110572                | 1.064806  | -0.027561 |
| 1                                                        | 7.812275                | -1.376740 | 0.210506  |
| 1                                                        | 6.970339                | -0.557272 | 1.511213  |
| 6                                                        | -6.030231               | 1.643683  | 0.031675  |
| 6                                                        | -5.661494               | -1.449790 | 0.015853  |
| 6                                                        | -7.145868               | 0.623302  | -0.295242 |
| 6                                                        | -6.964168               | -0.718886 | 0.417394  |
| 1                                                        | -8.110441               | 1.065981  | -0.022424 |
| 1                                                        | -7.812594               | -1.377128 | 0.199046  |
| 1                                                        | -7.180963               | 0.465385  | -1.380680 |
| 1                                                        | -6.969251               | -0.566568 | 1.504408  |
| 6                                                        | -6.214775               | 2.225019  | 1.459444  |
| 1                                                        | -6.219388               | 1.446186  | 2.228997  |
| 1                                                        | -5.412310               | 2.930834  | 1.695513  |
| 1                                                        | -7.169567               | 2.758992  | 1.511874  |
| 6                                                        | -6.072752               | 2.801568  | -0.988935 |
| 1                                                        | -7.065789               | 3.262901  | -0.969408 |
| 1                                                        | -5.331909               | 3.570309  | -0.755844 |
| 1                                                        | -5.888512               | 2.442896  | -2.007854 |
| 6                                                        | -5.779501               | -2.048035 | -1.410201 |
| 1                                                        | -4.847988               | -2.546039 | -1.697806 |
| 1                                                        | -6.585005               | -2.790058 | -1.429455 |
| 1                                                        | -6.002062               | -1.287280 | -2.165707 |
| 6                                                        | -5.386506               | -2.592595 | 1.016905  |
| 1                                                        | -4.502879               | -3.171091 | 0.736224  |
| 1                                                        | -5.236489               | -2.207512 | 2.031793  |
| 1                                                        | -6.247378               | -3.269435 | 1.036967  |
| 93                                                       | 0.000122                | -1.334723 | -0.014964 |
| 8                                                        | 0.054319                | -1.399758 | -1.790714 |
| 8                                                        | -0.054752               | -1.354901 | 1.761776  |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTBP)] <sup>+</sup> |                         |           |           |
|-----------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                                    | Coordinates (Angstroms) |           |           |
| Number                                                    | X                       | Y         | Z         |
| 6                                                         | 0.745523                | 3.439309  | -0.033131 |
| 6                                                         | 2.716844                | 2.202308  | -0.048791 |
| 6                                                         | 3.504796                | 3.352552  | -0.125809 |
| 6                                                         | 2.866405                | 4.586915  | -0.170099 |
| 6                                                         | 1.477713                | 4.633612  | -0.125083 |
| 6                                                         | -0.745453               | 3.439324  | 0.032727  |
| 6                                                         | -2.716791               | 2.202358  | 0.049085  |
| 6                                                         | -3.504654               | 3.352607  | 0.126789  |
| 6                                                         | -2.866237               | 4.586974  | 0.170676  |
| 6                                                         | -1.477577               | 4.633653  | 0.124918  |
| 1                                                         | 4.582894                | 3.256998  | -0.154757 |
| 1                                                         | 3.442270                | 5.504271  | -0.240858 |
| 1                                                         | 0.978693                | 5.592609  | -0.170419 |
| 1                                                         | -4.582735               | 3.257061  | 0.156449  |
| 1                                                         | -3.442072               | 5.504326  | 0.241738  |
| 1                                                         | -0.978495               | 5.592629  | 0.169967  |
| 7                                                         | -1.368699               | 2.244191  | 0.004752  |
| 7                                                         | 1.368759                | 2.244166  | -0.005074 |
| 7                                                         | -2.547774               | -0.194301 | -0.022067 |
| 6                                                         | -3.360484               | 0.863461  | 0.014378  |
| 6                                                         | -5.234157               | -0.439298 | -0.012953 |
| 6                                                         | -4.379637               | -1.584579 | -0.020803 |
| 7                                                         | -3.055903               | -1.418353 | -0.033979 |
| 7                                                         | -4.693440               | 0.778142  | 0.019350  |
| 7                                                         | 3.055896                | -1.418510 | 0.030687  |
| 6                                                         | 4.379656                | -1.584659 | 0.020540  |
| 6                                                         | 5.234140                | -0.439324 | 0.016218  |
| 6                                                         | 3.360477                | 0.863370  | -0.014143 |
| 7                                                         | 2.547713                | -0.194457 | 0.019076  |
| 7                                                         | 4.693445                | 0.778113  | -0.016037 |
| 6                                                         | 6.753969                | -0.531782 | 0.010894  |
| 6                                                         | 4.883752                | -3.023893 | 0.048752  |
| 6                                                         | 7.199469                | -1.965487 | 0.383158  |
| 6                                                         | 6.385116                | -3.052168 | -0.322632 |
| 6                                                         | 7.348070                | 0.472126  | 1.022401  |
| 1                                                         | 8.439580                | 0.381571  | 1.022984  |
| 1                                                         | 7.088226                | 1.501959  | 0.765092  |
| 1                                                         | 6.993136                | 0.271674  | 2.039638  |
| 6                                                         | 7.239198                | -0.153962 | -1.413743 |
| 1                                                         | 6.902397                | 0.852508  | -1.681127 |
| 1                                                         | 8.334071                | -0.169204 | -1.440236 |
| 1                                                         | 6.872046                | -0.847923 | -2.176874 |
| 6                                                         | 4.090657                | -3.887452 | -0.955814 |
| 1                                                         | 3.030287                | -3.933335 | -0.695809 |
| 1                                                         | 4.176768                | -3.494273 | -1.975069 |
| 1                                                         | 4.491183                | -4.907032 | -0.952510 |
| 6                                                         | 4.657499                | -3.580984 | 1.477920  |
| 1                                                         | 3.596644                | -3.536466 | 1.744163  |
| 1                                                         | 4.978834                | -4.627548 | 1.518517  |
| 1                                                         | 5.218875                | -3.025050 | 2.236359  |
| 1                                                         | 8.262669                | -2.073616 | 0.139900  |
| 1                                                         | 7.122515                | -2.093097 | 1.470518  |
| 1                                                         | 6.487887                | -2.946199 | -1.410385 |
| 1                                                         | 6.785666                | -4.041725 | -0.074751 |
| 6                                                         | -6.753972               | -0.531814 | -0.003765 |
| 6                                                         | -4.883757               | -3.023784 | -0.049537 |
| 6                                                         | -6.384068               | -3.052561 | 0.326050  |
| 1                                                         | -6.483804               | -2.947819 | 1.414212  |
| 6                                                         | -7.200459               | -1.965154 | -0.376259 |
| 1                                                         | -8.262961               | -2.073584 | -0.130095 |
| 1                                                         | -7.126589               | -2.091628 | -1.463960 |
| 1                                                         | -6.785263               | -4.041865 | 0.078198  |
| 6                                                         | -7.350734               | 0.473055  | -1.012752 |
| 1                                                         | -8.442222               | 0.382279  | -1.010795 |
| 1                                                         | -7.090487               | 1.502672  | -0.754990 |
| 1                                                         | -6.998236               | 0.273744  | -2.031062 |
| 6                                                         | -7.235452               | -0.155427 | 1.422515  |
| 1                                                         | -6.866248               | -0.850164 | 2.183951  |
| 1                                                         | -6.897954               | 0.850775  | 1.690023  |
| 1                                                         | -8.330251               | -0.170744 | 1.451901  |
| 6                                                         | -4.087807               | -3.888697 | 0.951592  |
| 1                                                         | -3.028170               | -3.934161 | 0.688543  |
| 1                                                         | -4.171062               | -3.496933 | 1.971626  |
| 1                                                         | -4.488287               | -4.908293 | 0.947983  |
| 6                                                         | -4.661547               | -3.578932 | -1.480098 |
| 1                                                         | -3.601461               | -3.533939 | -1.749319 |
| 1                                                         | -4.982865               | -4.625481 | -1.521175 |
| 1                                                         | -5.225168               | -3.022075 | -2.236194 |
| 93                                                        | -0.000036               | 0.013029  | -0.002175 |
| 8                                                         | -0.079025               | -0.017521 | 1.782038  |
| 8                                                         | 0.079033                | -0.013424 | -1.786449 |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTPhen)] <sup>+</sup> |                         |           |           |
|-------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                               | Coordinates (Angstroms) |           |           |
|                                                             | X                       | Y         | Z         |
| 6                                                           | 3.479584                | 3.197113  | 0.006410  |
| 6                                                           | 2.829175                | 4.412508  | 0.005088  |
| 6                                                           | 1.418001                | 4.455347  | 0.002590  |
| 6                                                           | 0.724925                | 3.214096  | 0.002680  |
| 6                                                           | 2.710998                | 2.015485  | 0.007646  |
| 6                                                           | 0.681210                | 5.685570  | 0.000794  |
| 6                                                           | -0.724936               | 3.214115  | -0.002863 |
| 6                                                           | -1.417984               | 4.455378  | -0.002634 |
| 6                                                           | -0.681162               | 5.685585  | -0.000898 |
| 6                                                           | -2.829161               | 4.412584  | -0.004831 |
| 1                                                           | -3.393167               | 5.341086  | -0.004851 |
| 6                                                           | -3.479600               | 3.197205  | -0.005977 |
| 6                                                           | -2.711037               | 2.015565  | -0.007475 |
| 1                                                           | 1.233992                | 6.620411  | 0.001341  |
| 1                                                           | 4.559792                | 3.121782  | 0.006157  |
| 1                                                           | 3.393211                | 5.340991  | 0.005236  |
| 1                                                           | -1.233926               | 6.620437  | -0.001433 |
| 1                                                           | -4.559810               | 3.121885  | -0.005419 |
| 7                                                           | -2.567213               | -0.380598 | -0.012292 |
| 6                                                           | -3.372118               | 0.686608  | -0.006494 |
| 6                                                           | -5.258222               | -0.597304 | 0.012442  |
| 6                                                           | -4.415769               | -1.749863 | -0.026895 |
| 7                                                           | -3.089280               | -1.597733 | -0.026149 |
| 7                                                           | 2.567179                | -0.380736 | 0.011485  |
| 6                                                           | 3.372064                | 0.686519  | 0.006660  |
| 6                                                           | 5.258254                | -0.597302 | -0.011382 |
| 6                                                           | 4.415827                | -1.749899 | 0.026979  |
| 7                                                           | 3.089337                | -1.597840 | 0.025279  |
| 7                                                           | -4.705284               | 0.615736  | 0.008483  |
| 7                                                           | 4.705235                | 0.615704  | -0.007432 |
| 7                                                           | -1.373717               | 2.026821  | -0.007845 |
| 7                                                           | 1.373680                | 2.026792  | 0.007689  |
| 6                                                           | -6.778742               | -0.674717 | 0.026854  |
| 6                                                           | -7.232404               | -2.112966 | 0.371036  |
| 1                                                           | -8.300636               | -2.204876 | 0.143508  |
| 1                                                           | -7.138093               | -2.268583 | 1.453413  |
| 6                                                           | -4.933279               | -3.184539 | -0.030964 |
| 6                                                           | -6.441127               | -3.188979 | -0.376278 |
| 1                                                           | -6.561471               | -3.053681 | -1.458895 |
| 1                                                           | -6.847248               | -4.180741 | -0.147046 |
| 6                                                           | -7.348640               | 0.310300  | 1.070249  |
| 1                                                           | -7.082230               | 1.343379  | 0.833423  |
| 1                                                           | -8.440907               | 0.230191  | 1.084162  |
| 1                                                           | -6.981329               | 0.082600  | 2.077280  |
| 6                                                           | -7.280725               | -0.257977 | -1.381007 |
| 1                                                           | -8.375975               | -0.262006 | -1.391444 |
| 1                                                           | -6.937778               | 0.751474  | -1.628619 |
| 1                                                           | -6.931816               | -0.936704 | -2.166083 |
| 6                                                           | -4.166249               | -4.025963 | -1.073973 |
| 1                                                           | -4.269312               | -3.604682 | -2.080393 |
| 1                                                           | -3.101401               | -4.086321 | -0.836117 |
| 1                                                           | -4.574320               | -5.042421 | -1.090599 |
| 6                                                           | -4.687394               | -3.784663 | 1.377387  |
| 1                                                           | -5.018594               | -4.828776 | 1.393655  |
| 1                                                           | -3.621737               | -3.757869 | 1.626059  |
| 1                                                           | -5.229706               | -3.245046 | 2.161013  |
| 6                                                           | 6.778793                | -0.674606 | -0.024938 |
| 6                                                           | 4.933415                | -3.184545 | 0.030918  |
| 6                                                           | 7.232780                | -2.112764 | -0.369097 |
| 1                                                           | 7.139275                | -2.268157 | -1.451574 |
| 1                                                           | 8.300848                | -2.204678 | -0.140796 |
| 6                                                           | 6.440993                | -3.188984 | 0.377386  |
| 1                                                           | 6.847346                | -4.180672 | 0.148245  |
| 6                                                           | 7.279961                | -0.258057 | 1.383265  |
| 1                                                           | 8.375205                | -0.262033 | 1.394315  |
| 1                                                           | 6.936818                | 0.751332  | 1.630851  |
| 1                                                           | 6.930650                | -0.936939 | 2.168028  |
| 6                                                           | 7.349184                | 0.310627  | -1.067860 |
| 1                                                           | 6.982384                | 0.083105  | -2.075117 |
| 1                                                           | 7.082625                | 1.343653  | -0.830966 |
| 1                                                           | 8.441462                | 0.230559  | -1.081245 |
| 6                                                           | 4.165643                | -4.026398 | 1.073030  |
| 1                                                           | 4.267936                | -3.605498 | 2.079689  |
| 1                                                           | 3.100975                | -4.086703 | 0.834355  |
| 1                                                           | 4.573739                | -5.042847 | 1.089570  |
| 6                                                           | 4.688659                | -3.784185 | -1.377839 |
| 1                                                           | 5.019887                | -4.828287 | -1.394209 |
| 1                                                           | 3.623196                | -3.757322 | -1.627334 |
| 1                                                           | 5.231578                | -3.244291 | -2.160854 |
| 1                                                           | 6.560506                | -3.053922 | 1.460127  |
| 93                                                          | -0.000062               | -0.198629 | -0.000660 |
| 8                                                           | -0.064750               | -0.229563 | 1.783596  |
| 8                                                           | 0.064589                | -0.229149 | -1.784931 |

| [NpO <sub>2</sub> BTP(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|-------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                         | Coordinates (Angstroms) |           |           |
|                                                       | X                       | Y         | Z         |
| 6                                                     | 1.200698                | 3.578259  | 0.003797  |
| 6                                                     | 1.154600                | 2.179643  | -0.000026 |
| 6                                                     | -1.156703               | 2.179299  | -0.000423 |
| 6                                                     | -1.203335               | 3.577892  | 0.002382  |
| 6                                                     | -0.001436               | 4.282566  | 0.004782  |
| 1                                                     | 2.160468                | 4.080897  | 0.005836  |
| 1                                                     | -2.163298               | 4.080178  | 0.002696  |
| 1                                                     | -0.001594               | 5.367841  | 0.007430  |
| 6                                                     | 2.398507                | 1.371276  | -0.003819 |
| 6                                                     | 4.650770                | 1.211546  | -0.007765 |
| 6                                                     | 4.514981                | -0.188119 | -0.018137 |
| 1                                                     | 5.628926                | 1.686668  | -0.004812 |
| 1                                                     | 5.368114                | -0.858371 | -0.025282 |
| 6                                                     | -2.399884               | 1.370256  | -0.000092 |
| 6                                                     | -4.651907               | 1.208215  | -0.001652 |
| 6                                                     | -4.514662               | -0.191342 | 0.007297  |
| 1                                                     | -5.630575               | 1.682270  | -0.006297 |
| 1                                                     | -5.367112               | -0.862486 | 0.011448  |
| 7                                                     | -0.001021               | 1.493539  | -0.001928 |
| 7                                                     | 2.250294                | 0.037925  | -0.010351 |
| 7                                                     | 3.314021                | -0.757544 | -0.017298 |
| 7                                                     | 3.584432                | 1.998755  | -0.000427 |
| 7                                                     | -2.250227               | 0.037206  | 0.005601  |
| 7                                                     | -3.313105               | -0.759477 | 0.008962  |
| 7                                                     | -3.586428               | 1.996589  | -0.005493 |
| 93                                                    | 0.000370                | -1.177507 | 0.001696  |
| 8                                                     | 0.060780                | -1.198850 | 1.783660  |
| 8                                                     | -0.059912               | -1.216265 | -1.780035 |
| 8                                                     | 0.002329                | -3.701022 | 0.005617  |
| 1                                                     | -0.055901               | -4.269376 | -0.779022 |
| 1                                                     | 0.065484                | -4.276239 | 0.784805  |

| [NpO <sub>2</sub> BTBP(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|--------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic Number                                          | Coordinates (Angstroms) |           |           |
|                                                        | X                       | Y         | Z         |
| 6                                                      | 0.840732                | 2.612995  | -0.050785 |
| 6                                                      | 2.789136                | 1.352024  | -0.104180 |
| 6                                                      | 3.587559                | 2.482517  | -0.293418 |
| 6                                                      | 2.960648                | 3.721057  | -0.385049 |
| 6                                                      | 1.577335                | 3.789912  | -0.264940 |
| 6                                                      | -0.643455               | 2.643999  | 0.100515  |
| 6                                                      | -2.656391               | 1.488668  | 0.081591  |
| 6                                                      | -3.398235               | 2.656917  | 0.272443  |
| 6                                                      | -2.709583               | 3.857365  | 0.414510  |
| 6                                                      | -1.323323               | 3.853036  | 0.327088  |
| 1                                                      | 4.661730                | 2.371867  | -0.374626 |
| 1                                                      | 3.541586                | 4.622406  | -0.552479 |
| 1                                                      | 1.081966                | 4.747885  | -0.358122 |
| 1                                                      | -4.478782               | 2.605266  | 0.315144  |
| 1                                                      | -3.246142               | 4.784269  | 0.590082  |
| 1                                                      | -0.778341               | 4.780099  | 0.450596  |
| 7                                                      | -1.310061               | 1.476629  | 0.009442  |
| 7                                                      | 1.448014                | 1.413849  | 0.009199  |
| 7                                                      | -2.626642               | -0.923311 | -0.117643 |
| 6                                                      | -3.367285               | 0.191948  | -0.062202 |
| 6                                                      | -5.305153               | -0.958606 | -0.283990 |
| 6                                                      | -4.549138               | -2.141407 | -0.362364 |
| 7                                                      | -3.226131               | -2.102709 | -0.267043 |
| 1                                                      | -6.390862               | -0.973297 | -0.343998 |
| 1                                                      | -5.000416               | -3.119474 | -0.492659 |
| 7                                                      | -4.711053               | 0.212781  | -0.129773 |
| 7                                                      | 3.086479                | -2.273104 | 0.192082  |
| 6                                                      | 4.407268                | -2.417656 | 0.160999  |
| 6                                                      | 5.253704                | -1.304096 | 0.025184  |
| 6                                                      | 3.416492                | 0.008539  | -0.019334 |
| 7                                                      | 2.593930                | -1.042477 | 0.098287  |
| 1                                                      | 6.335186                | -1.413172 | -0.010576 |
| 1                                                      | 4.783985                | -3.432009 | 0.241578  |
| 7                                                      | 4.755605                | -0.079611 | -0.064577 |
| 93                                                     | 0.019000                | -0.820806 | 0.028226  |
| 8                                                      | -0.116365               | -0.832551 | 1.815848  |
| 8                                                      | 0.140976                | -0.822891 | -1.755597 |
| 8                                                      | -0.689564               | -3.288287 | 0.132278  |
| 1                                                      | -1.637037               | -3.289052 | -0.129714 |
| 1                                                      | -0.673128               | -3.597563 | 1.053350  |

| [NpO <sub>2</sub> BTBP(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|--------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                       | Coordinates (Angstroms) |           |           |
|                                                        | X                       | Y         | Z         |
| 6                                                      | 0.840732                | 2.612995  | -0.050785 |
| 6                                                      | 2.789136                | 1.352024  | -0.104180 |
| 6                                                      | 3.587559                | 2.482517  | -0.293418 |
| 6                                                      | 2.960648                | 3.721057  | -0.385049 |
| 6                                                      | 1.577335                | 3.789912  | -0.264940 |
| 6                                                      | -0.643455               | 2.643999  | 0.100515  |
| 6                                                      | -2.656391               | 1.488668  | 0.081591  |
| 6                                                      | -3.398235               | 2.656917  | 0.272443  |
| 6                                                      | -2.709583               | 3.857365  | 0.414510  |
| 6                                                      | -1.323323               | 3.853036  | 0.327088  |
| 1                                                      | 4.661730                | 2.371867  | -0.374626 |
| 1                                                      | 3.541586                | 4.622406  | -0.552479 |
| 1                                                      | 1.081966                | 4.747885  | -0.358122 |
| 1                                                      | -4.478782               | 2.605266  | 0.315144  |
| 1                                                      | -3.246142               | 4.784269  | 0.590082  |
| 1                                                      | -0.778341               | 4.780099  | 0.450596  |
| 7                                                      | -1.310061               | 1.476629  | 0.009442  |
| 7                                                      | 1.448014                | 1.413849  | 0.009199  |
| 7                                                      | -2.626642               | -0.923311 | -0.117643 |
| 6                                                      | -3.367285               | 0.191948  | -0.062202 |
| 6                                                      | -5.305153               | -0.958606 | -0.283990 |
| 6                                                      | -4.549138               | -2.141407 | -0.362364 |
| 7                                                      | -3.226131               | -2.102709 | -0.267043 |
| 1                                                      | -6.390862               | -0.973297 | -0.343998 |
| 1                                                      | -5.000416               | -3.119474 | -0.492659 |
| 7                                                      | -4.711053               | 0.212781  | -0.129773 |
| 7                                                      | 3.086479                | -2.273104 | 0.192082  |
| 6                                                      | 4.407268                | -2.417656 | 0.160999  |
| 6                                                      | 5.253704                | -1.304096 | 0.025184  |
| 6                                                      | 3.416492                | 0.008539  | -0.019334 |
| 7                                                      | 2.593930                | -1.042477 | 0.098287  |
| 1                                                      | 6.335186                | -1.413172 | -0.010576 |
| 1                                                      | 4.783985                | -3.432009 | 0.241578  |
| 7                                                      | 4.755605                | -0.079611 | -0.064577 |
| 93                                                     | 0.019000                | -0.820806 | 0.028226  |
| 8                                                      | -0.116365               | -0.832551 | 1.815848  |
| 8                                                      | 0.140976                | -0.822891 | -1.755597 |
| 8                                                      | -0.689564               | -3.288287 | 0.132278  |
| 1                                                      | -1.637037               | -3.289052 | -0.129714 |
| 1                                                      | -0.673128               | -3.597563 | 1.053350  |

| [NpO <sub>2</sub> BTPhen(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|----------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                         | Coordinates (Angstroms) |           |           |
|                                                          | X                       | Y         | Z         |
| 6                                                        | -3.629013               | 2.219359  | -0.041479 |
| 6                                                        | -3.031125               | 3.461316  | -0.018871 |
| 6                                                        | -1.624017               | 3.563456  | 0.007536  |
| 6                                                        | -0.874299               | 2.353687  | 0.009755  |
| 6                                                        | -2.806199               | 1.075258  | -0.032485 |
| 6                                                        | -0.948982               | 4.828259  | 0.029503  |
| 6                                                        | 0.577454                | 2.421272  | 0.023168  |
| 6                                                        | 1.205109                | 3.700006  | 0.039346  |
| 6                                                        | 0.410668                | 4.893563  | 0.046273  |
| 6                                                        | 2.614670                | 3.737631  | 0.041669  |
| 1                                                        | 3.126141                | 4.695795  | 0.055427  |
| 6                                                        | 3.331330                | 2.560736  | 0.020453  |
| 6                                                        | 2.626350                | 1.340255  | 0.003922  |
| 1                                                        | -1.546846               | 5.734891  | 0.030685  |
| 1                                                        | -4.704942               | 2.098737  | -0.064466 |
| 1                                                        | -3.633833               | 4.365002  | -0.022449 |
| 1                                                        | 0.918892                | 5.853110  | 0.061261  |
| 1                                                        | 4.413818                | 2.548555  | 0.013791  |
| 7                                                        | 2.675820                | -1.077918 | -0.015266 |
| 6                                                        | 3.381226                | 0.062842  | -0.035852 |
| 6                                                        | 5.357071                | -1.037703 | -0.153564 |
| 6                                                        | 4.640143                | -2.246520 | -0.149775 |
| 7                                                        | 3.314637                | -2.243387 | -0.074003 |
| 1                                                        | 6.443280                | -1.021420 | -0.203036 |
| 1                                                        | 5.123183                | -3.216581 | -0.202760 |
| 7                                                        | -2.569921               | -1.322063 | -0.017420 |
| 6                                                        | -3.412783               | -0.278977 | -0.048830 |
| 6                                                        | -5.226647               | -1.623061 | -0.099081 |
| 6                                                        | -4.360444               | -2.728224 | -0.058881 |
| 7                                                        | -3.041398               | -2.563403 | -0.018781 |
| 1                                                        | -6.306364               | -1.747913 | -0.136184 |
| 1                                                        | -4.718733               | -3.752394 | -0.059201 |
| 7                                                        | 4.724069                | 0.122407  | -0.095661 |
| 7                                                        | -4.750214               | -0.386130 | -0.091394 |
| 7                                                        | 1.290599                | 1.270982  | 0.010501  |
| 7                                                        | -1.471609               | 1.141780  | -0.006238 |
| 93                                                       | 0.012153                | -1.051909 | 0.020806  |
| 8                                                        | 0.040808                | -1.056866 | 1.813386  |
| 8                                                        | -0.004375               | -1.063162 | -1.766744 |
| 8                                                        | 0.798487                | -3.493556 | 0.214179  |
| 1                                                        | 0.725895                | -3.774201 | 1.141719  |
| 1                                                        | 1.762932                | -3.462188 | 0.024659  |

| [NpO <sub>2</sub> (C2-BTP)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                           | Coordinates (Angstroms) |           |           |
|                                                            | X                       | Y         | Z         |
| 6                                                          | -1.200710               | 3.564471  | -0.066035 |
| 6                                                          | -1.155172               | 2.166488  | -0.063258 |
| 6                                                          | 1.155428                | 2.166931  | 0.062704  |
| 6                                                          | 1.200516                | 3.564832  | 0.066281  |
| 6                                                          | -0.000245               | 4.268423  | 0.000295  |
| 1                                                          | -2.159831               | 4.065198  | -0.119573 |
| 1                                                          | 2.159455                | 4.065887  | 0.120187  |
| 1                                                          | -0.000426               | 5.353880  | 0.000554  |
| 6                                                          | -2.392764               | 1.351948  | -0.129582 |
| 6                                                          | -4.661162               | 1.194770  | -0.257384 |
| 6                                                          | -4.516111               | -0.229666 | -0.242970 |
| 6                                                          | 2.393064                | 1.352495  | 0.129089  |
| 6                                                          | 4.661299                | 1.194622  | 0.257528  |
| 6                                                          | 4.515840                | -0.229745 | 0.243113  |
| 7                                                          | 0.000244                | 1.482318  | -0.000474 |
| 7                                                          | -2.236693               | 0.026837  | -0.117273 |
| 7                                                          | -3.302223               | -0.768803 | -0.174798 |
| 7                                                          | -3.580854               | 1.966967  | -0.199587 |
| 7                                                          | 2.236580                | 0.027425  | 0.116625  |
| 7                                                          | 3.301809                | -0.768593 | 0.174473  |
| 7                                                          | 3.581243                | 1.967213  | 0.199353  |
| 6                                                          | -5.996762               | 1.885829  | -0.296444 |
| 6                                                          | -6.513351               | 2.209122  | 1.123317  |
| 1                                                          | -6.729321               | 1.271699  | -0.828535 |
| 1                                                          | -5.871044               | 2.818226  | -0.855496 |
| 1                                                          | -7.472707               | 2.730430  | 1.057100  |
| 1                                                          | -6.662073               | 1.302563  | 1.719750  |
| 1                                                          | -5.806715               | 2.855310  | 1.653088  |
| 6                                                          | -5.698687               | -1.166354 | -0.313842 |
| 6                                                          | -5.356958               | -2.654511 | -0.212532 |
| 1                                                          | -6.231165               | -0.969846 | -1.255655 |
| 1                                                          | -6.405164               | -0.888142 | 0.479932  |
| 1                                                          | -6.276526               | -3.244186 | -0.271128 |
| 1                                                          | -4.694892               | -2.968192 | -1.024600 |
| 1                                                          | -4.859880               | -2.886476 | 0.734191  |
| 6                                                          | 5.997046                | 1.885325  | 0.296821  |
| 6                                                          | 6.512526                | 2.210458  | -1.122959 |
| 1                                                          | 6.729890                | 1.270329  | 0.827456  |
| 1                                                          | 5.871946                | 2.816956  | 0.857293  |
| 1                                                          | 7.472080                | 2.731414  | -1.056901 |
| 1                                                          | 6.660438                | 1.304588  | -1.720647 |
| 1                                                          | 5.805554                | 2.857492  | -1.651221 |
| 6                                                          | 5.698236                | -1.166672 | 0.314479  |
| 6                                                          | 5.356491                | -2.654671 | 0.211029  |
| 1                                                          | 6.229402                | -0.971323 | 1.257293  |
| 1                                                          | 6.405854                | -0.887665 | -0.477977 |
| 1                                                          | 6.275943                | -3.244514 | 0.269746  |
| 1                                                          | 4.693676                | -2.969294 | 1.022120  |
| 1                                                          | 4.860302                | -2.885413 | -0.736474 |
| 93                                                         | -0.000061               | -1.171646 | 0.000085  |
| 8                                                          | -0.092105               | -1.211500 | 1.786587  |
| 8                                                          | 0.092635                | -1.211105 | -1.786355 |
| 8                                                          | -0.000334               | -3.706174 | 0.000004  |
| 1                                                          | -0.032971               | -4.274999 | 0.785075  |
| 1                                                          | 0.050421                | -4.278681 | -0.781461 |

| [NpO <sub>2</sub> (C2-BTP)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                           | Coordinates (Angstroms) |           |           |
|                                                            | X                       | Y         | Z         |
| 6                                                          | 0.655447                | 3.130718  | -0.163247 |
| 6                                                          | 2.668039                | 1.971645  | -0.217165 |
| 6                                                          | 3.400410                | 3.138096  | -0.451898 |
| 6                                                          | 2.707635                | 4.338622  | -0.562482 |
| 6                                                          | 1.324382                | 4.338434  | -0.419663 |
| 6                                                          | -0.826168               | 3.084412  | 0.009194  |
| 6                                                          | -2.766722               | 1.810343  | 0.087065  |
| 6                                                          | -3.573763               | 2.942660  | 0.222642  |
| 6                                                          | -2.957226               | 4.187735  | 0.285065  |
| 6                                                          | -1.574198               | 4.261616  | 0.177257  |
| 1                                                          | 4.477017                | 3.079523  | -0.551586 |
| 1                                                          | 3.236850                | 5.265008  | -0.762390 |
| 1                                                          | 0.778360                | 5.266861  | -0.526827 |
| 1                                                          | -4.648248               | 2.827678  | 0.285441  |
| 1                                                          | -3.546335               | 5.090016  | 0.415363  |
| 1                                                          | -1.085575               | 5.225430  | 0.238491  |
| 7                                                          | -1.423413               | 1.876137  | -0.006465 |
| 7                                                          | 1.327726                | 1.967545  | -0.080368 |
| 7                                                          | -2.599544               | -0.597951 | 0.044916  |
| 6                                                          | -3.398765               | 0.465406  | 0.034862  |
| 6                                                          | -5.295549               | -0.799574 | -0.086796 |
| 6                                                          | -4.457516               | -1.964043 | -0.089263 |
| 7                                                          | -3.142070               | -1.818539 | -0.012537 |
| 7                                                          | -4.741847               | 0.399984  | -0.019071 |
| 7                                                          | 3.178522                | -1.613963 | 0.174046  |
| 6                                                          | 4.505040                | -1.717319 | 0.089995  |
| 6                                                          | 5.297392                | -0.547543 | -0.112864 |
| 6                                                          | 3.366969                | 0.664905  | -0.111480 |
| 7                                                          | 2.608686                | -0.418287 | 0.069104  |
| 7                                                          | 4.702770                | 0.638980  | -0.205047 |
| 6                                                          | 5.063433                | -3.114461 | 0.176168  |
| 6                                                          | 5.198511                | -3.774081 | -1.211680 |
| 1                                                          | 4.378941                | -3.704940 | 0.792690  |
| 1                                                          | 6.033785                | -3.102295 | 0.683146  |
| 1                                                          | 5.585938                | -4.791938 | -1.105473 |
| 1                                                          | 4.224607                | -3.827604 | -1.708385 |
| 1                                                          | 5.882809                | -3.218690 | -1.862760 |
| 6                                                          | 6.801247                | -0.566046 | -0.183570 |
| 6                                                          | 7.439506                | -0.352481 | 1.206051  |
| 1                                                          | 7.110889                | 0.242788  | -0.852630 |
| 1                                                          | 7.151717                | -1.508159 | -0.615010 |
| 1                                                          | 8.529776                | -0.341349 | 1.116261  |
| 1                                                          | 7.120292                | 0.602679  | 1.634621  |
| 1                                                          | 7.165265                | -1.149778 | 1.905385  |
| 6                                                          | -5.024068               | -3.359756 | -0.171960 |
| 6                                                          | -3.999160               | -4.495218 | -0.140327 |
| 1                                                          | -5.624486               | -3.425160 | -1.090833 |
| 1                                                          | -5.745989               | -3.483367 | 0.647842  |
| 1                                                          | -4.517115               | -5.455672 | -0.214001 |
| 1                                                          | -3.294369               | -4.427100 | -0.974566 |
| 1                                                          | -3.427202               | -4.495280 | 0.793132  |
| 6                                                          | -6.796511               | -0.912087 | -0.157256 |
| 6                                                          | -7.550020               | 0.417980  | -0.141971 |
| 1                                                          | -7.128227               | -1.548454 | 0.676405  |
| 1                                                          | -7.049379               | -1.484034 | -1.062273 |
| 1                                                          | -8.626065               | 0.230596  | -0.200153 |
| 1                                                          | -7.349743               | 0.979084  | 0.775545  |
| 1                                                          | -7.265229               | 1.047342  | -0.990076 |
| 93                                                         | 0.033327                | -0.341005 | 0.088512  |
| 8                                                          | 0.089687                | -0.438672 | -1.698248 |
| 8                                                          | -0.038374               | -0.265781 | 1.881034  |
| 8                                                          | -0.560038               | -2.828254 | 0.396412  |
| 1                                                          | -1.523220               | -2.848971 | 0.185488  |
| 1                                                          | -0.500521               | -3.006172 | 1.349826  |

| [NpO <sub>2</sub> (C2-BTPhen)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|---------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                                        | Coordinates (Angstroms) |           |           |
| Number                                                        | X                       | Y         | Z         |
| 6                                                             | -3.526426               | 2.905829  | 0.102823  |
| 6                                                             | -2.875879               | 4.115160  | -0.010806 |
| 6                                                             | -1.467819               | 4.150109  | -0.105865 |
| 6                                                             | -0.775447               | 2.907648  | -0.080242 |
| 6                                                             | -2.758454               | 1.723520  | 0.116225  |
| 6                                                             | -0.736943               | 5.377920  | -0.221539 |
| 6                                                             | 0.674752                | 2.904104  | -0.162286 |
| 6                                                             | 1.359757                | 4.147458  | -0.270546 |
| 6                                                             | 0.622246                | 5.376387  | -0.302014 |
| 6                                                             | 2.768327                | 4.113880  | -0.337627 |
| 1                                                             | 3.323218                | 5.043930  | -0.422688 |
| 6                                                             | 3.427852                | 2.905329  | -0.288985 |
| 6                                                             | 2.668375                | 1.722377  | -0.179224 |
| 1                                                             | -1.291699               | 6.311440  | -0.241551 |
| 1                                                             | -4.604065               | 2.835160  | 0.181918  |
| 1                                                             | -3.436499               | 5.045591  | -0.026127 |
| 1                                                             | 1.173215                | 6.308362  | -0.387716 |
| 1                                                             | 4.507439                | 2.837413  | -0.330286 |
| 7                                                             | 2.603762                | -0.687365 | -0.038718 |
| 6                                                             | 3.361093                | 0.410331  | -0.109409 |
| 6                                                             | 5.311979                | -0.779080 | -0.039370 |
| 6                                                             | 4.527153                | -1.968689 | 0.053919  |
| 7                                                             | 3.198946                | -1.874980 | 0.044278  |
| 7                                                             | -2.632528               | -0.676770 | 0.226672  |
| 6                                                             | -3.422833               | 0.401499  | 0.233023  |
| 6                                                             | -5.321339               | -0.847779 | 0.441776  |
| 6                                                             | -4.497621               | -2.012912 | 0.403672  |
| 7                                                             | -3.172035               | -1.885039 | 0.309301  |
| 7                                                             | 4.703018                | 0.398696  | -0.116643 |
| 7                                                             | -4.754979               | 0.354358  | 0.346986  |
| 7                                                             | 1.332679                | 1.721119  | -0.123336 |
| 7                                                             | -1.425450               | 1.727078  | 0.025256  |
| 6                                                             | 6.816685                | -0.775430 | -0.006989 |
| 6                                                             | 7.355484                | -0.628325 | 1.433079  |
| 1                                                             | 7.157657                | 0.071892  | -0.609644 |
| 1                                                             | 7.211238                | -1.688591 | -0.462276 |
| 1                                                             | 8.448880                | -0.599803 | 1.417351  |
| 1                                                             | 6.993982                | 0.299099  | 1.887858  |
| 1                                                             | 7.047604                | -1.464454 | 2.070264  |
| 6                                                             | 5.101021                | -3.360375 | 0.122396  |
| 6                                                             | 5.353317                | -3.963158 | -1.275132 |
| 1                                                             | 4.390579                | -3.989175 | 0.668543  |
| 1                                                             | 6.031324                | -3.351291 | 0.699116  |
| 1                                                             | 5.752365                | -4.977048 | -1.176633 |
| 1                                                             | 4.423129                | -4.016632 | -1.850159 |
| 1                                                             | 6.072992                | -3.371691 | -1.851304 |
| 6                                                             | -6.822278               | -0.881512 | 0.566629  |
| 6                                                             | -7.522244               | -1.110566 | -0.789536 |
| 1                                                             | -7.133889               | 0.082522  | 0.978940  |
| 1                                                             | -7.125212               | -1.658451 | 1.276429  |
| 1                                                             | -8.607657               | -1.087095 | -0.654088 |
| 1                                                             | -7.250454               | -0.327530 | -1.504685 |
| 1                                                             | -7.257787               | -2.079250 | -1.225466 |
| 6                                                             | -5.002314               | -3.434256 | 0.450605  |
| 6                                                             | -4.880761               | -4.145202 | -0.911938 |
| 1                                                             | -6.039391               | -3.458933 | 0.794657  |
| 1                                                             | -4.401285               | -3.975175 | 1.190073  |
| 1                                                             | -5.222808               | -5.180891 | -0.824393 |
| 1                                                             | -5.485128               | -3.652096 | -1.680930 |
| 1                                                             | -3.839854               | -4.153425 | -1.249170 |
| 93                                                            | -0.051372               | -0.534596 | 0.062076  |
| 8                                                             | 0.022171                | -0.435154 | 1.847169  |
| 8                                                             | -0.114535               | -0.659156 | -1.728245 |
| 8                                                             | 0.643585                | -3.016209 | -0.029881 |
| 1                                                             | 0.507186                | -3.296935 | -0.950149 |
| 1                                                             | 1.622740                | -2.970664 | 0.084325  |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTP)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|----------------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic                                                                     | Coordinates (Angstroms) |           |           |
| Number                                                                     | X                       | Y         | Z         |
| 6                                                                          | -1.202039               | 3.470816  | -0.050416 |
| 6                                                                          | -1.157187               | 2.073022  | -0.039202 |
| 6                                                                          | 1.158236                | 2.073221  | -0.039780 |
| 6                                                                          | 1.202940                | 3.471006  | -0.051624 |
| 6                                                                          | 0.000398                | 4.174459  | -0.057690 |
| 1                                                                          | -2.162213               | 3.972178  | -0.052914 |
| 1                                                                          | 2.163060                | 3.972471  | -0.055634 |
| 1                                                                          | 0.000299                | 5.259909  | -0.067337 |
| 6                                                                          | -2.397617               | 1.258231  | -0.028672 |
| 6                                                                          | -4.674075               | 1.094865  | -0.002839 |
| 6                                                                          | -4.524707               | -0.326246 | 0.013300  |
| 6                                                                          | 2.398560                | 1.258435  | -0.027089 |
| 6                                                                          | 4.674929                | 1.094031  | -0.004349 |
| 6                                                                          | 4.524872                | -0.326772 | 0.024637  |
| 7                                                                          | 0.000578                | 1.389660  | -0.035357 |
| 7                                                                          | -2.238999               | -0.069748 | -0.032061 |
| 7                                                                          | -3.302537               | -0.860510 | -0.009382 |
| 7                                                                          | -3.586433               | 1.865340  | -0.015100 |
| 7                                                                          | 2.239338                | -0.069469 | -0.021564 |
| 7                                                                          | 3.302447                | -0.860629 | 0.004728  |
| 7                                                                          | 3.587668                | 1.865027  | -0.021831 |
| 6                                                                          | 6.027942                | 1.791079  | 0.024521  |
| 6                                                                          | 5.694139                | -1.305982 | 0.039712  |
| 6                                                                          | 7.155768                | 0.780025  | -0.289806 |
| 6                                                                          | 6.987645                | -0.556890 | 0.436447  |
| 6                                                                          | 6.206720                | 2.393061  | 1.443933  |
| 1                                                                          | 7.153980                | 2.941110  | 1.489082  |
| 1                                                                          | 5.394453                | 3.090166  | 1.672225  |
| 1                                                                          | 6.222762                | 1.624016  | 2.223247  |
| 6                                                                          | 6.056452                | 2.935680  | -1.011181 |
| 1                                                                          | 7.043408                | 3.410384  | -0.998424 |
| 1                                                                          | 5.876229                | 2.561199  | -2.025148 |
| 1                                                                          | 5.305376                | 3.697490  | -0.788268 |
| 6                                                                          | 5.821742                | -1.918019 | -1.379112 |
| 1                                                                          | 6.633624                | -2.653484 | -1.389799 |
| 1                                                                          | 4.894365                | -2.425344 | -1.663862 |
| 1                                                                          | 6.039365                | -1.162751 | -2.141493 |
| 6                                                                          | 5.429569                | -2.441178 | 1.051947  |
| 1                                                                          | 5.277177                | -2.046974 | 2.063036  |
| 1                                                                          | 4.548714                | -3.026927 | 0.777347  |
| 1                                                                          | 6.295265                | -3.111885 | 1.078287  |
| 1                                                                          | 7.194371                | 0.610905  | -1.373491 |
| 1                                                                          | 8.115172                | 1.236011  | -0.020317 |
| 1                                                                          | 7.844516                | -1.207479 | 0.227621  |
| 1                                                                          | 6.987894                | -0.392400 | 1.521768  |
| 6                                                                          | -6.026624               | 1.792373  | 0.035900  |
| 6                                                                          | -5.694528               | -1.304919 | 0.021466  |
| 6                                                                          | -7.155582               | 0.785004  | -0.285991 |
| 6                                                                          | -6.986980               | -0.558699 | 0.427340  |
| 1                                                                          | -8.114260               | 1.238943  | -0.010544 |
| 1                                                                          | -7.844542               | -1.206863 | 0.213841  |
| 1                                                                          | -7.196109               | 0.626068  | -1.371153 |
| 1                                                                          | -6.985308               | -0.404418 | 1.514152  |
| 6                                                                          | -6.201954               | 2.380583  | 1.461468  |
| 1                                                                          | -6.215961               | 1.604048  | 2.233335  |
| 1                                                                          | -5.389123               | 3.075469  | 1.694463  |
| 1                                                                          | -7.149107               | 2.928140  | 1.514254  |
| 6                                                                          | -6.056746               | 2.947112  | -0.988461 |
| 1                                                                          | -7.043325               | 3.422334  | -0.968636 |
| 1                                                                          | -5.304617               | 3.706153  | -0.759740 |
| 1                                                                          | -5.879212               | 2.582512  | -2.006502 |
| 6                                                                          | -5.825039               | -1.903926 | -1.402631 |
| 1                                                                          | -4.898735               | -2.409901 | -1.693331 |
| 1                                                                          | -6.637748               | -2.638370 | -1.418746 |
| 1                                                                          | -6.042943               | -1.141615 | -2.157910 |
| 6                                                                          | -5.429190               | -2.449391 | 1.022920  |
| 1                                                                          | -4.549888               | -3.033995 | 0.741044  |
| 1                                                                          | -5.273621               | -2.064322 | 2.037016  |
| 1                                                                          | -6.295867               | -3.118991 | 1.045449  |
| 93                                                                         | 0.000330                | -1.271391 | -0.021022 |
| 8                                                                          | 0.053966                | -1.332831 | -1.805716 |
| 8                                                                          | -0.053988               | -1.289287 | 1.764545  |
| 8                                                                          | -0.009054               | -3.805950 | 0.003651  |
| 1                                                                          | 0.042633                | -4.384250 | -0.773499 |
| 1                                                                          | -0.068468               | -4.369170 | 0.791260  |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTBP)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|-----------------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                                            | Coordinates (Angstroms) |           |           |
|                                                                             | X                       | Y         | Z         |
| 6                                                                           | -0.711279               | 3.455999  | -0.101519 |
| 6                                                                           | -2.688427               | 2.236963  | -0.145323 |
| 6                                                                           | -3.463696               | 3.390309  | -0.288025 |
| 6                                                                           | -2.812904               | 4.616113  | -0.371800 |
| 6                                                                           | -1.427291               | 4.651560  | -0.278013 |
| 6                                                                           | 0.772816                | 3.463412  | 0.058005  |
| 6                                                                           | 2.751526                | 2.247309  | 0.136522  |
| 6                                                                           | 3.518682                | 3.398907  | 0.329808  |
| 6                                                                           | 2.862460                | 4.622158  | 0.405265  |
| 6                                                                           | 1.478834                | 4.658207  | 0.271362  |
| 1                                                                           | -4.541452               | 3.305172  | -0.340366 |
| 1                                                                           | -3.377117               | 5.533343  | -0.507916 |
| 1                                                                           | -0.913033               | 5.600606  | -0.355540 |
| 1                                                                           | 4.593544                | 3.312026  | 0.426029  |
| 1                                                                           | 3.419889                | 5.538599  | 0.571623  |
| 1                                                                           | 0.962138                | 5.605769  | 0.351610  |
| 7                                                                           | 1.410659                | 2.278862  | 0.007244  |
| 7                                                                           | -1.342902               | 2.265328  | -0.064164 |
| 7                                                                           | 2.619643                | -0.147044 | -0.081134 |
| 6                                                                           | 3.411603                | 0.917480  | 0.071799  |
| 6                                                                           | 5.304872                | -0.356618 | 0.125231  |
| 6                                                                           | 4.477386                | -1.505283 | -0.057096 |
| 7                                                                           | 3.154590                | -1.358372 | -0.148011 |
| 7                                                                           | 4.741861                | 0.849495  | 0.175912  |
| 7                                                                           | -3.163423               | -1.372453 | -0.010115 |
| 6                                                                           | -4.485207               | -1.489884 | 0.098863  |
| 6                                                                           | -5.289612               | -0.308229 | 0.088641  |
| 6                                                                           | -3.359464               | 0.911641  | -0.072346 |
| 7                                                                           | -2.587443               | -0.176687 | -0.091505 |
| 7                                                                           | -4.695800               | 0.878097  | 0.004213  |
| 6                                                                           | -6.807274               | -0.329478 | 0.207304  |
| 6                                                                           | -5.049649               | -2.904958 | 0.186675  |
| 6                                                                           | -7.339352               | -1.760807 | -0.037774 |
| 6                                                                           | -6.517077               | -2.838202 | 0.673242  |
| 6                                                                           | -7.432701               | 0.638765  | -0.819585 |
| 1                                                                           | -8.524195               | 0.591130  | -0.743212 |
| 1                                                                           | -7.120612               | 1.670437  | -0.639260 |
| 1                                                                           | -7.154858               | 0.369072  | -1.844764 |
| 6                                                                           | -7.165174               | 0.155231  | 1.637591  |
| 1                                                                           | -6.763899               | 1.157598  | 1.816197  |
| 1                                                                           | -8.254457               | 0.195236  | 1.745576  |
| 1                                                                           | -6.772088               | -0.510319 | 2.413096  |
| 6                                                                           | -4.226914               | -3.757904 | 1.177096  |
| 1                                                                           | -3.200975               | -3.915109 | 0.833080  |
| 1                                                                           | -4.186142               | -3.293562 | 2.168447  |
| 1                                                                           | -4.698604               | -4.740655 | 1.283697  |
| 6                                                                           | -4.967743               | -3.547043 | -1.222044 |
| 1                                                                           | -3.931790               | -3.578684 | -1.575693 |
| 1                                                                           | -5.342990               | -4.575175 | -1.178945 |
| 1                                                                           | -5.558371               | -3.001526 | -1.965153 |
| 1                                                                           | -8.382933               | -1.805352 | 0.293813  |
| 1                                                                           | -7.355569               | -1.958073 | -1.117274 |
| 1                                                                           | -6.526873               | -2.659479 | 1.756225  |
| 1                                                                           | -6.977013               | -3.821698 | 0.523796  |
| 6                                                                           | 6.822504                | -0.428859 | 0.230535  |
| 6                                                                           | 5.004948                | -2.935322 | -0.111800 |
| 6                                                                           | 6.533149                | -2.914939 | -0.350686 |
| 1                                                                           | 6.727636                | -2.714081 | -1.412102 |
| 6                                                                           | 7.264851                | -1.884217 | 0.512557  |
| 1                                                                           | 8.346327                | -1.957041 | 0.349024  |
| 1                                                                           | 7.102935                | -2.108472 | 1.574712  |
| 1                                                                           | 6.928973                | -3.917822 | -0.153559 |
| 6                                                                           | 7.320709                | 0.491054  | 1.365430  |
| 1                                                                           | 8.410213                | 0.411110  | 1.444844  |
| 1                                                                           | 7.065201                | 1.536452  | 1.175347  |
| 1                                                                           | 6.890476                | 0.202548  | 2.331121  |
| 6                                                                           | 7.405615                | 0.074952  | -1.116200 |
| 1                                                                           | 7.108480                | -0.555721 | -1.960581 |
| 1                                                                           | 7.070896                | 1.096519  | -1.322276 |
| 1                                                                           | 8.499672                | 0.075317  | -1.061950 |
| 6                                                                           | 4.317992                | -3.717406 | -1.251769 |
| 1                                                                           | 3.239637                | -3.791267 | -1.091786 |
| 1                                                                           | 4.489565                | -3.239631 | -2.223148 |
| 1                                                                           | 4.731737                | -4.730827 | -1.296851 |
| 6                                                                           | 4.665059                | -3.616648 | 1.238839  |
| 1                                                                           | 3.583928                | -3.610744 | 1.409942  |
| 1                                                                           | 5.006145                | -4.657640 | 1.221104  |
| 1                                                                           | 5.143123                | -3.117952 | 2.088568  |
| 93                                                                          | 0.051947                | 0.006137  | -0.127581 |
| 8                                                                           | 0.001201                | 0.064380  | -1.921694 |
| 8                                                                           | 0.087328                | -0.074864 | 1.660896  |
| 8                                                                           | -0.633562               | -2.462354 | -0.438397 |
| 1                                                                           | -1.597073               | -2.429358 | -0.225210 |
| 1                                                                           | -0.587050               | -2.624979 | -1.395477 |

| [NpO <sub>2</sub> (CyMe <sub>4</sub> -BTPhen)(H <sub>2</sub> O)] <sup>+</sup> |                         |           |           |
|-------------------------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                                              | Coordinates (Angstroms) |           |           |
|                                                                               | X                       | Y         | Z         |
| 6                                                                             | 3.442442                | 3.246413  | -0.028215 |
| 6                                                                             | 2.787595                | 4.458061  | -0.019200 |
| 6                                                                             | 1.377477                | 4.492671  | -0.016449 |
| 6                                                                             | 0.687225                | 3.247692  | -0.031517 |
| 6                                                                             | 2.678271                | 2.061456  | -0.046736 |
| 6                                                                             | 0.643927                | 5.724066  | 0.005395  |
| 6                                                                             | -0.764962               | 3.252031  | -0.008204 |
| 6                                                                             | -1.453863               | 4.496346  | 0.020848  |
| 6                                                                             | -0.717479               | 5.726102  | 0.022333  |
| 6                                                                             | -2.864735               | 4.461013  | 0.053728  |
| 1                                                                             | -3.422773               | 5.392875  | 0.076529  |
| 6                                                                             | -3.520977               | 3.249643  | 0.060189  |
| 6                                                                             | -2.756229               | 2.065575  | 0.028694  |
| 1                                                                             | 1.199608                | 6.657192  | 0.011268  |
| 1                                                                             | 4.522576                | 3.177155  | -0.021169 |
| 1                                                                             | 3.346696                | 5.389466  | -0.009273 |
| 1                                                                             | -1.269755               | 6.661123  | 0.041630  |
| 1                                                                             | -4.601019               | 3.178814  | 0.089106  |
| 7                                                                             | -2.632684               | -0.334308 | -0.032699 |
| 6                                                                             | -3.425298               | 0.740698  | 0.034546  |
| 6                                                                             | -5.324341               | -0.522070 | 0.120996  |
| 6                                                                             | -4.498348               | -1.681172 | 0.022305  |
| 7                                                                             | -3.172056               | -1.544186 | -0.046077 |
| 7                                                                             | 2.608325                | -0.350685 | -0.131182 |
| 6                                                                             | 3.367591                | 0.745175  | -0.043462 |
| 6                                                                             | 5.310977                | -0.458387 | 0.081339  |
| 6                                                                             | 4.521357                | -1.647698 | 0.027474  |
| 7                                                                             | 3.199022                | -1.539954 | -0.093049 |
| 7                                                                             | -4.757528               | 0.684088  | 0.109057  |
| 7                                                                             | 4.702767                | 0.723831  | 0.052253  |
| 7                                                                             | -1.420598               | 2.069726  | -0.005638 |
| 7                                                                             | 1.341350                | 2.061674  | -0.056055 |
| 6                                                                             | -6.843796               | -0.582772 | 0.204292  |
| 6                                                                             | -7.297365               | -2.020505 | 0.551151  |
| 1                                                                             | -8.375993               | -2.098158 | 0.372095  |
| 1                                                                             | -7.155072               | -2.191411 | 1.625993  |
| 6                                                                             | -5.031069               | -3.110220 | 0.025935  |
| 6                                                                             | -6.553865               | -3.095168 | -0.245767 |
| 1                                                                             | -6.724727               | -2.944763 | -1.319564 |
| 1                                                                             | -6.959186               | -4.085610 | -0.009103 |
| 6                                                                             | -7.353967               | 0.394506  | 1.284954  |
| 1                                                                             | -7.086017               | 1.427496  | 1.049367  |
| 1                                                                             | -8.445370               | 0.326652  | 1.348647  |
| 1                                                                             | -6.943089               | 0.149546  | 2.270890  |
| 6                                                                             | -7.404763               | -0.142906 | -1.173702 |
| 1                                                                             | -8.499444               | -0.134487 | -1.135053 |
| 1                                                                             | -7.061577               | 0.865671  | -1.424670 |
| 1                                                                             | -7.099345               | -0.815576 | -1.981888 |
| 6                                                                             | -4.324844               | -3.947208 | -1.062347 |
| 1                                                                             | -4.471875               | -3.512387 | -2.057657 |
| 1                                                                             | -3.250776               | -4.020645 | -0.875482 |
| 1                                                                             | -4.744788               | -4.959066 | -1.071225 |
| 6                                                                             | -4.722181               | -3.729022 | 1.413422  |
| 1                                                                             | -5.065235               | -4.769289 | 1.436226  |
| 1                                                                             | -3.645035               | -3.716798 | 1.607640  |
| 1                                                                             | -5.217551               | -3.190998 | 2.228547  |
| 6                                                                             | 6.827957                | -0.467097 | 0.210099  |
| 6                                                                             | 5.099953                | -3.059046 | 0.063189  |
| 6                                                                             | 7.378631                | -1.880887 | -0.090174 |
| 1                                                                             | 7.407732                | -2.031944 | -1.176894 |
| 1                                                                             | 8.419483                | -1.927974 | 0.249669  |
| 6                                                                             | 6.562279                | -2.996986 | 0.565883  |
| 1                                                                             | 7.034682                | -3.968029 | 0.378594  |
| 6                                                                             | 7.172241                | -0.035959 | 1.660467  |
| 1                                                                             | 8.260333                | 0.011880  | 1.776826  |
| 1                                                                             | 6.758284                | 0.953879  | 1.875859  |
| 1                                                                             | 6.782065                | -0.735854 | 2.406579  |
| 6                                                                             | 7.447201                | 0.548960  | -0.773821 |
| 1                                                                             | 7.180539                | 0.315283  | -1.810747 |
| 1                                                                             | 7.119043                | 1.568441  | -0.556536 |
| 1                                                                             | 8.538696                | 0.513322  | -0.691041 |
| 6                                                                             | 4.278146                | -3.959853 | 1.011352  |
| 1                                                                             | 4.223290                | -3.535995 | 2.019992  |
| 1                                                                             | 3.257044                | -4.115304 | 0.652360  |
| 1                                                                             | 4.760137                | -4.940802 | 1.083147  |
| 6                                                                             | 5.036863                | -3.644613 | -1.370808 |
| 1                                                                             | 5.421018                | -4.670318 | -1.365598 |
| 1                                                                             | 4.004646                | -3.670195 | -1.735638 |
| 1                                                                             | 5.629478                | -3.064329 | -2.085323 |
| 1                                                                             | 6.560374                | -2.865004 | 1.655571  |
| 93                                                                            | -0.053148               | -0.197816 | -0.128284 |
| 8                                                                             | 0.074253                | -0.280147 | 1.655087  |
| 8                                                                             | -0.169791               | -0.148144 | -1.919496 |
| 8                                                                             | 0.679043                | -2.660045 | -0.402922 |
| 1                                                                             | 1.652258                | -2.598893 | -0.242960 |
| 1                                                                             | 0.582861                | -2.885768 | -1.343069 |

NpO<sub>2</sub>(BTP)(NO<sub>3</sub>)

| Atomic<br>Number | Coordinates (Angstroms) |           |           |
|------------------|-------------------------|-----------|-----------|
|                  | X                       | Y         | Z         |
| 6                | -4.074259               | -0.566180 | -0.016097 |
| 6                | -2.684866               | -0.742305 | -0.002391 |
| 6                | -2.318907               | 1.536177  | -0.011724 |
| 6                | -3.693680               | 1.803832  | -0.026917 |
| 6                | -4.579781               | 0.730555  | -0.028884 |
| 1                | -4.720350               | -1.435419 | -0.016875 |
| 1                | -4.035095               | 2.831607  | -0.036509 |
| 1                | -5.651654               | 0.902574  | -0.040313 |
| 6                | -2.101087               | -2.108960 | 0.006621  |
| 6                | -2.365783               | -4.352053 | 0.005333  |
| 6                | -0.969808               | -4.475834 | 0.005436  |
| 1                | -3.015835               | -5.224413 | 0.005439  |
| 1                | -0.465986               | -5.437003 | 0.002370  |
| 6                | -1.337037               | 2.651769  | -0.005147 |
| 6                | -0.888961               | 4.865588  | 0.003458  |
| 6                | 0.475720                | 4.547670  | 0.024685  |
| 1                | -1.234526               | 5.897162  | -0.002107 |
| 1                | 1.254197                | 5.303601  | 0.040167  |
| 7                | -1.825221               | 0.288346  | 0.000053  |
| 7                | -0.761899               | -2.206429 | 0.013622  |
| 7                | -0.184970               | -3.401775 | 0.012978  |
| 7                | -2.940893               | -3.157180 | 0.005885  |
| 7                | -0.034262               | 2.326429  | 0.007416  |
| 7                | 0.886406                | 3.282421  | 0.023112  |
| 7                | -1.807817               | 3.909664  | -0.011308 |
| 93               | 0.885652                | -0.146176 | 0.006999  |
| 8                | 0.822036                | -0.064412 | -1.785278 |
| 8                | 0.813186                | -0.208536 | 1.799923  |
| 7                | 3.790993                | -0.576321 | -0.026657 |
| 8                | 3.275386                | 0.593658  | 0.104429  |
| 8                | 2.954859                | -1.546177 | -0.138148 |
| 8                | 4.994274                | -0.754706 | -0.044058 |

NpO<sub>2</sub>(BTBP)(NO<sub>3</sub>)

| Atomic<br>Number | Coordinates (Angstroms) |           |           |
|------------------|-------------------------|-----------|-----------|
|                  | X                       | Y         | Z         |
| 6                | -0.718199               | 2.913408  | 0.190407  |
| 6                | -2.694196               | 1.728237  | 0.323086  |
| 6                | -3.385104               | 2.831947  | 0.835063  |
| 6                | -2.683834               | 4.016901  | 1.033874  |
| 6                | -1.335817               | 4.067924  | 0.694396  |
| 6                | 0.718561                | 2.913278  | -0.190896 |
| 6                | 2.694484                | 1.727883  | -0.322883 |
| 6                | 3.385566                | 2.831344  | -0.835175 |
| 6                | 2.684398                | 4.016260  | -1.034562 |
| 6                | 1.336332                | 4.067537  | -0.695303 |
| 1                | -4.440290               | 2.741539  | 1.060280  |
| 1                | -3.181953               | 4.889951  | 1.444737  |
| 1                | -0.761929               | 4.975757  | 0.843788  |
| 1                | 4.440771                | 2.740788  | -1.060250 |
| 1                | 3.182635                | 4.889121  | -1.445687 |
| 1                | 0.762575                | 4.975374  | -0.845187 |
| 7                | 1.383790                | 1.759745  | -0.032243 |
| 7                | -1.383548               | 1.759862  | 0.032235  |
| 7                | 2.707105                | -0.544811 | 0.497370  |
| 6                | 3.423088                | 0.472918  | -0.007735 |
| 6                | 5.376208                | -0.640588 | 0.197407  |
| 6                | 4.665800                | -1.669778 | 0.826150  |
| 7                | 3.342786                | -1.615565 | 0.956858  |
| 1                | 6.449410                | -0.702817 | 0.028143  |
| 1                | 5.147817                | -2.557232 | 1.224095  |
| 7                | 4.752772                | 0.459387  | -0.200339 |
| 7                | -3.343448               | -1.615619 | -0.955351 |
| 6                | -4.666382               | -1.669669 | -0.823839 |
| 6                | -5.376378               | -0.640119 | -0.195239 |
| 6                | -3.423011               | 0.473231  | 0.008492  |
| 7                | -2.707402               | -0.544700 | -0.496673 |
| 1                | -6.449525               | -0.702117 | -0.025545 |
| 1                | -5.148695               | -2.557278 | -1.221081 |
| 7                | -4.752635               | 0.459939  | 0.201753  |
| 93               | -0.000011               | -0.674819 | -0.000216 |
| 8                | 0.447905                | -0.610733 | -1.742105 |
| 8                | -0.448079               | -0.611352 | 1.741642  |
| 7                | -0.000094               | -3.638973 | -0.000780 |
| 8                | 1.077638                | -2.955440 | 0.104110  |
| 8                | -1.077884               | -2.955373 | -0.105226 |
| 8                | -0.000097               | -4.858862 | -0.001229 |

NpO<sub>2</sub>(BTPhen)(NO<sub>3</sub>)

| Atomic<br>Number | Coordinates (Angstroms) |           |           |
|------------------|-------------------------|-----------|-----------|
|                  | X                       | Y         | Z         |
| 6                | -3.389384               | 2.804624  | 0.092980  |
| 6                | -2.691327               | 3.969805  | 0.306638  |
| 6                | -1.280828               | 3.950979  | 0.296494  |
| 6                | -0.636062               | 2.700526  | 0.071830  |
| 6                | -2.664231               | 1.612167  | -0.124199 |
| 6                | -0.509020               | 5.140369  | 0.498845  |
| 6                | 0.817702                | 2.655506  | 0.054738  |
| 6                | 1.543012                | 3.866319  | 0.251462  |
| 6                | 0.850685                | 5.100070  | 0.474612  |
| 6                | 2.951446                | 3.801285  | 0.215994  |
| 1                | 3.533063                | 4.707787  | 0.360682  |
| 6                | 3.571503                | 2.593186  | -0.000291 |
| 6                | 2.770397                | 1.442789  | -0.171202 |
| 1                | -1.034886               | 6.075690  | 0.669786  |
| 1                | -4.471346               | 2.772551  | 0.083071  |
| 1                | -3.212684               | 4.907364  | 0.480444  |
| 1                | 1.436906                | 6.002414  | 0.625143  |
| 1                | 4.648881                | 2.496032  | -0.040320 |
| 7                | 2.662337                | -0.966522 | -0.334989 |
| 6                | 3.430570                | 0.131802  | -0.392342 |
| 6                | 5.295619                | -1.053192 | -0.859261 |
| 6                | 4.502685                | -2.206858 | -0.862182 |
| 7                | 3.200945                | -2.151368 | -0.594116 |
| 1                | 6.367122                | -1.092662 | -1.045477 |
| 1                | 4.903756                | -3.193213 | -1.073322 |
| 7                | -2.693790               | -0.786220 | -0.416501 |
| 6                | -3.404012               | 0.352023  | -0.383145 |
| 6                | -5.341985               | -0.699428 | -0.870255 |
| 6                | -4.608922               | -1.885853 | -0.990435 |
| 7                | -3.300185               | -1.917870 | -0.754133 |
| 1                | -6.419966               | -0.672387 | -1.016845 |
| 1                | -5.065123               | -2.830391 | -1.270027 |
| 7                | 4.753883                | 0.134681  | -0.632485 |
| 7                | -4.731032               | 0.440399  | -0.580071 |
| 7                | 1.437294                | 1.470955  | -0.148830 |
| 7                | -1.331919               | 1.559385  | -0.131735 |
| 93               | -0.022492               | -0.898471 | 0.069059  |
| 8                | 0.021677                | -0.372288 | 1.790430  |
| 8                | -0.034302               | -1.306768 | -1.683851 |
| 7                | -0.186519               | -3.656792 | 1.128219  |
| 8                | -1.231839               | -2.990144 | 0.804474  |
| 8                | 0.932626                | -3.085973 | 0.878315  |
| 8                | -0.252925               | -4.764660 | 1.635024  |

| NpO <sub>2</sub> (C2-BTP)(NO <sub>3</sub> ) |                         |           |           |
|---------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                            | Coordinates (Angstroms) |           |           |
|                                             | X                       | Y         | Z         |
| 6                                           | -1.198605               | 3.831750  | 0.069679  |
| 6                                           | -1.153022               | 2.432264  | 0.066524  |
| 6                                           | 1.153276                | 2.432268  | -0.067726 |
| 6                                           | 1.198796                | 3.831747  | -0.072307 |
| 6                                           | 0.000075                | 4.535814  | -0.001687 |
| 1                                           | -2.158043               | 4.330860  | 0.127302  |
| 1                                           | 2.158216                | 4.330843  | -0.130388 |
| 1                                           | 0.000040                | 5.621707  | -0.002259 |
| 6                                           | -2.403966               | 1.633315  | 0.135358  |
| 6                                           | -4.677073               | 1.543179  | 0.259800  |
| 6                                           | -4.572991               | 0.122468  | 0.238673  |
| 6                                           | 2.404241                | 1.633266  | -0.135695 |
| 6                                           | 4.677417                | 1.542926  | -0.258528 |
| 6                                           | 4.573200                | 0.122224  | -0.237433 |
| 7                                           | 0.000147                | 1.748545  | -0.000258 |
| 7                                           | -2.283325               | 0.303013  | 0.123630  |
| 7                                           | -3.374526               | -0.452740 | 0.175523  |
| 7                                           | -3.575117               | 2.284157  | 0.206199  |
| 7                                           | 2.283460                | 0.302973  | -0.124132 |
| 7                                           | 3.374637                | -0.452882 | -0.175198 |
| 7                                           | 3.575488                | 2.284007  | -0.205724 |
| 6                                           | -5.993155               | 2.276268  | 0.303215  |
| 6                                           | -6.497351               | 2.630669  | -1.111193 |
| 1                                           | -5.841061               | 3.197810  | 0.874375  |
| 1                                           | -6.744875               | 1.677863  | 0.827301  |
| 1                                           | -7.440865               | 3.181955  | -1.047506 |
| 1                                           | -5.767089               | 3.256999  | -1.633334 |
| 1                                           | -6.669718               | 1.733747  | -1.716038 |
| 6                                           | -5.775628               | -0.791719 | 0.298736  |
| 6                                           | -5.453432               | -2.283937 | 0.179832  |
| 1                                           | -6.477615               | -0.492921 | -0.492347 |
| 1                                           | -6.304735               | -0.597854 | 1.243685  |
| 1                                           | -6.380990               | -2.862962 | 0.234258  |
| 1                                           | -4.956415               | -2.511410 | -0.767281 |
| 1                                           | -4.787142               | -2.615037 | 0.980321  |
| 6                                           | 5.993592                | 2.275902  | -0.301050 |
| 6                                           | 6.496731                | 2.630486  | 1.113685  |
| 1                                           | 5.842009                | 3.197371  | -0.872469 |
| 1                                           | 6.745658                | 1.677360  | -0.824478 |
| 1                                           | 7.440334                | 3.181695  | 1.050638  |
| 1                                           | 5.766111                | 3.256946  | 1.635169  |
| 1                                           | 6.668570                | 1.733644  | 1.718800  |
| 6                                           | 5.775818                | -0.792057 | -0.296498 |
| 6                                           | 5.453473                | -2.284214 | -0.177213 |
| 1                                           | 6.477409                | -0.493004 | 0.494832  |
| 1                                           | 6.305421                | -0.598581 | -1.241251 |
| 1                                           | 6.381037                | -2.863307 | -0.230820 |
| 1                                           | 4.955861                | -2.511285 | 0.769688  |
| 1                                           | 4.787672                | -2.615605 | -0.977984 |
| 93                                          | 0.000048                | -0.992732 | -0.000347 |
| 8                                           | 0.030389                | -0.931435 | 1.795401  |
| 8                                           | -0.030395               | -0.930861 | -1.796077 |
| 7                                           | -0.000570               | -3.941961 | -0.000721 |
| 8                                           | 1.086632                | -3.261058 | 0.056479  |
| 8                                           | -1.087519               | -3.260543 | -0.057745 |
| 8                                           | -0.000851               | -5.160380 | -0.000582 |

| NpO <sub>2</sub> (C2-BTBP)(NO <sub>3</sub> ) |                         |           |           |
|----------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                             | Coordinates (Angstroms) |           |           |
|                                              | X                       | Y         | Z         |
| 6                                            | 0.668418                | 3.321024  | -0.249427 |
| 6                                            | 2.650051                | 2.143554  | -0.404629 |
| 6                                            | 3.333136                | 3.254895  | -0.910215 |
| 6                                            | 2.626669                | 4.439726  | -1.089621 |
| 6                                            | 1.279468                | 4.483022  | -0.743489 |
| 6                                            | -0.768327               | 3.303633  | 0.133577  |
| 6                                            | -2.719544               | 2.076453  | 0.291523  |
| 6                                            | -3.431320               | 3.172357  | 0.791161  |
| 6                                            | -2.755477               | 4.375746  | 0.966070  |
| 6                                            | -1.409415               | 4.452038  | 0.621434  |
| 1                                            | 4.386241                | 3.167382  | -1.146913 |
| 1                                            | 3.119317                | 5.319589  | -1.492907 |
| 1                                            | 0.702385                | 5.390611  | -0.881572 |
| 1                                            | -4.482228               | 3.059801  | 1.026718  |
| 1                                            | -3.271102               | 5.244612  | 1.364450  |
| 1                                            | -0.856044               | 5.374847  | 0.755667  |
| 7                                            | -1.410990               | 2.135019  | -0.006678 |
| 7                                            | 1.340946                | 2.169663  | -0.104524 |
| 7                                            | -2.678100               | -0.175537 | -0.549994 |
| 6                                            | -3.410806               | 0.794093  | 0.006210  |
| 6                                            | -5.326395               | -0.437207 | -0.047726 |
| 6                                            | -4.591911               | -1.438273 | -0.739404 |
| 7                                            | -3.290501               | -1.272772 | -0.970217 |
| 7                                            | -4.721160               | 0.700359  | 0.277758  |
| 7                                            | 3.310895                | -1.184083 | 0.868653  |
| 6                                            | 4.619365                | -1.315974 | 0.639699  |
| 6                                            | 5.320614                | -0.305072 | -0.065543 |
| 6                                            | 3.375542                | 0.881020  | -0.116579 |
| 7                                            | 2.669189                | -0.108097 | 0.445793  |
| 7                                            | 4.683831                | 0.818348  | -0.394334 |
| 6                                            | 5.207735                | -2.618341 | 1.124463  |
| 6                                            | 4.773490                | -3.794496 | 0.226152  |
| 1                                            | 4.833623                | -2.789780 | 2.139909  |
| 1                                            | 6.298963                | -2.555600 | 1.183514  |
| 1                                            | 5.150238                | -4.739473 | 0.631630  |
| 1                                            | 3.681313                | -3.842412 | 0.172629  |
| 1                                            | 5.163022                | -3.682356 | -0.792688 |
| 6                                            | 6.779876                | -0.396888 | -0.435463 |
| 6                                            | 7.696296                | 0.159378  | 0.672081  |
| 1                                            | 6.923899                | 0.184458  | -1.351865 |
| 1                                            | 7.047103                | -1.435494 | -0.656322 |
| 1                                            | 8.744410                | 0.105581  | 0.359996  |
| 1                                            | 7.454028                | 1.206513  | 0.881511  |
| 1                                            | 7.590681                | -0.406020 | 1.604517  |
| 6                                            | -5.148512               | -2.760757 | -1.204647 |
| 6                                            | -4.697693               | -3.909535 | -0.278285 |
| 1                                            | -4.761229               | -2.945324 | -2.212676 |
| 1                                            | -6.240424               | -2.722241 | -1.272094 |
| 1                                            | -5.055766               | -4.869443 | -0.665104 |
| 1                                            | -3.605184               | -3.936434 | -0.218718 |
| 1                                            | -5.094105               | -3.783681 | 0.736352  |
| 6                                            | -6.783464               | -0.613440 | 0.315864  |
| 6                                            | -7.383895               | 0.527334  | 1.138606  |
| 1                                            | -6.886586               | -1.565271 | 0.854867  |
| 1                                            | -7.355828               | -0.747884 | -0.613433 |
| 1                                            | -8.432039               | 0.309000  | 1.367471  |
| 1                                            | -6.846243               | 0.661946  | 2.082106  |
| 1                                            | -7.340210               | 1.475574  | 0.594842  |
| 93                                           | -0.003525               | -0.291900 | -0.043298 |
| 8                                            | 0.454811                | -0.245127 | -1.782755 |
| 8                                            | -0.461538               | -0.230172 | 1.695868  |
| 7                                            | 0.024947                | -3.290271 | -0.017279 |
| 8                                            | -1.060589               | -2.619641 | -0.109448 |
| 8                                            | 1.098053                | -2.598451 | 0.062291  |
| 8                                            | 0.035863                | -4.512351 | -0.005997 |

| NpO <sub>2</sub> (C2-BTPhen)(NO <sub>3</sub> ) |                         |           |           |
|------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                               | Coordinates (Angstroms) |           |           |
|                                                | X                       | Y         | Z         |
| 6                                              | -3.504726               | 3.145553  | 0.092731  |
| 6                                              | -2.852491               | 4.347489  | -0.045353 |
| 6                                              | -1.443178               | 4.374701  | -0.101488 |
| 6                                              | -0.751961               | 3.132206  | -0.005838 |
| 6                                              | -2.736765               | 1.962463  | 0.171954  |
| 6                                              | -0.718748               | 5.600676  | -0.252418 |
| 6                                              | 0.701828                | 3.135690  | -0.059268 |
| 6                                              | 1.378900                | 4.379430  | -0.219958 |
| 6                                              | 0.640475                | 5.602780  | -0.312358 |
| 6                                              | 2.788010                | 4.356146  | -0.282553 |
| 1                                              | 3.333142                | 5.287972  | -0.408459 |
| 6                                              | 3.453635                | 3.157313  | -0.185207 |
| 6                                              | 2.698933                | 1.974958  | -0.019965 |
| 1                                              | -1.280517               | 6.528221  | -0.322386 |
| 1                                              | -4.583719               | 3.073818  | 0.141296  |
| 1                                              | -3.408555               | 5.278813  | -0.114741 |
| 1                                              | 1.191101                | 6.531911  | -0.432026 |
| 1                                              | 4.533131                | 3.088408  | -0.228345 |
| 7                                              | 2.652830                | -0.426889 | 0.175789  |
| 6                                              | 3.405694                | 0.676367  | 0.104650  |
| 6                                              | 5.357645                | -0.490387 | 0.282821  |
| 6                                              | 4.575484                | -1.660721 | 0.456278  |
| 7                                              | 3.244410                | -1.588942 | 0.391367  |
| 7                                              | -2.683159               | -0.446092 | 0.261669  |
| 6                                              | -3.430043               | 0.659204  | 0.319273  |
| 6                                              | -5.361404               | -0.501560 | 0.663565  |
| 6                                              | -4.576659               | -1.687335 | 0.682717  |
| 7                                              | -3.263741               | -1.618720 | 0.480461  |
| 7                                              | 4.745490                | 0.684069  | 0.141445  |
| 7                                              | -4.760370               | 0.672740  | 0.504835  |
| 7                                              | 1.366527                | 1.962962  | 0.044472  |
| 7                                              | -1.403464               | 1.954327  | 0.128464  |
| 6                                              | 6.865906                | -0.477455 | 0.290562  |
| 6                                              | 7.438253                | -0.317007 | 1.712947  |
| 1                                              | 7.190414                | 0.364988  | -0.328592 |
| 1                                              | 7.253301                | -1.393810 | -0.166937 |
| 1                                              | 8.531947                | -0.278279 | 1.679070  |
| 1                                              | 7.076130                | 0.609290  | 2.170935  |
| 1                                              | 7.148339                | -1.151401 | 2.360969  |
| 6                                              | 5.113890                | -3.055670 | 0.662220  |
| 6                                              | 4.918300                | -3.924397 | -0.596222 |
| 1                                              | 4.556397                | -3.503360 | 1.492715  |
| 1                                              | 6.168008                | -3.026473 | 0.954700  |
| 1                                              | 5.251818                | -4.949619 | -0.404543 |
| 1                                              | 3.860505                | -3.944497 | -0.876142 |
| 1                                              | 5.492264                | -3.532804 | -1.444393 |
| 6                                              | -6.864086               | -0.495993 | 0.782179  |
| 6                                              | -7.546736               | -0.582238 | -0.598315 |
| 1                                              | -7.156698               | 0.437273  | 1.274076  |
| 1                                              | -7.197681               | -1.326476 | 1.412737  |
| 1                                              | -8.635349               | -0.557055 | -0.484130 |
| 1                                              | -7.247662               | 0.261279  | -1.228889 |
| 1                                              | -7.282751               | -1.507174 | -1.122353 |
| 6                                              | -5.154551               | -3.066601 | 0.910292  |
| 6                                              | -4.111776               | -4.188437 | 0.944045  |
| 1                                              | -5.893096               | -3.262980 | 0.119093  |
| 1                                              | -5.729951               | -3.056187 | 1.847472  |
| 1                                              | -4.616114               | -5.154202 | 1.055581  |
| 1                                              | -3.506105               | -4.201553 | 0.034578  |
| 1                                              | -3.421308               | -4.058099 | 1.782465  |
| 93                                             | -0.017420               | -0.474591 | -0.170501 |
| 8                                              | -0.026868               | -0.905292 | 1.576969  |
| 8                                              | 0.012091                | 0.058780  | -1.890486 |
| 7                                              | -0.028846               | -3.268736 | -1.231973 |
| 8                                              | -1.108069               | -2.657996 | -0.915997 |
| 8                                              | 1.057797                | -2.632620 | -1.003060 |
| 8                                              | -0.034654               | -4.392509 | -1.713257 |

| NpO <sub>2</sub> (CyMe <sub>4</sub> -BTP)(NO <sub>3</sub> ) |                         |           |           |
|-------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                            | Coordinates (Angstroms) |           |           |
|                                                             | X                       | Y         | Z         |
| 6                                                           | -1.196030               | 3.694758  | -0.059467 |
| 6                                                           | -1.152079               | 2.295475  | -0.050063 |
| 6                                                           | 1.159433                | 2.293323  | -0.040255 |
| 6                                                           | 1.206004                | 3.692520  | -0.048725 |
| 6                                                           | 0.005649                | 4.397494  | -0.059769 |
| 1                                                           | -2.156323               | 4.195501  | -0.065644 |
| 1                                                           | 2.167192                | 4.191556  | -0.046069 |
| 1                                                           | 0.006705                | 5.483387  | -0.067622 |
| 6                                                           | -2.404156               | 1.494632  | -0.040670 |
| 6                                                           | -4.683671               | 1.384192  | -0.000199 |
| 6                                                           | -4.564973               | -0.031432 | 0.031291  |
| 6                                                           | 2.410235                | 1.490388  | -0.025184 |
| 6                                                           | 4.689817                | 1.377204  | 0.008254  |
| 6                                                           | 4.569730                | -0.038648 | 0.030583  |
| 7                                                           | 0.003026                | 1.611135  | -0.042802 |
| 7                                                           | -2.273151               | 0.161703  | -0.049374 |
| 7                                                           | -3.356041               | -0.595786 | -0.011563 |
| 7                                                           | -3.579558               | 2.131107  | -0.024944 |
| 7                                                           | 2.277533                | 0.157752  | -0.030578 |
| 7                                                           | 3.359668                | -0.601240 | -0.001165 |
| 7                                                           | 3.586584                | 2.125389  | -0.008905 |
| 6                                                           | 6.031195                | 2.102068  | 0.039328  |
| 6                                                           | 5.751844                | -1.001702 | 0.057975  |
| 6                                                           | 7.175878                | 1.109568  | -0.276070 |
| 6                                                           | 7.032288                | -0.230297 | 0.451756  |
| 6                                                           | 6.203577                | 2.710717  | 1.454361  |
| 1                                                           | 7.139661                | 3.279023  | 1.500064  |
| 1                                                           | 5.375779                | 3.389468  | 1.683055  |
| 1                                                           | 6.234396                | 1.942433  | 2.234064  |
| 6                                                           | 6.038983                | 3.243372  | -0.999163 |
| 1                                                           | 7.014142                | 3.743448  | -0.986654 |
| 1                                                           | 5.868829                | 2.860435  | -2.011864 |
| 1                                                           | 5.266636                | 3.985483  | -0.781618 |
| 6                                                           | 5.889905                | -1.629927 | -1.351827 |
| 1                                                           | 6.708223                | -2.359105 | -1.352239 |
| 1                                                           | 4.966768                | -2.148257 | -1.628688 |
| 1                                                           | 6.101663                | -0.880808 | -2.122887 |
| 6                                                           | 5.491431                | -2.129709 | 1.080019  |
| 1                                                           | 5.345778                | -1.725272 | 2.088397  |
| 1                                                           | 4.604418                | -2.710323 | 0.816248  |
| 1                                                           | 6.356031                | -2.802968 | 1.106517  |
| 1                                                           | 7.210455                | 0.937387  | -1.359750 |
| 1                                                           | 8.129607                | 1.583029  | -0.012905 |
| 1                                                           | 7.902232                | -0.864816 | 0.244488  |
| 1                                                           | 7.029497                | -0.062651 | 1.536922  |
| 6                                                           | -6.024228               | 2.110595  | 0.027148  |
| 6                                                           | -5.747457               | -0.993299 | 0.075762  |
| 6                                                           | -7.170718               | 1.115723  | -0.273928 |
| 6                                                           | -7.025340               | -0.216651 | 0.467385  |
| 1                                                           | -8.123218               | 1.592603  | -0.012466 |
| 1                                                           | -7.896889               | -0.852345 | 0.270778  |
| 1                                                           | -7.209165               | 0.932207  | -1.355614 |
| 1                                                           | -7.017548               | -0.037501 | 1.550695  |
| 6                                                           | -6.192132               | 2.735045  | 1.435814  |
| 1                                                           | -6.222586               | 1.975373  | 2.223950  |
| 1                                                           | -5.362587               | 3.414727  | 1.655156  |
| 1                                                           | -7.127109               | 3.305481  | 1.477485  |
| 6                                                           | -6.033784               | 3.240305  | -1.023973 |
| 1                                                           | -7.008173               | 3.741968  | -1.013981 |
| 1                                                           | -5.259671               | 3.983711  | -0.817251 |
| 1                                                           | -5.867414               | 2.845838  | -2.032864 |
| 6                                                           | -5.893390               | -1.637726 | -1.325842 |
| 1                                                           | -4.971556               | -2.158621 | -1.602013 |
| 1                                                           | -6.711469               | -2.367063 | -1.313148 |
| 1                                                           | -6.109855               | -0.897421 | -2.104061 |
| 6                                                           | -5.481182               | -2.109559 | 1.109354  |
| 1                                                           | -4.594563               | -2.692058 | 0.848154  |
| 1                                                           | -5.331758               | -1.693636 | 2.112539  |
| 1                                                           | -6.344832               | -2.783480 | 1.147306  |
| 93                                                          | 0.000173                | -1.133686 | -0.042592 |
| 8                                                           | -0.056773               | -1.087324 | -1.838399 |
| 8                                                           | 0.059777                | -1.059819 | 1.752122  |
| 7                                                           | -0.026204               | -4.084706 | -0.003627 |
| 8                                                           | -1.104201               | -3.393272 | 0.090204  |
| 8                                                           | -0.035835               | -5.302978 | 0.017858  |
| 8                                                           | 1.062863                | -3.414351 | -0.121799 |

| NpO <sub>2</sub> (CyMe <sub>4</sub> -BTBP)(NO <sub>3</sub> ) |                         |           |           |
|--------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                             | Coordinates (Angstroms) |           |           |
|                                                              | X                       | Y         | Z         |
| 6                                                            | 0.714083                | 3.517855  | -0.226199 |
| 6                                                            | 2.689885                | 2.346098  | -0.455712 |
| 6                                                            | 3.358391                | 3.467599  | -0.959470 |
| 6                                                            | 2.644235                | 4.650033  | -1.114893 |
| 6                                                            | 1.307366                | 4.684279  | -0.732353 |
| 6                                                            | -0.703329               | 3.517602  | 0.222692  |
| 6                                                            | -2.679813               | 2.348239  | 0.459115  |
| 6                                                            | -3.343979               | 3.470120  | 0.968365  |
| 6                                                            | -2.627995               | 4.651613  | 1.121576  |
| 6                                                            | -1.292963               | 4.684175  | 0.732629  |
| 1                                                            | 4.407444                | 3.388360  | -1.214769 |
| 1                                                            | 3.122737                | 5.534747  | -1.524526 |
| 1                                                            | 0.724036                | 5.590572  | -0.848761 |
| 1                                                            | -4.391708               | 3.391412  | 1.228854  |
| 1                                                            | -3.103460               | 5.536408  | 1.534545  |
| 1                                                            | -0.707300               | 5.589143  | 0.847307  |
| 7                                                            | -1.379666               | 2.362338  | 0.119710  |
| 7                                                            | 1.388533                | 2.362398  | -0.121539 |
| 7                                                            | -2.734305               | 0.034151  | -0.226145 |
| 6                                                            | -3.429192               | 1.088914  | 0.220075  |
| 6                                                            | -5.424344               | -0.016085 | 0.136731  |
| 6                                                            | -4.713325               | -1.144093 | -0.343876 |
| 7                                                            | -3.393529               | -1.071017 | -0.528208 |
| 7                                                            | -4.753317               | 1.101445  | 0.410989  |
| 7                                                            | 3.374519                | -1.070460 | 0.549182  |
| 6                                                            | 4.699612                | -1.142136 | 0.411304  |
| 6                                                            | 5.422390                | -0.023382 | -0.076132 |
| 6                                                            | 3.432228                | 1.084440  | -0.210982 |
| 7                                                            | 2.724124                | 0.029568  | 0.210725  |
| 7                                                            | 4.760423                | 1.093668  | -0.373188 |
| 6                                                            | 6.931672                | -0.035938 | -0.293509 |
| 6                                                            | 5.334255                | -2.464464 | 0.832830  |
| 6                                                            | 7.557983                | -1.218565 | 0.483314  |
| 6                                                            | 6.788482                | -2.531104 | 0.309803  |
| 6                                                            | 7.553594                | 1.287052  | 0.197844  |
| 1                                                            | 8.640218                | 1.256335  | 0.057448  |
| 1                                                            | 7.156734                | 2.143381  | -0.353097 |
| 1                                                            | 7.355175                | 1.447025  | 1.263921  |
| 6                                                            | 7.186321                | -0.173474 | -1.816060 |
| 1                                                            | 6.722029                | 0.656928  | -2.357965 |
| 1                                                            | 8.264275                | -0.156083 | -2.015083 |
| 1                                                            | 6.780488                | -1.106082 | -2.221069 |
| 6                                                            | 4.519957                | -3.642943 | 0.254954  |
| 1                                                            | 3.473473                | -3.601053 | 0.564285  |
| 1                                                            | 4.538705                | -3.631793 | -0.840800 |
| 1                                                            | 4.959627                | -4.589568 | 0.591078  |
| 6                                                            | 5.295723                | -2.537934 | 2.379503  |
| 1                                                            | 4.263114                | -2.463555 | 2.734090  |
| 1                                                            | 5.708873                | -3.495838 | 2.716098  |
| 1                                                            | 5.874796                | -1.733853 | 2.848605  |
| 1                                                            | 8.597014                | -1.342281 | 0.153291  |
| 1                                                            | 7.605293                | -0.957433 | 1.548971  |
| 1                                                            | 6.772952                | -2.809698 | -0.751764 |
| 1                                                            | 7.312124                | -3.343609 | 0.828132  |
| 6                                                            | -6.931889               | -0.016740 | 0.364898  |
| 6                                                            | -5.351260               | -2.482254 | -0.705351 |
| 6                                                            | -6.803441               | -2.526678 | -0.173342 |
| 1                                                            | -6.785489               | -2.774410 | 0.895750  |
| 6                                                            | -7.565935               | -1.214996 | -0.381125 |
| 1                                                            | -8.605676               | -1.324008 | -0.048305 |
| 1                                                            | -7.611151               | -0.981030 | -1.453294 |
| 1                                                            | -7.333979               | -3.350770 | -0.665579 |
| 6                                                            | -7.549741               | 1.297149  | -0.155766 |
| 1                                                            | -8.635389               | 1.276791  | -0.006314 |
| 1                                                            | -7.143475               | 2.164645  | 0.370436  |
| 1                                                            | -7.358513               | 1.428737  | -1.226995 |
| 6                                                            | -7.180112               | -0.115484 | 1.891186  |
| 1                                                            | -6.777070               | -1.039880 | 2.317180  |
| 1                                                            | -6.708950               | 0.725580  | 2.410205  |
| 1                                                            | -8.256939               | -0.087588 | 2.094835  |
| 6                                                            | -4.531039               | -3.630908 | -0.076264 |
| 1                                                            | -3.486286               | -3.600799 | -0.393154 |
| 1                                                            | -4.547324               | -3.567769 | 1.017671  |
| 1                                                            | -4.969092               | -4.593727 | -0.365092 |
| 6                                                            | -5.320321               | -2.626667 | -2.246487 |
| 1                                                            | -4.290732               | -2.560027 | -2.610701 |
| 1                                                            | -5.727544               | -3.602379 | -2.535481 |
| 1                                                            | -5.910055               | -1.850005 | -2.747475 |
| 93                                                           | -0.003838               | -0.086259 | -0.040534 |
| 8                                                            | -0.208130               | -0.066979 | 1.746922  |
| 8                                                            | 0.202446                | 0.023054  | -1.825296 |
| 7                                                            | 0.020996                | -3.081320 | -0.124870 |
| 8                                                            | 1.093271                | -2.388775 | -0.193100 |
| 8                                                            | -1.062645               | -2.411165 | -0.019894 |
| 8                                                            | 0.031129                | -4.303396 | -0.159281 |

| NpO <sub>2</sub> (CyMe <sub>4</sub> -BTPhen)(NO <sub>3</sub> ) |                         |           |           |
|----------------------------------------------------------------|-------------------------|-----------|-----------|
| Atomic<br>Number                                               | Coordinates (Angstroms) |           |           |
|                                                                | X                       | Y         | Z         |
| 6                                                              | 3.449892                | 3.405154  | -0.452399 |
| 6                                                              | 2.791876                | 4.611995  | -0.431150 |
| 6                                                              | 1.397493                | 4.642258  | -0.218925 |
| 6                                                              | 0.722947                | 3.394553  | -0.084662 |
| 6                                                              | 2.706385                | 2.222634  | -0.241032 |
| 6                                                              | 0.672342                | 5.873293  | -0.120804 |
| 6                                                              | -0.721285               | 3.395196  | 0.079117  |
| 6                                                              | -1.394973               | 4.643664  | 0.210614  |
| 6                                                              | -0.669198               | 5.873995  | 0.108558  |
| 6                                                              | -2.789091               | 4.614792  | 0.424910  |
| 1                                                              | -3.330354               | 5.548562  | 0.553309  |
| 6                                                              | -3.447633               | 3.408336  | 0.451265  |
| 6                                                              | -2.705109               | 2.224863  | 0.241846  |
| 1                                                              | 1.220860                | 6.806271  | -0.218253 |
| 1                                                              | 4.519902                | 3.331756  | -0.598988 |
| 1                                                              | 3.333814                | 5.545075  | -0.561622 |
| 1                                                              | -1.217169               | 6.807557  | 0.203478  |
| 1                                                              | -4.517373               | 3.335886  | 0.600446  |
| 7                                                              | -2.708839               | -0.127977 | -0.281520 |
| 6                                                              | -3.423971               | 0.933527  | 0.118022  |
| 6                                                              | -5.383004               | -0.236737 | 0.160901  |
| 6                                                              | -4.674807               | -1.325561 | -0.403850 |
| 7                                                              | -3.356514               | -1.236471 | -0.589086 |
| 7                                                              | 2.705672                | -0.131345 | 0.278162  |
| 6                                                              | 3.424316                | 0.931281  | -0.112064 |
| 6                                                              | 5.384345                | -0.238023 | -0.136975 |
| 6                                                              | 4.670606                | -1.328722 | 0.417007  |
| 7                                                              | 3.350482                | -1.240386 | 0.589560  |
| 7                                                              | -4.738823               | 0.912688  | 0.361984  |
| 7                                                              | 4.741659                | 0.911498  | -0.342342 |
| 7                                                              | -1.380952               | 2.215013  | 0.081427  |
| 7                                                              | 1.381895                | 2.213998  | -0.083123 |
| 6                                                              | -6.861583               | -0.299834 | 0.524898  |
| 6                                                              | -7.337537               | -1.772468 | 0.497038  |
| 1                                                              | -8.433782               | -1.786859 | 0.538567  |
| 1                                                              | -6.990008               | -2.275425 | 1.408931  |
| 6                                                              | -5.300766               | -2.661226 | -0.788630 |
| 6                                                              | -6.841567               | -2.544187 | -0.730524 |
| 1                                                              | -7.201326               | -2.051720 | -1.644124 |
| 1                                                              | -7.272807               | -3.552491 | -0.738946 |
| 6                                                              | -7.076000               | 0.286266  | 1.936619  |
| 1                                                              | -6.762846               | 1.332741  | 1.983553  |
| 1                                                              | -8.137941               | 0.228739  | 2.202209  |
| 1                                                              | -6.508223               | -0.272994 | 2.688862  |
| 6                                                              | -7.648310               | 0.557030  | -0.497645 |
| 1                                                              | -8.712009               | 0.566695  | -0.232746 |
| 1                                                              | -7.282179               | 1.588657  | -0.494550 |
| 1                                                              | -7.556226               | 0.170127  | -1.517931 |
| 6                                                              | -4.856465               | -3.049918 | -2.215589 |
| 1                                                              | -5.171937               | -2.298508 | -2.949649 |
| 1                                                              | -3.769750               | -3.150809 | -2.270296 |
| 1                                                              | -5.312776               | -4.007145 | -2.493635 |
| 6                                                              | -4.775250               | -3.732469 | 0.201019  |
| 1                                                              | -5.157543               | -4.719171 | -0.086013 |
| 1                                                              | -3.681164               | -3.758851 | 0.183217  |
| 1                                                              | -5.093474               | -3.532282 | 1.230679  |
| 6                                                              | 6.867328                | -0.298722 | -0.483304 |
| 6                                                              | 5.292676                | -2.666039 | 0.802311  |
| 6                                                              | 7.344358                | -1.770996 | -0.455153 |
| 1                                                              | 7.008846                | -2.270742 | -1.373257 |
| 1                                                              | 8.441058                | -1.784141 | -0.482929 |
| 6                                                              | 6.833984                | -2.548220 | 0.762988  |
| 1                                                              | 7.265404                | -3.556439 | 0.771928  |
| 6                                                              | 7.640519                | 0.554901  | 0.552220  |
| 1                                                              | 8.707404                | 0.566708  | 0.300582  |
| 1                                                              | 7.273330                | 1.586161  | 0.548779  |
| 1                                                              | 7.536144                | 0.163822  | 1.569723  |
| 6                                                              | 7.098764                | 0.292872  | -1.889953 |
| 1                                                              | 6.540802                | -0.263911 | -2.651322 |
| 1                                                              | 6.785502                | 1.339320  | -1.936803 |
| 1                                                              | 8.163957                | 0.237100  | -2.142591 |
| 6                                                              | 4.831795                | -3.063022 | 2.221702  |
| 1                                                              | 5.136943                | -2.315067 | 2.963592  |
| 1                                                              | 3.744726                | -3.165923 | 2.262465  |
| 1                                                              | 5.286219                | -4.021024 | 2.500122  |
| 6                                                              | 4.778950                | -3.732025 | -0.199340 |
| 1                                                              | 5.159095                | -4.720053 | 0.085998  |
| 1                                                              | 3.684694                | -3.759499 | -0.193466 |
| 1                                                              | 5.107960                | -3.525485 | -1.224312 |
| 1                                                              | 7.182746                | -2.059936 | 1.683118  |
| 93                                                             | -0.000273               | -0.237641 | -0.010736 |
| 8                                                              | 0.161222                | -0.171991 | -1.800893 |
| 8                                                              | -0.162804               | -0.194981 | 1.779875  |
| 7                                                              | 0.002357                | -3.244522 | -0.029208 |
| 8                                                              | -1.080484               | -2.565208 | -0.061141 |
| 8                                                              | 1.084198                | -2.563724 | 0.010772  |
| 8                                                              | 0.003388                | -4.467123 | -0.036724 |