

Electronic Supplementary Information (ESI)

**Tweaking the proton transfer triggered proton transfer of 3,5-bis(2-hydroxyphenyl)-1H-1,2,4-triazole**

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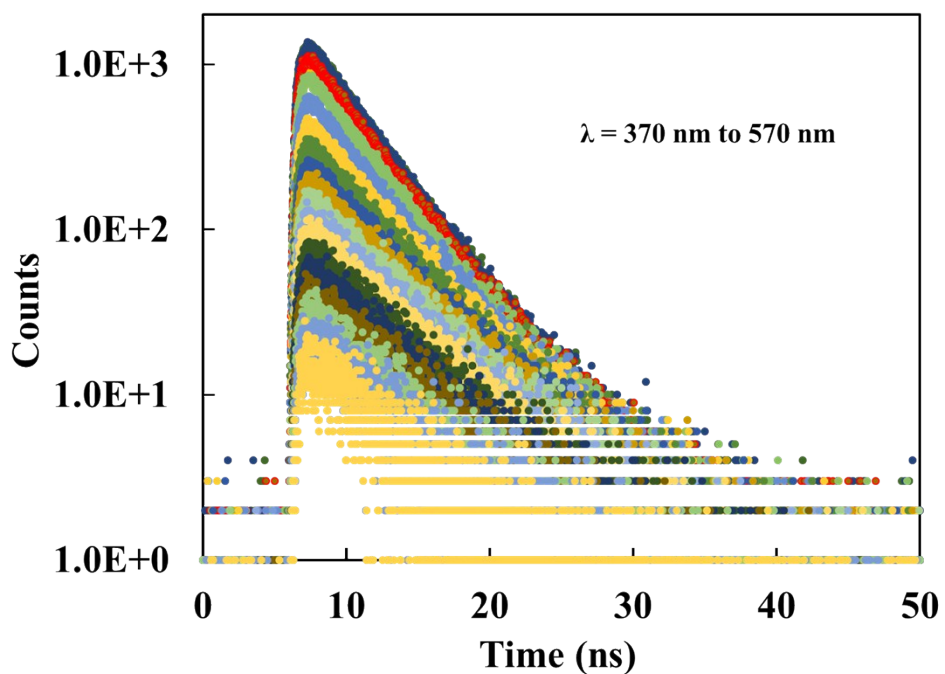


Figure S1: Fluorescence decay of bis-HPTA in DMF recorded at different emission wavelength. ( $\lambda_{\text{ex}} = 308 \text{ nm}$ ).

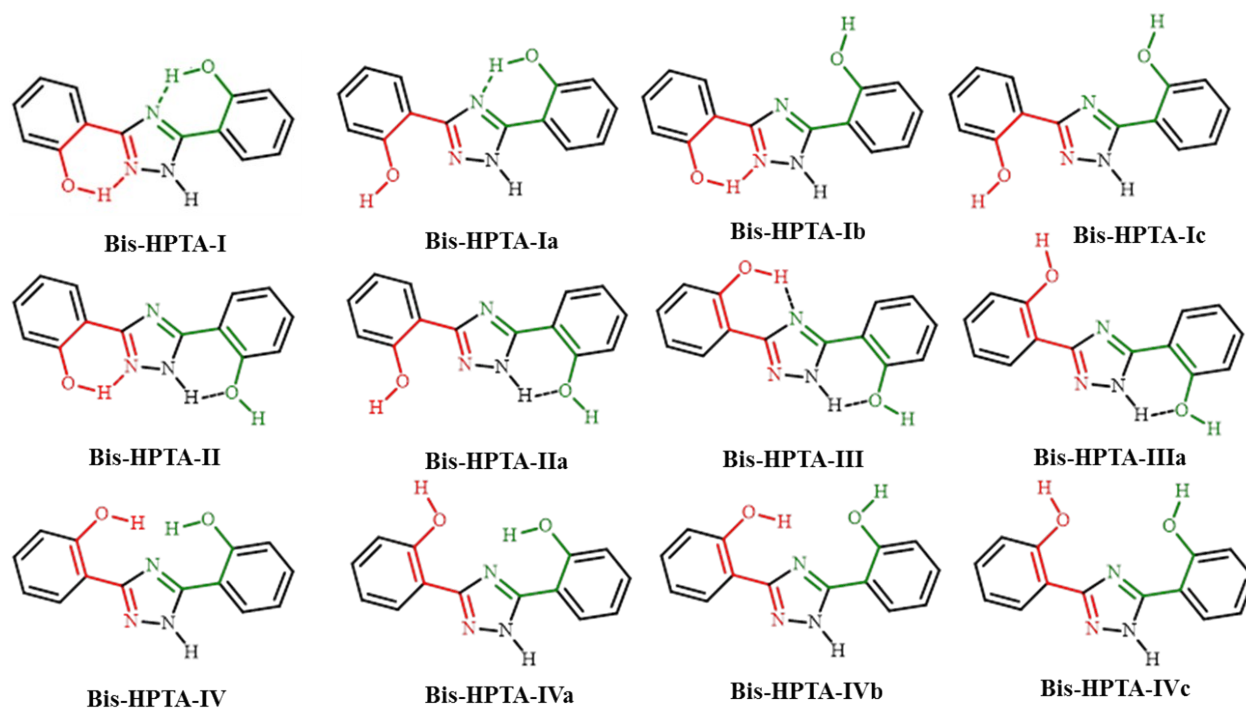
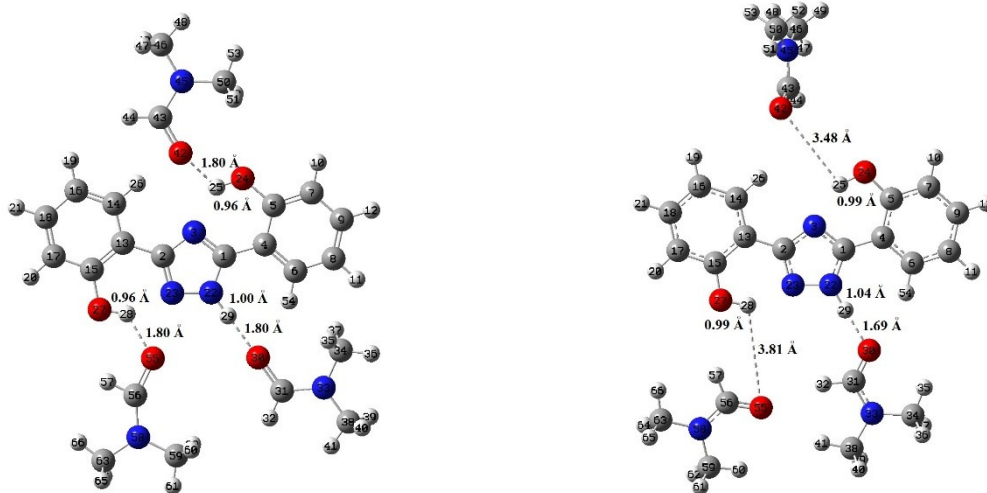


Figure S2. Different conformers of bis-HPTA.

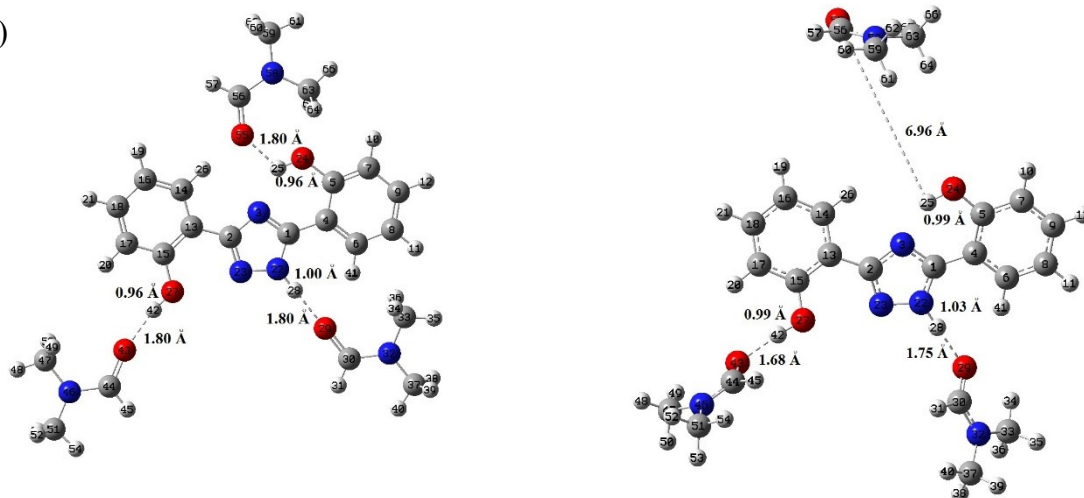
Table S1. The ground state optimized energy of different conformers in DMF. Optimized geometries of the conformers along with the Cartesian coordinates are given in table S6.

| Conformer     | Relative energy (eV) |
|---------------|----------------------|
| Bis-HPTA-I    | 0                    |
| Bis-HPTA-III  | 0.076                |
| Bis-HPTA-II   | 0.107                |
| Bis-HPTA-IV   | 0.116                |
| Bis-HPTA-IVb  | 0.271                |
| Bis-HPTA-Ia   | 0.277                |
| Bis-HPTA-IVa  | 0.283                |
| Bis-HPTA-Ib   | 0.313                |
| Bis-HPTA-IIa  | 0.412                |
| Bis-HPTA-IIIa | 0.459                |
| Bis-HPTA-Ic   | 0.610                |
| Bis-HPTA-IVc  | 0.635                |

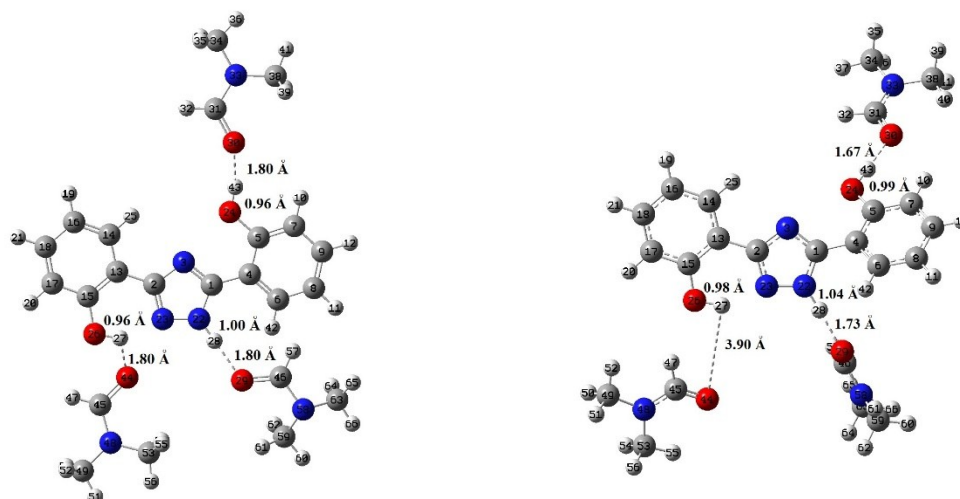
(a)



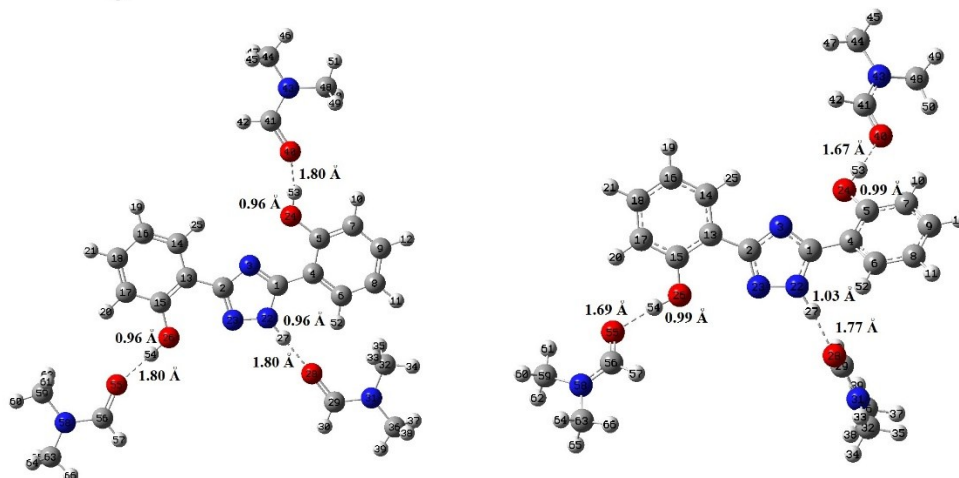
(b)



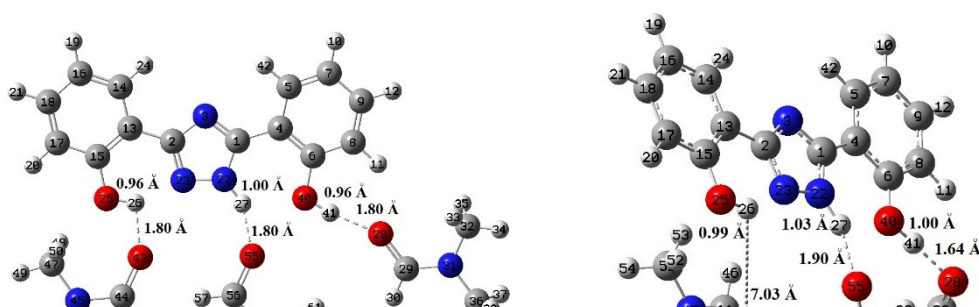
(c)



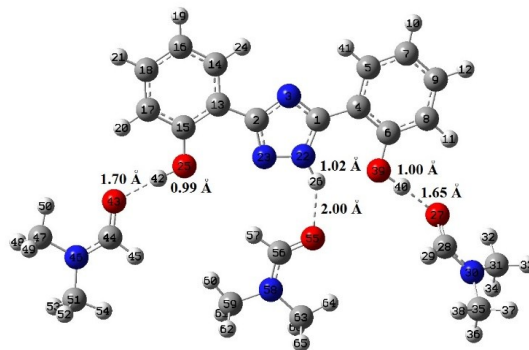
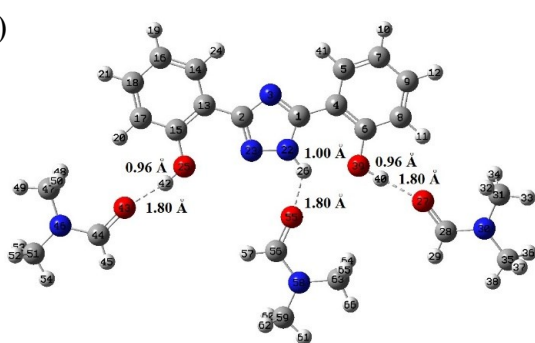
(d)



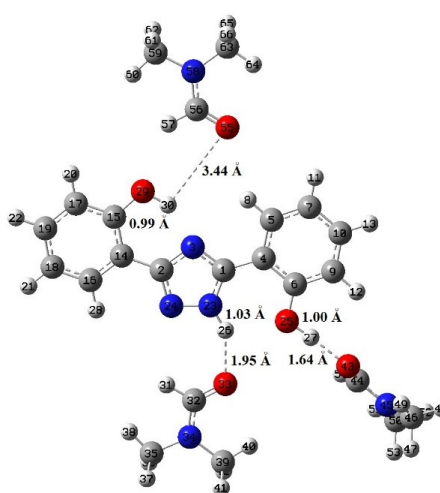
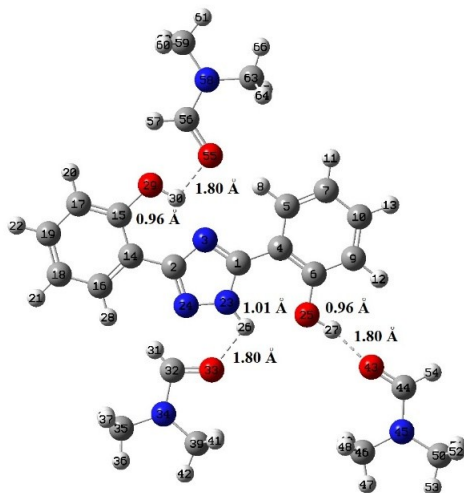
(e)



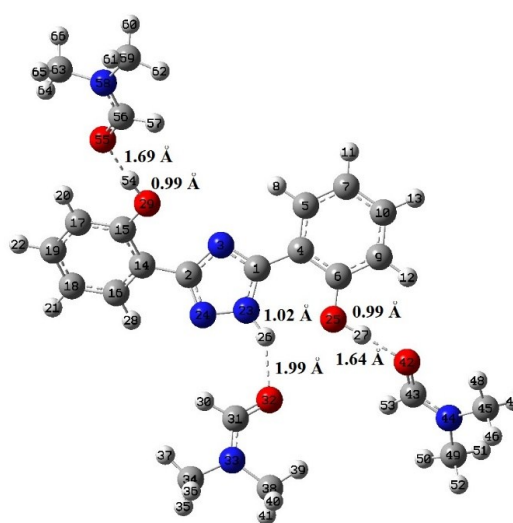
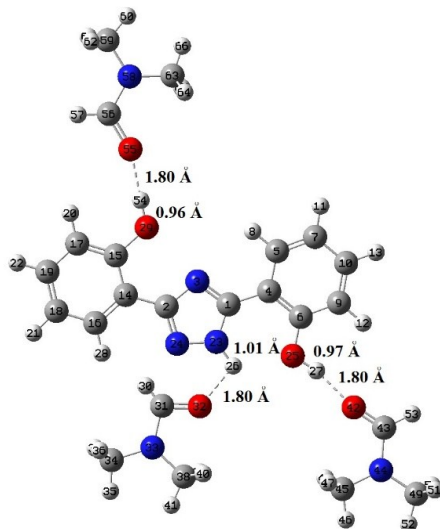
(f)



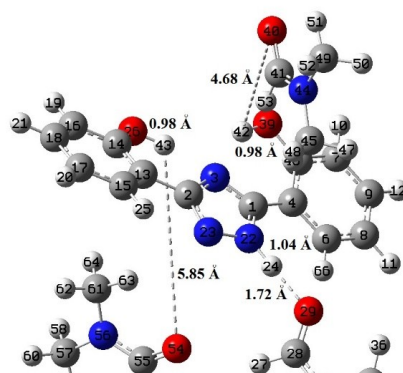
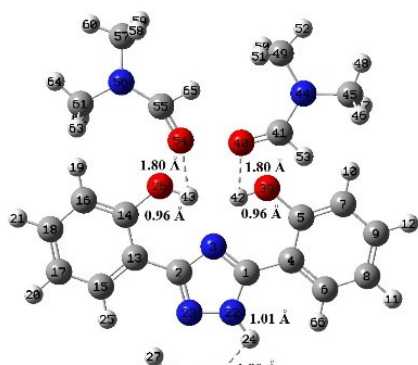
(g)



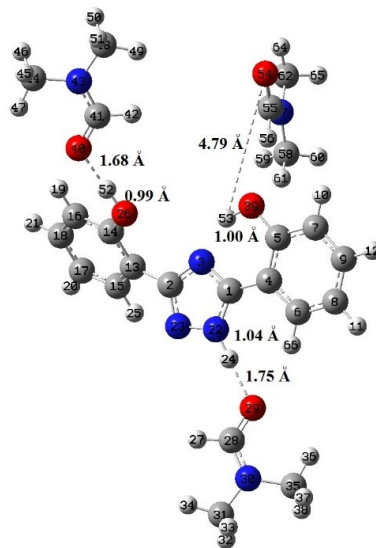
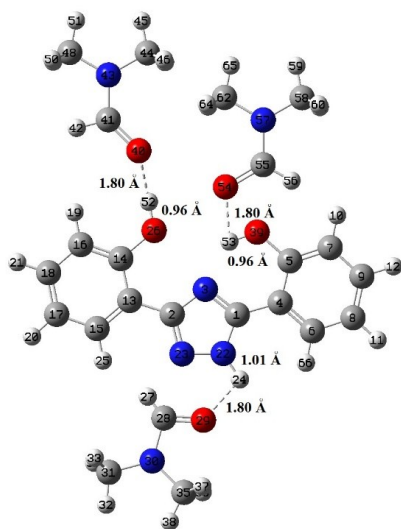
(h)



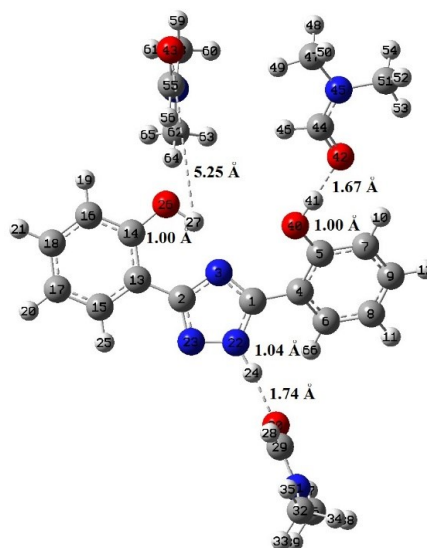
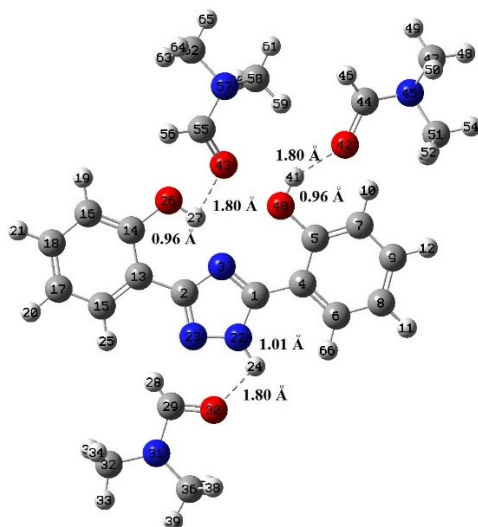
(i)



(j)



(k)



(l)

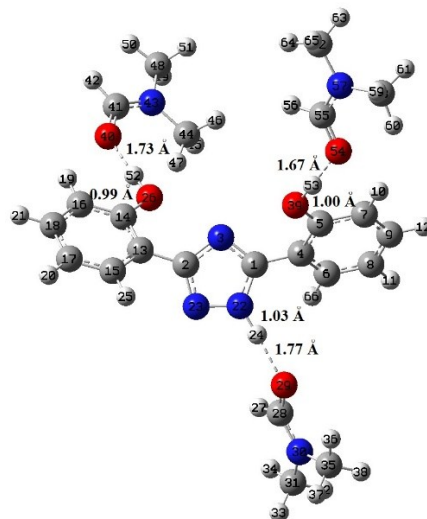
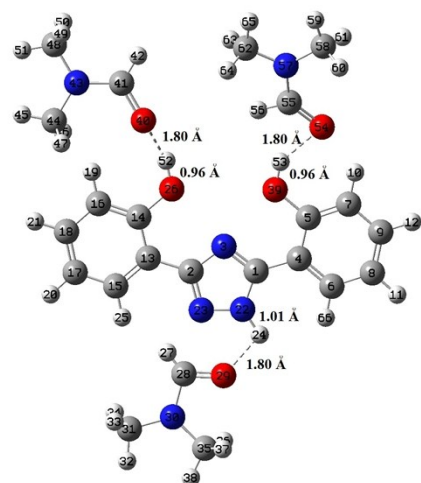


Figure S3: The input (left) and output (right) structures of bis-HPTA DMF complexes. (a) bis-HPTA-I, (b) bis-HPTA-Ia, (c) bi-HPTA-Ib, (d) bis-HPTA-Ic, (e) bis-HPTA-II, (f) bis-HPTA-IIa, (g) bis-HPTA-III, (h) bis-HPTA-IIa, (i) bis-HPTA-IV, (j) bis-HPTA-IVa, (k) bis-HPTA-IVb, (l) bis-HPTA-IVc.

Table S2. The optimized Cartesian coordinates of optimized bis-HPTA DMF complexes.

(a)bis-HPTA-I DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 0.671062                | 1.471032  | -0.22195  |
| 2           | 6             | 0.526642                | -0.663539 | -0.287598 |
| 3           | 7             | 1.426816                | 0.361555  | -0.27481  |
| 4           | 6             | 1.207489                | 2.829003  | -0.189733 |
| 5           | 6             | 2.61311                 | 3.023787  | -0.20668  |
| 6           | 6             | 0.364877                | 3.957693  | -0.141492 |
| 7           | 6             | 3.134225                | 4.32601   | -0.174695 |
| 8           | 6             | 0.890387                | 5.244693  | -0.110233 |
| 9           | 6             | 2.28165                 | 5.424506  | -0.12676  |
| 10          | 1             | 4.212337                | 4.45062   | -0.188589 |
| 11          | 1             | 0.225428                | 6.101311  | -0.073392 |
| 12          | 1             | 2.701195                | 6.425903  | -0.102607 |
| 13          | 6             | 0.86582                 | -2.087739 | -0.337628 |
| 14          | 6             | 2.210352                | -2.501975 | -0.376771 |
| 15          | 6             | -0.151606               | -3.074744 | -0.343784 |
| 16          | 6             | 2.545516                | -3.852756 | -0.419528 |
| 17          | 6             | 0.19196                 | -4.432747 | -0.387606 |
| 18          | 6             | 1.529799                | -4.81878  | -0.424673 |
| 19          | 1             | 3.588467                | -4.151283 | -0.44954  |
| 20          | 1             | -0.606063               | -5.168638 | -0.391361 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 21 | 1 | 1.780502  | -5.87508  | -0.458021 |
| 22 | 7 | -0.631245 | 1.118029  | -0.204543 |
| 23 | 7 | -0.736451 | -0.233352 | -0.245409 |
| 24 | 8 | 3.493965  | 1.994616  | -0.253258 |
| 25 | 1 | 2.985295  | 1.141391  | -0.275408 |
| 26 | 1 | 2.995964  | -1.752792 | -0.374074 |
| 27 | 8 | -1.477157 | -2.765309 | -0.307861 |
| 28 | 1 | -1.579015 | -1.78399  | -0.277477 |
| 29 | 1 | -1.494625 | 1.701234  | -0.158291 |
| 30 | 8 | -2.874962 | 2.683051  | -0.083492 |
| 31 | 6 | -4.032176 | 2.229077  | 0.059636  |
| 32 | 1 | -4.22139  | 1.149669  | 0.131709  |
| 33 | 7 | -5.13819  | 2.979658  | 0.13826   |
| 34 | 6 | -5.085974 | 4.436318  | 0.06096   |
| 35 | 1 | -4.051204 | 4.751334  | -0.063009 |
| 36 | 1 | -5.680167 | 4.785737  | -0.78986  |
| 37 | 1 | -5.49511  | 4.873002  | 0.978005  |
| 38 | 6 | -6.453554 | 2.366002  | 0.310621  |
| 39 | 1 | -6.911671 | 2.717865  | 1.241053  |
| 40 | 1 | -7.10622  | 2.638096  | -0.525613 |
| 41 | 1 | -6.349196 | 1.280606  | 0.347972  |
| 42 | 8 | 5.559373  | -1.190138 | -0.502314 |
| 43 | 6 | 6.220532  | -0.933612 | 0.512494  |
| 44 | 1 | 5.741974  | -0.547557 | 1.427256  |
| 45 | 7 | 7.555577  | -1.081012 | 0.643899  |
| 46 | 6 | 8.238546  | -0.749323 | 1.88873   |
| 47 | 1 | 7.51343   | -0.399086 | 2.625871  |
| 48 | 1 | 8.751234  | -1.630903 | 2.288902  |
| 49 | 1 | 8.979584  | 0.039611  | 1.719475  |
| 50 | 6 | 8.376504  | -1.578891 | -0.453446 |
| 51 | 1 | 7.737845  | -1.771529 | -1.314609 |
| 52 | 1 | 9.137409  | -0.837544 | -0.721108 |
| 53 | 1 | 8.880464  | -2.505694 | -0.157575 |
| 54 | 1 | -0.7119   | 3.821382  | -0.128588 |
| 55 | 8 | -5.25701  | -0.983253 | 0.320907  |
| 56 | 6 | -5.160375 | -2.215002 | 0.213681  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 57 | 1 | -4.189983 | -2.699424 | 0.02291   |
| 58 | 7 | -6.177655 | -3.094349 | 0.311139  |
| 59 | 6 | -7.544244 | -2.652755 | 0.563739  |
| 60 | 1 | -7.554226 | -1.567872 | 0.660179  |
| 61 | 1 | -8.196654 | -2.951978 | -0.263974 |
| 62 | 1 | -7.920967 | -3.105321 | 1.487487  |
| 63 | 6 | -5.958142 | -4.528889 | 0.164528  |
| 64 | 1 | -6.26313  | -5.055728 | 1.075209  |
| 65 | 1 | -6.539969 | -4.91922  | -0.677588 |
| 66 | 1 | -4.89968  | -4.723763 | -0.017812 |

(b) bis-HPTA-Ia DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -0.496945               | 1.934465  | -0.005962 |
| 2           | 6             | 0.090972                | -0.094073 | -0.390652 |
| 3           | 7             | -0.973402               | 0.682624  | -0.006406 |
| 4           | 6             | -1.282443               | 3.113493  | 0.351141  |
| 5           | 6             | -2.636543               | 2.952842  | 0.744604  |
| 6           | 6             | -0.734545               | 4.410722  | 0.316334  |
| 7           | 6             | -3.398704               | 4.078636  | 1.089428  |
| 8           | 6             | -1.497645               | 5.522298  | 0.659403  |
| 9           | 6             | -2.834629               | 5.350579  | 1.04709   |
| 10          | 1             | -4.432104               | 3.93162   | 1.387314  |
| 11          | 1             | -1.057786               | 6.5137    | 0.62536   |
| 12          | 1             | -3.438378               | 6.212238  | 1.316435  |
| 13          | 6             | -0.035188               | -1.553387 | -0.548759 |
| 14          | 6             | -1.325203               | -2.094062 | -0.713676 |
| 15          | 6             | 1.066906                | -2.443935 | -0.529739 |
| 16          | 6             | -1.539898               | -3.461849 | -0.864613 |
| 17          | 6             | 0.845532                | -3.82488  | -0.682839 |
| 18          | 6             | -0.442132               | -4.329698 | -0.849413 |
| 19          | 1             | -2.547004               | -3.844188 | -0.997055 |
| 20          | 1             | 1.701147                | -4.492951 | -0.665251 |
| 21          | 1             | -0.58559                | -5.400021 | -0.967685 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | 0.799698  | 1.901127  | -0.376408 |
| 23 | 7 | 1.190456  | 0.623185  | -0.624101 |
| 24 | 8 | -3.237337 | 1.738226  | 0.803499  |
| 25 | 1 | -2.574499 | 1.047888  | 0.526869  |
| 26 | 1 | -2.167984 | -1.411556 | -0.729205 |
| 27 | 8 | 2.317581  | -1.956104 | -0.352633 |
| 28 | 1 | 1.482026  | 2.672948  | -0.482081 |
| 29 | 8 | 2.597754  | 3.999598  | -0.718587 |
| 30 | 6 | 3.755291  | 4.000942  | -0.254454 |
| 31 | 1 | 4.117845  | 3.173877  | 0.372066  |
| 32 | 7 | 4.663191  | 4.965743  | -0.450513 |
| 33 | 6 | 4.363148  | 6.144095  | -1.259321 |
| 34 | 1 | 3.344779  | 6.067779  | -1.636865 |
| 35 | 1 | 4.462789  | 7.048844  | -0.650835 |
| 36 | 1 | 5.062466  | 6.205865  | -2.099412 |
| 37 | 6 | 5.999371  | 4.881416  | 0.132934  |
| 38 | 1 | 6.756583  | 4.886321  | -0.657734 |
| 39 | 1 | 6.175817  | 5.734643  | 0.79577   |
| 40 | 1 | 6.094112  | 3.959352  | 0.708912  |
| 41 | 1 | 0.300206  | 4.545129  | 0.015731  |
| 42 | 1 | 2.99073   | -2.687807 | -0.318267 |
| 43 | 8 | 4.23942   | -3.818361 | -0.297745 |
| 44 | 6 | 4.860348  | -4.076355 | 0.753637  |
| 45 | 1 | 4.608358  | -3.577049 | 1.699567  |
| 46 | 7 | 5.864797  | -4.954712 | 0.857322  |
| 47 | 6 | 6.340376  | -5.711136 | -0.298172 |
| 48 | 1 | 6.245527  | -6.784263 | -0.103844 |
| 49 | 1 | 5.745219  | -5.44319  | -1.169616 |
| 50 | 1 | 7.393529  | -5.478872 | -0.487142 |
| 51 | 6 | 6.53638   | -5.194073 | 2.132006  |
| 52 | 1 | 6.435915  | -6.245858 | 2.418299  |
| 53 | 1 | 7.600478  | -4.950744 | 2.048857  |
| 54 | 1 | 6.089618  | -4.571106 | 2.908555  |
| 55 | 8 | -7.770519 | -2.960073 | -1.797638 |
| 56 | 6 | -7.519164 | -3.069723 | -0.590004 |
| 57 | 1 | -7.233398 | -4.038462 | -0.148697 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 7 | -7.55545  | -2.072617 | 0.318256  |
| 59 | 6 | -7.23682  | -2.309678 | 1.721344  |
| 60 | 1 | -6.989927 | -3.362511 | 1.871491  |
| 61 | 1 | -6.37996  | -1.699247 | 2.026552  |
| 62 | 1 | -8.092846 | -2.053924 | 2.35534   |
| 63 | 6 | -7.911962 | -0.710816 | -0.062279 |
| 64 | 1 | -7.084049 | -0.028281 | 0.15876   |
| 65 | 1 | -8.12786  | -0.686124 | -1.129635 |
| 66 | 1 | -8.794999 | -0.382728 | 0.49698   |

(c) bi-HPTA-Ib DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 0.91246                 | 0.156356  | -1.366961 |
| 2           | 6             | -0.460199               | -1.445752 | -1.119504 |
| 3           | 7             | 0.844438                | -1.177151 | -1.411838 |
| 4           | 6             | 2.076589                | 1.011434  | -1.656693 |
| 5           | 6             | 3.33716                 | 0.781947  | -1.056719 |
| 6           | 6             | 1.929437                | 2.09335   | -2.542285 |
| 7           | 6             | 4.413648                | 1.629443  | -1.371425 |
| 8           | 6             | 2.999055                | 2.933495  | -2.84884  |
| 9           | 6             | 4.244338                | 2.691647  | -2.258784 |
| 10          | 1             | 5.377432                | 1.448661  | -0.90597  |
| 11          | 1             | 2.864564                | 3.757938  | -3.541391 |
| 12          | 1             | 5.090796                | 3.332869  | -2.487748 |
| 13          | 6             | -1.043416               | -2.789975 | -1.049199 |
| 14          | 6             | -0.251927               | -3.923339 | -1.30904  |
| 15          | 6             | -2.408115               | -2.978351 | -0.71843  |
| 16          | 6             | -0.783546               | -5.2088   | -1.246434 |
| 17          | 6             | -2.940566               | -4.273438 | -0.655866 |
| 18          | 6             | -2.135337               | -5.379955 | -0.917438 |
| 19          | 1             | -0.153936               | -6.068737 | -1.451702 |
| 20          | 1             | -3.989043               | -4.390293 | -0.399879 |
| 21          | 1             | -2.563171               | -6.376913 | -0.86509  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | -0.303948 | 0.663172  | -1.061071 |
| 23 | 7 | -1.190468 | -0.346021 | -0.898536 |
| 24 | 8 | 3.465573  | -0.235479 | -0.174317 |
| 25 | 1 | 0.792068  | -3.772469 | -1.562913 |
| 26 | 8 | -3.24936  | -1.940877 | -0.451491 |
| 27 | 1 | -2.75185  | -1.09172  | -0.535846 |
| 28 | 1 | -0.594835 | 1.648317  | -0.901743 |
| 29 | 8 | -1.169373 | 3.257454  | -0.636169 |
| 30 | 8 | 5.896501  | -0.374178 | 0.91243   |
| 31 | 6 | 6.168895  | -1.272294 | 1.735749  |
| 32 | 1 | 5.428663  | -2.037029 | 2.008175  |
| 33 | 7 | 7.343633  | -1.40999  | 2.361178  |
| 34 | 6 | 7.574446  | -2.492171 | 3.314619  |
| 35 | 1 | 8.408288  | -3.117081 | 2.979416  |
| 36 | 1 | 7.815301  | -2.080445 | 4.299907  |
| 37 | 1 | 6.67886   | -3.110051 | 3.397316  |
| 38 | 6 | 8.44845   | -0.484213 | 2.12501   |
| 39 | 1 | 9.317714  | -1.032627 | 1.748183  |
| 40 | 1 | 8.139984  | 0.259977  | 1.392795  |
| 41 | 1 | 8.723469  | 0.012813  | 3.060933  |
| 42 | 1 | 0.96214   | 2.261344  | -3.006651 |
| 43 | 1 | 4.3833    | -0.27159  | 0.212339  |
| 44 | 8 | -5.538553 | 0.83747   | 1.393955  |
| 45 | 6 | -6.026551 | -0.268958 | 1.121969  |
| 46 | 6 | -1.366357 | 3.673652  | 0.522824  |
| 47 | 1 | -5.424166 | -1.058868 | 0.64631   |
| 48 | 7 | -7.301938 | -0.643933 | 1.357932  |
| 49 | 6 | -7.78163  | -1.973645 | 1.000637  |
| 50 | 1 | -8.133198 | -2.505036 | 1.891944  |
| 51 | 1 | -8.609814 | -1.901956 | 0.286948  |
| 52 | 1 | -6.973152 | -2.548115 | 0.544556  |
| 53 | 6 | -8.258612 | 0.262067  | 1.981704  |
| 54 | 1 | -8.634055 | -0.170166 | 2.915924  |
| 55 | 1 | -7.763872 | 1.209293  | 2.192943  |
| 56 | 1 | -9.107455 | 0.434899  | 1.310841  |
| 57 | 1 | -1.160657 | 3.03976   | 1.397016  |

|    |   |           |          |           |
|----|---|-----------|----------|-----------|
| 58 | 7 | -1.831936 | 4.889361 | 0.837498  |
| 59 | 6 | -2.165096 | 5.869341 | -0.19262  |
| 60 | 1 | -1.551138 | 6.766943 | -0.065594 |
| 61 | 1 | -1.977049 | 5.434095 | -1.172739 |
| 62 | 1 | -3.220331 | 6.149711 | -0.111711 |
| 63 | 6 | -2.030791 | 5.290309 | 2.227624  |
| 64 | 1 | -3.082981 | 5.537321 | 2.401978  |
| 65 | 1 | -1.743551 | 4.474428 | 2.892971  |
| 66 | 1 | -1.419112 | 6.168648 | 2.457695  |

(d) bis-HPTA-Ic DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 0.933059                | 0.45452   | -1.021483 |
| 2           | 6             | -0.702883               | -0.866485 | -0.665736 |
| 3           | 7             | 0.616387                | -0.838553 | -1.045503 |
| 4           | 6             | 2.210934                | 1.08592   | -1.396887 |
| 5           | 6             | 3.453287                | 0.613574  | -0.911055 |
| 6           | 6             | 2.19777                 | 2.201578  | -2.252668 |
| 7           | 6             | 4.638405                | 1.260506  | -1.302375 |
| 8           | 6             | 3.375276                | 2.842472  | -2.636635 |
| 9           | 6             | 4.598316                | 2.361589  | -2.157172 |
| 10          | 1             | 5.586344                | 0.893277  | -0.921308 |
| 11          | 1             | 3.338743                | 3.697337  | -3.304105 |
| 12          | 1             | 5.527365                | 2.844515  | -2.446654 |
| 13          | 6             | -1.443807               | -2.139803 | -0.57228  |
| 14          | 6             | -0.75373                | -3.327973 | -0.886142 |
| 15          | 6             | -2.804923               | -2.247348 | -0.189265 |
| 16          | 6             | -1.362901               | -4.579142 | -0.833217 |
| 17          | 6             | -3.41713                | -3.513524 | -0.136523 |
| 18          | 6             | -2.707373               | -4.668713 | -0.455368 |
| 19          | 1             | -0.796993               | -5.47109  | -1.083668 |
| 20          | 1             | -4.460158               | -3.57266  | 0.159832  |
| 21          | 1             | -3.204187               | -5.633671 | -0.40686  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | -0.152444 | 1.169213  | -0.644737 |
| 23 | 7 | -1.204448 | 0.347277  | -0.410347 |
| 24 | 8 | 3.466592  | -0.436686 | -0.057474 |
| 25 | 1 | 0.286766  | -3.244453 | -1.178438 |
| 26 | 8 | -3.505969 | -1.131773 | 0.127519  |
| 27 | 1 | -0.245244 | 2.18507   | -0.474758 |
| 28 | 8 | -0.522161 | 3.907813  | -0.144483 |
| 29 | 6 | -0.268228 | 4.379674  | 0.980302  |
| 30 | 1 | 0.155293  | 3.752178  | 1.777917  |
| 31 | 7 | -0.468242 | 5.653134  | 1.348626  |
| 32 | 6 | -1.02637  | 6.635792  | 0.424265  |
| 33 | 1 | -1.231669 | 6.1519    | -0.529284 |
| 34 | 1 | -1.954446 | 7.04737   | 0.83439   |
| 35 | 1 | -0.314131 | 7.453937  | 0.275061  |
| 36 | 6 | -0.137752 | 6.11763   | 2.692838  |
| 37 | 1 | 0.606371  | 6.919241  | 2.642691  |
| 38 | 1 | -1.034618 | 6.49981   | 3.191086  |
| 39 | 1 | 0.269514  | 5.293283  | 3.280671  |
| 40 | 8 | 5.905633  | -1.118289 | 0.782579  |
| 41 | 6 | 6.175171  | -2.323437 | 0.965702  |
| 42 | 1 | 5.439329  | -3.109492 | 0.747002  |
| 43 | 7 | 7.340814  | -2.78808  | 1.430017  |
| 44 | 6 | 7.57033   | -4.218929 | 1.612791  |
| 45 | 1 | 8.411112  | -4.547282 | 0.993423  |
| 46 | 1 | 7.800331  | -4.431209 | 2.661761  |
| 47 | 1 | 6.678016  | -4.777339 | 1.325339  |
| 48 | 6 | 8.439044  | -1.88962  | 1.776183  |
| 49 | 1 | 9.315672  | -2.120853 | 1.162441  |
| 50 | 1 | 8.129102  | -0.861229 | 1.598261  |
| 51 | 1 | 8.703578  | -2.01675  | 2.830861  |
| 52 | 1 | 1.244091  | 2.55658   | -2.632266 |
| 53 | 1 | 4.393238  | -0.667095 | 0.226087  |
| 54 | 1 | -4.452242 | -1.349051 | 0.340058  |
| 55 | 8 | -6.09333  | -1.555136 | 0.714128  |
| 56 | 6 | -6.92248  | -0.753519 | 0.237483  |
| 57 | 1 | -6.604304 | 0.072134  | -0.414295 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 7 | -8.243725 | -0.794599 | 0.448733  |
| 59 | 6 | -8.85189  | -1.821242 | 1.290691  |
| 60 | 1 | -9.590191 | -2.385828 | 0.712221  |
| 61 | 1 | -8.075334 | -2.494814 | 1.649141  |
| 62 | 1 | -9.355221 | -1.353961 | 2.14351   |
| 63 | 6 | -9.139293 | 0.191706  | -0.14967  |
| 64 | 1 | -9.871517 | -0.306466 | -0.793142 |
| 65 | 1 | -9.672554 | 0.740062  | 0.633506  |
| 66 | 1 | -8.563576 | 0.899021  | -0.748824 |

(e) bis-HPTA-II DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.323244                | 1.812728  | -0.212055 |
| 2           | 6             | 3.168779                | 0.779999  | -0.460845 |
| 3           | 7             | 2.639771                | 1.941073  | 0.00845   |
| 4           | 6             | 0.331061                | 2.837606  | 0.128126  |
| 5           | 6             | 0.786555                | 4.07452   | 0.624114  |
| 6           | 6             | -1.061424               | 2.63811   | -0.017914 |
| 7           | 6             | -0.0994                 | 5.09099   | 0.966787  |
| 8           | 6             | -1.953931               | 3.666534  | 0.328547  |
| 9           | 6             | -1.476451               | 4.881069  | 0.815456  |
| 10          | 1             | 0.27619                 | 6.036411  | 1.344707  |
| 11          | 1             | -3.019273               | 3.498908  | 0.207873  |
| 12          | 1             | -2.181677               | 5.664937  | 1.076213  |
| 13          | 6             | 4.596117                | 0.441594  | -0.443164 |
| 14          | 6             | 5.532973                | 1.339852  | 0.098773  |
| 15          | 6             | 5.062485                | -0.787731 | -0.970875 |
| 16          | 6             | 6.892911                | 1.041945  | 0.122862  |
| 17          | 6             | 6.432193                | -1.085117 | -0.945416 |
| 18          | 6             | 7.340178                | -0.178074 | -0.403242 |
| 19          | 1             | 7.598073                | 1.750351  | 0.545912  |
| 20          | 1             | 6.763565                | -2.033596 | -1.356747 |
| 21          | 1             | 8.398253                | -0.423198 | -0.391292 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | 1.084446  | 0.611589  | -0.792603 |
| 23 | 7 | 2.250584  | -0.05643  | -0.957271 |
| 24 | 1 | 5.168724  | 2.279218  | 0.501387  |
| 25 | 8 | 4.228846  | -1.716903 | -1.514251 |
| 26 | 1 | 3.300005  | -1.383962 | -1.466823 |
| 27 | 1 | 0.211163  | 0.173694  | -1.112458 |
| 28 | 8 | -4.116282 | 1.232798  | -0.726993 |
| 29 | 6 | -4.814805 | 0.738767  | 0.183707  |
| 30 | 1 | -4.36229  | 0.400145  | 1.125656  |
| 31 | 7 | -6.139653 | 0.569287  | 0.127738  |
| 32 | 6 | -6.913107 | 0.965166  | -1.046692 |
| 33 | 1 | -6.240011 | 1.379914  | -1.795084 |
| 34 | 1 | -7.431333 | 0.093993  | -1.459852 |
| 35 | 1 | -7.657181 | 1.716855  | -0.764217 |
| 36 | 6 | -6.878782 | -0.014485 | 1.244544  |
| 37 | 1 | -7.620082 | 0.698997  | 1.61824   |
| 38 | 1 | -7.395597 | -0.922541 | 0.918442  |
| 39 | 1 | -6.190478 | -0.267842 | 2.052327  |
| 40 | 8 | -1.493246 | 1.446226  | -0.492345 |
| 41 | 1 | -2.491086 | 1.399292  | -0.549173 |
| 42 | 1 | 1.855679  | 4.219335  | 0.731617  |
| 43 | 8 | -1.778492 | -2.614872 | 3.248859  |
| 44 | 6 | -0.603245 | -2.22372  | 3.253119  |
| 45 | 7 | 0.481975  | -2.980001 | 2.988367  |
| 46 | 1 | -0.347347 | -1.177051 | 3.48493   |
| 47 | 6 | 0.360125  | -4.394703 | 2.656849  |
| 48 | 1 | -0.69322  | -4.671904 | 2.668309  |
| 49 | 1 | 0.777954  | -4.585966 | 1.662372  |
| 50 | 1 | 0.905784  | -5.001523 | 3.387794  |
| 51 | 6 | 1.827108  | -2.417216 | 3.019865  |
| 52 | 1 | 2.305702  | -2.518011 | 2.039773  |
| 53 | 1 | 1.778102  | -1.358165 | 3.280393  |
| 54 | 1 | 2.440212  | -2.936427 | 3.764601  |
| 55 | 8 | -0.66547  | -1.242488 | -2.033929 |
| 56 | 6 | -1.678314 | -1.822832 | -1.609106 |
| 57 | 1 | -2.147036 | -1.529755 | -0.658141 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 7 | -2.308514 | -2.839236 | -2.22326  |
| 59 | 6 | -1.836652 | -3.367912 | -3.49898  |
| 60 | 1 | -2.615698 | -3.259361 | -4.261232 |
| 61 | 1 | -0.94842  | -2.817009 | -3.804714 |
| 62 | 1 | -1.591905 | -4.430488 | -3.396536 |
| 63 | 6 | -3.49124  | -3.464089 | -1.640327 |
| 64 | 1 | -4.342231 | -3.37674  | -2.324004 |
| 65 | 1 | -3.303487 | -4.525641 | -1.447115 |
| 66 | 1 | -3.74244  | -2.972951 | -0.698645 |

(f) bis-HPTA-IIa DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.097179                | -2.263354 | 0.046177  |
| 2           | 6             | -1.038683               | -2.192992 | 0.001218  |
| 3           | 7             | 0.023448                | -3.056714 | -0.001659 |
| 4           | 6             | 2.484006                | -2.743069 | 0.062634  |
| 5           | 6             | 2.721541                | -4.130127 | 0.019722  |
| 6           | 6             | 3.59511                 | -1.870045 | 0.121573  |
| 7           | 6             | 4.013468                | -4.648223 | 0.034191  |
| 8           | 6             | 4.898387                | -2.394313 | 0.137316  |
| 9           | 6             | 5.104746                | -3.771594 | 0.093566  |
| 10          | 1             | 4.169849                | -5.7217   | 0.000405  |
| 11          | 1             | 5.738588                | -1.708602 | 0.184441  |
| 12          | 1             | 6.119197                | -4.159704 | 0.106607  |
| 13          | 6             | -2.427666               | -2.691344 | -0.041304 |
| 14          | 6             | -2.623175               | -4.086868 | -0.074387 |
| 15          | 6             | -3.577948               | -1.862499 | -0.051417 |
| 16          | 6             | -3.890987               | -4.661042 | -0.116757 |
| 17          | 6             | -4.858111               | -2.446273 | -0.094697 |
| 18          | 6             | -5.016443               | -3.829501 | -0.12723  |
| 19          | 1             | -3.999235               | -5.740958 | -0.141051 |
| 20          | 1             | -5.725347               | -1.793269 | -0.102393 |
| 21          | 1             | -6.016112               | -4.253637 | -0.160205 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | 0.682223  | -0.973842 | 0.075551  |
| 23 | 7 | -0.672487 | -0.907363 | 0.047558  |
| 24 | 1 | -1.742595 | -4.718883 | -0.065976 |
| 25 | 8 | -3.439462 | -0.514039 | -0.018826 |
| 26 | 1 | 1.221187  | -0.104469 | 0.11775   |
| 27 | 8 | 5.53745   | 0.957977  | 0.302321  |
| 28 | 6 | 5.707105  | 1.892591  | -0.508858 |
| 29 | 1 | 4.998909  | 2.066402  | -1.330403 |
| 30 | 7 | 6.726424  | 2.757683  | -0.478821 |
| 31 | 6 | 7.765326  | 2.678844  | 0.545293  |
| 32 | 1 | 7.554484  | 1.838199  | 1.204074  |
| 33 | 1 | 8.742376  | 2.53917   | 0.071872  |
| 34 | 1 | 7.784615  | 3.606002  | 1.127139  |
| 35 | 6 | 6.847787  | 3.825523  | -1.46808  |
| 36 | 1 | 6.835336  | 4.800977  | -0.971504 |
| 37 | 1 | 7.78769   | 3.721827  | -2.019426 |
| 38 | 1 | 6.015696  | 3.77495   | -2.17212  |
| 39 | 8 | 3.360106  | -0.53719  | 0.164546  |
| 40 | 1 | 4.203576  | -0.001807 | 0.199262  |
| 41 | 1 | 1.864804  | -4.793431 | -0.02526  |
| 42 | 1 | -4.324924 | -0.065513 | -0.041836 |
| 43 | 8 | -5.807958 | 0.772871  | -0.083948 |
| 44 | 6 | -5.872553 | 2.016821  | -0.148857 |
| 45 | 1 | -4.963199 | 2.633511  | -0.166749 |
| 46 | 7 | -7.006321 | 2.7271    | -0.202299 |
| 47 | 6 | -8.315371 | 2.079678  | -0.191819 |
| 48 | 1 | -8.899876 | 2.43801   | 0.661613  |
| 49 | 1 | -8.856078 | 2.317357  | -1.113845 |
| 50 | 1 | -8.180219 | 1.002051  | -0.115591 |
| 51 | 6 | -6.986476 | 4.185446  | -0.279844 |
| 52 | 1 | -7.47898  | 4.520558  | -1.198307 |
| 53 | 1 | -7.511641 | 4.614985  | 0.579263  |
| 54 | 1 | -5.95532  | 4.542252  | -0.279752 |
| 55 | 8 | 1.246236  | 1.889838  | 0.207431  |
| 56 | 6 | 0.150538  | 2.455979  | 0.357397  |
| 57 | 1 | -0.785796 | 1.879233  | 0.36945   |

|    |   |           |          |           |
|----|---|-----------|----------|-----------|
| 58 | 7 | -0.027827 | 3.780473 | 0.516642  |
| 59 | 6 | -1.358881 | 4.350865 | 0.691189  |
| 60 | 1 | -2.107032 | 3.556657 | 0.662376  |
| 61 | 1 | -1.427949 | 4.867534 | 1.654591  |
| 62 | 1 | -1.572797 | 5.068675 | -0.108006 |
| 63 | 6 | 1.099489  | 4.706084 | 0.527926  |
| 64 | 1 | 2.021428  | 4.14413  | 0.38481   |
| 65 | 1 | 0.989764  | 5.441176 | -0.276747 |
| 66 | 1 | 1.140071  | 5.237782 | 1.48481   |

(g) bis-HPTA-III DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -0.314886               | -0.081072 | -0.147252 |
| 2           | 6             | -1.330722               | 1.80647   | -0.072733 |
| 3           | 7             | -1.54414                | 0.456523  | -0.10788  |
| 4           | 6             | -0.032274               | -1.517131 | -0.195526 |
| 5           | 6             | -1.108384               | -2.42617  | -0.171723 |
| 6           | 6             | 1.285943                | -2.026135 | -0.269468 |
| 7           | 6             | -0.892764               | -3.800327 | -0.219978 |
| 8           | 1             | -2.122013               | -2.043996 | -0.11403  |
| 9           | 6             | 1.498259                | -3.413605 | -0.320236 |
| 10          | 6             | 0.417193                | -4.291692 | -0.295145 |
| 11          | 1             | -1.736781               | -4.482049 | -0.199891 |
| 12          | 1             | 2.515849                | -3.786236 | -0.37948  |
| 13          | 1             | 0.598729                | -5.361938 | -0.334525 |
| 14          | 6             | -2.432624               | 2.774268  | -0.025506 |
| 15          | 6             | -3.778542               | 2.332267  | -0.009955 |
| 16          | 6             | -2.177575               | 4.15773   | 0.004514  |
| 17          | 6             | -4.821222               | 3.270091  | 0.035074  |
| 18          | 6             | -3.214249               | 5.085292  | 0.049103  |
| 19          | 6             | -4.542135               | 4.634107  | 0.064209  |
| 20          | 1             | -5.843936               | 2.905943  | 0.04608   |
| 21          | 1             | -2.993691               | 6.147781  | 0.071401  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 1 | -5.360711 | 5.347227  | 0.098653  |
| 23 | 7 | 0.583106  | 0.93039   | -0.135002 |
| 24 | 7 | -0.039661 | 2.135225  | -0.087379 |
| 25 | 8 | 2.310837  | -1.14341  | -0.291102 |
| 26 | 1 | 1.608741  | 0.905954  | -0.151093 |
| 27 | 1 | 3.202987  | -1.593455 | -0.347586 |
| 28 | 1 | -1.1454   | 4.492721  | -0.008363 |
| 29 | 8 | -4.115378 | 1.014826  | -0.037035 |
| 30 | 1 | -3.278345 | 0.479194  | -0.069666 |
| 31 | 1 | 2.38088   | 3.660682  | -0.04414  |
| 32 | 6 | 3.322494  | 3.092205  | -0.053303 |
| 33 | 8 | 3.319554  | 1.850367  | -0.10483  |
| 34 | 7 | 4.42017   | 3.868023  | -0.004193 |
| 35 | 6 | 4.320002  | 5.322297  | 0.056341  |
| 36 | 1 | 4.793209  | 5.697753  | 0.96991   |
| 37 | 1 | 4.818672  | 5.773677  | -0.808016 |
| 38 | 1 | 3.270159  | 5.620803  | 0.053966  |
| 39 | 6 | 5.76123   | 3.293589  | -0.006509 |
| 40 | 1 | 5.682913  | 2.208983  | -0.064681 |
| 41 | 1 | 6.327235  | 3.666518  | -0.866822 |
| 42 | 1 | 6.291655  | 3.573813  | 0.910064  |
| 43 | 8 | 4.697023  | -2.248628 | -0.499294 |
| 44 | 6 | 5.540653  | -2.143084 | 0.416083  |
| 45 | 7 | 6.786904  | -2.624939 | 0.368324  |
| 46 | 6 | 7.286201  | -3.338879 | -0.804373 |
| 47 | 1 | 8.164983  | -2.823625 | -1.20504  |
| 48 | 1 | 7.571803  | -4.358198 | -0.525207 |
| 49 | 1 | 6.505115  | -3.372304 | -1.562002 |
| 50 | 6 | 7.709174  | -2.460359 | 1.489271  |
| 51 | 1 | 7.216476  | -1.918932 | 2.29844   |
| 52 | 1 | 8.028847  | -3.439703 | 1.859169  |
| 53 | 1 | 8.592288  | -1.897858 | 1.170064  |
| 54 | 1 | 5.297903  | -1.626361 | 1.354476  |
| 55 | 8 | -4.701064 | -2.65377  | 0.062824  |
| 56 | 6 | -5.767606 | -2.024903 | 0.113459  |
| 57 | 1 | -5.782957 | -0.924568 | 0.073931  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 7 | -6.997993 | -2.570611 | 0.219835  |
| 59 | 6 | -8.195017 | -1.739835 | 0.270157  |
| 60 | 1 | -7.915825 | -0.686301 | 0.208322  |
| 61 | 1 | -8.860996 | -1.978583 | -0.566427 |
| 62 | 1 | -8.737171 | -1.907459 | 1.207412  |
| 63 | 6 | -7.187717 | -4.014297 | 0.290142  |
| 64 | 1 | -6.214567 | -4.502138 | 0.249513  |
| 65 | 1 | -7.69215  | -4.283399 | 1.224833  |
| 66 | 1 | -7.802967 | -4.356255 | -0.549572 |

(h) bis-HPTA-IIIa DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -0.136188               | -0.686858 | -0.771293 |
| 2           | 6             | 1.275133                | 0.899034  | -0.954996 |
| 3           | 7             | 1.133236                | -0.445699 | -1.124624 |
| 4           | 6             | -0.7624                 | -2.013815 | -0.783833 |
| 5           | 6             | 0.016894                | -3.126614 | -1.153613 |
| 6           | 6             | -2.117499               | -2.223979 | -0.437431 |
| 7           | 6             | -0.517102               | -4.411822 | -1.18226  |
| 8           | 1             | 1.055014                | -2.957774 | -1.417543 |
| 9           | 6             | -2.65455                | -3.521791 | -0.465461 |
| 10          | 6             | -1.860462               | -4.605508 | -0.835047 |
| 11          | 1             | 0.10488                 | -5.253386 | -1.470135 |
| 12          | 1             | -3.695795               | -3.664237 | -0.194058 |
| 13          | 1             | -2.292012               | -5.602234 | -0.850529 |
| 14          | 6             | 2.493813                | 1.671583  | -1.274997 |
| 15          | 6             | 3.786509                | 1.252316  | -0.881812 |
| 16          | 6             | 2.366364                | 2.88061   | -1.980324 |
| 17          | 6             | 4.903807                | 2.036196  | -1.219552 |
| 18          | 6             | 3.474927                | 3.661747  | -2.308514 |
| 19          | 6             | 4.7489                  | 3.228435  | -1.926742 |
| 20          | 1             | 5.890293                | 1.703904  | -0.910658 |
| 21          | 1             | 3.346815                | 4.58762   | -2.860421 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 1 | 5.626716  | 3.817796  | -2.176756 |
| 23 | 7 | -0.718183 | 0.482336  | -0.409475 |
| 24 | 7 | 0.167099  | 1.503818  | -0.517423 |
| 25 | 8 | -2.861806 | -1.149768 | -0.081422 |
| 26 | 1 | -1.664024 | 0.676702  | -0.069238 |
| 27 | 1 | -3.808432 | -1.39541  | 0.126076  |
| 28 | 1 | 1.3719    | 3.197423  | -2.279262 |
| 29 | 8 | 3.918251  | 0.111428  | -0.16014  |
| 30 | 1 | -1.490322 | 3.398289  | 0.723282  |
| 31 | 6 | -2.539224 | 3.132866  | 0.921316  |
| 32 | 8 | -2.975583 | 2.003532  | 0.641626  |
| 33 | 7 | -3.252417 | 4.130821  | 1.474591  |
| 34 | 6 | -2.645686 | 5.425117  | 1.76638   |
| 35 | 1 | -3.16616  | 6.22027   | 1.221914  |
| 36 | 1 | -2.703131 | 5.638747  | 2.839134  |
| 37 | 1 | -1.59705  | 5.418334  | 1.463581  |
| 38 | 6 | -4.662038 | 3.965922  | 1.811558  |
| 39 | 1 | -4.970823 | 2.952046  | 1.560695  |
| 40 | 1 | -4.814188 | 4.140614  | 2.882021  |
| 41 | 1 | -5.270056 | 4.683533  | 1.24991   |
| 42 | 8 | -5.372847 | -1.738283 | 0.505334  |
| 43 | 6 | -6.307129 | -1.11092  | -0.036752 |
| 44 | 7 | -7.607554 | -1.325868 | 0.189005  |
| 45 | 6 | -8.062779 | -2.353399 | 1.122171  |
| 46 | 1 | -8.670686 | -1.895931 | 1.90922   |
| 47 | 1 | -8.671085 | -3.093346 | 0.591988  |
| 48 | 1 | -7.197201 | -2.842364 | 1.565933  |
| 49 | 6 | -8.636006 | -0.545215 | -0.494268 |
| 50 | 1 | -8.168197 | 0.176465  | -1.165671 |
| 51 | 1 | -9.283493 | -1.207151 | -1.077956 |
| 52 | 1 | -9.247723 | -0.007169 | 0.236876  |
| 53 | 1 | -6.107482 | -0.310924 | -0.76253  |
| 54 | 1 | 4.867439  | -0.058745 | 0.080991  |
| 55 | 8 | 6.450055  | -0.450774 | 0.527703  |
| 56 | 6 | 6.666518  | -1.395315 | 1.313957  |
| 57 | 1 | 5.839208  | -1.968101 | 1.755359  |

|    |   |          |           |          |
|----|---|----------|-----------|----------|
| 58 | 7 | 7.878154 | -1.811758 | 1.701545 |
| 59 | 6 | 8.036926 | -2.926446 | 2.631863 |
| 60 | 1 | 8.613056 | -3.729806 | 2.161771 |
| 61 | 1 | 8.564327 | -2.593506 | 3.531533 |
| 62 | 1 | 7.05733  | -3.313289 | 2.917542 |
| 63 | 6 | 9.097671 | -1.17042  | 1.21733  |
| 64 | 1 | 8.831334 | -0.378671 | 0.519095 |
| 65 | 1 | 9.655002 | -0.746142 | 2.0589   |
| 66 | 1 | 9.729234 | -1.908541 | 0.712715 |

(i) bis-HPTA-IV DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 0.232286                | 0.372302  | 0.867242  |
| 2           | 6             | 0.595397                | -1.207466 | -0.544282 |
| 3           | 7             | 0.710436                | -0.883101 | 0.786003  |
| 4           | 6             | 0.160247                | 1.179071  | 2.084421  |
| 5           | 6             | 0.850292                | 0.771724  | 3.252928  |
| 6           | 6             | -0.575058               | 2.381215  | 2.119183  |
| 7           | 6             | 0.791232                | 1.559034  | 4.410908  |
| 8           | 6             | -0.631641               | 3.157293  | 3.271525  |
| 9           | 6             | 0.055889                | 2.740465  | 4.420496  |
| 10          | 1             | 1.330608                | 1.224011  | 5.29106   |
| 11          | 1             | -1.207564               | 4.076777  | 3.277923  |
| 12          | 1             | 0.016666                | 3.338274  | 5.326157  |
| 13          | 6             | 0.98554                 | -2.50863  | -1.102073 |
| 14          | 6             | 1.18487                 | -3.635701 | -0.271325 |
| 15          | 6             | 1.145205                | -2.663838 | -2.492312 |
| 16          | 6             | 1.531348                | -4.871697 | -0.834411 |
| 17          | 6             | 1.489285                | -3.891293 | -3.050174 |
| 18          | 6             | 1.682539                | -4.999091 | -2.212712 |
| 19          | 1             | 1.67553                 | -5.719431 | -0.171945 |
| 20          | 1             | 1.610557                | -3.985406 | -4.124501 |
| 21          | 1             | 1.953997                | -5.962377 | -2.634379 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | -0.139632 | 0.764574  | -0.366806 |
| 23 | 7 | 0.073783  | -0.223583 | -1.271591 |
| 24 | 1 | -0.552549 | 1.664389  | -0.684865 |
| 25 | 1 | 0.996705  | -1.797422 | -3.128452 |
| 26 | 8 | 1.0375    | -3.589819 | 1.083217  |
| 27 | 1 | -2.924829 | 2.334961  | -1.987152 |
| 28 | 6 | -2.294597 | 3.223938  | -1.846271 |
| 29 | 8 | -1.198673 | 3.150895  | -1.253134 |
| 30 | 7 | -2.816586 | 4.343575  | -2.360821 |
| 31 | 6 | -4.109438 | 4.337503  | -3.040304 |
| 32 | 1 | -4.808879 | 5.00297   | -2.524294 |
| 33 | 1 | -3.992563 | 4.680431  | -4.073248 |
| 34 | 1 | -4.52023  | 3.326605  | -3.046064 |
| 35 | 6 | -2.119679 | 5.623896  | -2.268925 |
| 36 | 1 | -1.179972 | 5.481617  | -1.737892 |
| 37 | 1 | -1.919398 | 6.010859  | -3.273326 |
| 38 | 1 | -2.740571 | 6.346758  | -1.73     |
| 39 | 8 | 1.59495   | -0.363857 | 3.308815  |
| 40 | 8 | 5.798589  | -0.320394 | 0.595888  |
| 41 | 6 | 4.923856  | 0.319502  | -0.003192 |
| 42 | 1 | 1.530314  | -0.828158 | 2.446161  |
| 43 | 1 | 0.8407    | -2.66774  | 1.348606  |
| 44 | 7 | 5.141002  | 1.305943  | -0.898069 |
| 45 | 6 | 4.036355  | 1.998996  | -1.550388 |
| 46 | 1 | 3.085873  | 1.593258  | -1.1991   |
| 47 | 1 | 4.069731  | 3.069827  | -1.321459 |
| 48 | 1 | 4.094526  | 1.871328  | -2.636919 |
| 49 | 6 | 6.491317  | 1.724269  | -1.254975 |
| 50 | 1 | 6.633235  | 2.783922  | -1.015672 |
| 51 | 1 | 7.207726  | 1.125646  | -0.693792 |
| 52 | 1 | 6.658363  | 1.583053  | -2.328533 |
| 53 | 1 | 3.852523  | 0.119177  | 0.159587  |
| 54 | 8 | -4.50337  | -0.579128 | 0.216761  |
| 55 | 6 | -5.331816 | -1.480806 | 0.401378  |
| 56 | 7 | -5.056057 | -2.79736  | 0.504767  |
| 57 | 6 | -6.109616 | -3.781404 | 0.724103  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 1 | -5.935019 | -4.324837 | 1.659159  |
| 59 | 1 | -7.077505 | -3.279984 | 0.783993  |
| 60 | 1 | -6.13548  | -4.502345 | -0.100304 |
| 61 | 6 | -3.689974 | -3.297401 | 0.401731  |
| 62 | 1 | -3.608921 | -4.002084 | -0.433125 |
| 63 | 1 | -3.016725 | -2.457562 | 0.234958  |
| 64 | 1 | -3.407029 | -3.814828 | 1.324995  |
| 65 | 1 | -6.407551 | -1.260952 | 0.499134  |
| 66 | 1 | -1.107886 | 2.706065  | 1.231088  |

(j) bis-HPTA-Iva DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.724491               | 0.362447  | -0.097747 |
| 2           | 6             | -0.840902               | -1.393531 | 0.753782  |
| 3           | 7             | -0.535952               | -0.177785 | 0.208275  |
| 4           | 6             | -1.885948               | 1.677363  | -0.713444 |
| 5           | 6             | -0.729206               | 2.437665  | -1.029379 |
| 6           | 6             | -3.154259               | 2.214479  | -1.00738  |
| 7           | 6             | -0.869383               | 3.700879  | -1.622873 |
| 8           | 6             | -3.283973               | 3.46877   | -1.59575  |
| 9           | 6             | -2.134181               | 4.211054  | -1.902579 |
| 10          | 1             | 0.028212                | 4.264488  | -1.857098 |
| 11          | 1             | -4.269795               | 3.866089  | -1.81447  |
| 12          | 1             | -2.225418               | 5.1909    | -2.362063 |
| 13          | 6             | 0.13697                 | -2.349421 | 1.30436   |
| 14          | 6             | 1.402057                | -2.570677 | 0.709557  |
| 15          | 6             | -0.203757               | -3.082786 | 2.45503   |
| 16          | 6             | 2.286037                | -3.499502 | 1.286924  |
| 17          | 6             | 0.672272                | -4.007398 | 3.02156   |
| 18          | 6             | 1.924935                | -4.209245 | 2.431177  |
| 19          | 1             | 3.252712                | -3.661511 | 0.819754  |
| 20          | 1             | 0.386211                | -4.554743 | 3.914095  |
| 21          | 1             | 2.62472                 | -4.921057 | 2.859981  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | -2.697148 | -0.502689 | 0.256928  |
| 23 | 7 | -2.153769 | -1.625312 | 0.795802  |
| 24 | 1 | -3.725266 | -0.429938 | 0.150388  |
| 25 | 1 | -1.173999 | -2.905356 | 2.907956  |
| 26 | 8 | 1.724861  | -1.900415 | -0.422814 |
| 27 | 1 | -5.785144 | -2.233433 | -0.433669 |
| 28 | 6 | -6.192722 | -1.219554 | -0.315797 |
| 29 | 8 | -5.453546 | -0.25611  | -0.031014 |
| 30 | 7 | -7.516288 | -1.146342 | -0.505578 |
| 31 | 6 | -8.303386 | -2.331804 | -0.834286 |
| 32 | 1 | -9.062642 | -2.50523  | -0.064933 |
| 33 | 1 | -8.802703 | -2.196164 | -1.798981 |
| 34 | 1 | -7.651445 | -3.204962 | -0.892179 |
| 35 | 6 | -8.23607  | 0.119391  | -0.393233 |
| 36 | 1 | -7.52969  | 0.911521  | -0.150361 |
| 37 | 1 | -8.733886 | 0.348858  | -1.340954 |
| 38 | 1 | -8.993265 | 0.048354  | 0.394366  |
| 39 | 8 | 0.525954  | 1.988886  | -0.779288 |
| 40 | 8 | 4.135892  | -2.489841 | -1.410664 |
| 41 | 6 | 4.867113  | -1.547991 | -1.780673 |
| 42 | 1 | 4.548065  | -0.502946 | -1.665622 |
| 43 | 7 | 6.075874  | -1.685582 | -2.337985 |
| 44 | 6 | 6.665866  | -3.001311 | -2.570498 |
| 45 | 1 | 6.858123  | -3.138986 | -3.639482 |
| 46 | 1 | 7.613431  | -3.084024 | -2.028459 |
| 47 | 1 | 5.976857  | -3.768676 | -2.221628 |
| 48 | 6 | 6.862921  | -0.523347 | -2.742283 |
| 49 | 1 | 6.317253  | 0.392803  | -2.511017 |
| 50 | 1 | 7.818455  | -0.512773 | -2.208399 |
| 51 | 1 | 7.059944  | -0.558159 | -3.818545 |
| 52 | 1 | 2.63184   | -2.149139 | -0.749678 |
| 53 | 1 | 0.457189  | 1.082296  | -0.363463 |
| 54 | 8 | 4.348011  | 3.791387  | 0.312459  |
| 55 | 6 | 3.306159  | 3.53854   | 0.935643  |
| 56 | 1 | 2.412891  | 3.14254   | 0.427555  |
| 57 | 7 | 3.127263  | 3.703473  | 2.263824  |

|    |   |           |          |           |
|----|---|-----------|----------|-----------|
| 58 | 6 | 1.858467  | 3.374777 | 2.903099  |
| 59 | 1 | 2.002671  | 2.597523 | 3.661767  |
| 60 | 1 | 1.434276  | 4.261317 | 3.387498  |
| 61 | 1 | 1.153053  | 3.009941 | 2.154334  |
| 62 | 6 | 4.190816  | 4.215182 | 3.119077  |
| 63 | 1 | 4.436764  | 3.482164 | 3.895454  |
| 64 | 1 | 5.072966  | 4.409063 | 2.509979  |
| 65 | 1 | 3.871209  | 5.143808 | 3.605035  |
| 66 | 1 | -4.044852 | 1.639963 | -0.771173 |

(k) bis-HPTA-IVb DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.576979                | 0.131345  | 0.446834  |
| 2           | 6             | 1.149289                | 2.097523  | -0.284775 |
| 3           | 7             | 0.555823                | 0.934639  | 0.127951  |
| 4           | 6             | 1.523245                | -1.22854  | 0.998279  |
| 5           | 6             | 0.511751                | -2.149306 | 0.627977  |
| 6           | 6             | 2.508515                | -1.636803 | 1.917541  |
| 7           | 6             | 0.515032                | -3.438183 | 1.190525  |
| 8           | 6             | 2.508652                | -2.916348 | 2.467335  |
| 9           | 6             | 1.501945                | -3.816198 | 2.098612  |
| 10          | 1             | -0.262482               | -4.137431 | 0.899618  |
| 11          | 1             | 3.275404                | -3.20351  | 3.179336  |
| 12          | 1             | 1.482041                | -4.817142 | 2.520103  |
| 13          | 6             | 0.362413                | 3.252771  | -0.729982 |
| 14          | 6             | -1.052361               | 3.17836   | -0.778878 |
| 15          | 6             | 0.988834                | 4.450037  | -1.121435 |
| 16          | 6             | -1.794125               | 4.287073  | -1.21399  |
| 17          | 6             | 0.249092                | 5.548246  | -1.550908 |
| 18          | 6             | -1.149894               | 5.461176  | -1.596265 |
| 19          | 1             | -2.876169               | 4.205354  | -1.245728 |
| 20          | 1             | 0.753624                | 6.462159  | -1.847984 |
| 21          | 1             | -1.739168               | 6.31027   | -1.930352 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | 2.729013  | 0.804031  | 0.226003  |
| 23 | 7 | 2.48055   | 2.054078  | -0.239129 |
| 24 | 1 | 3.711144  | 0.483301  | 0.323083  |
| 25 | 1 | 2.072167  | 4.503221  | -1.081983 |
| 26 | 8 | -1.738589 | 2.060646  | -0.417944 |
| 27 | 1 | -1.079197 | 1.368406  | -0.133475 |
| 28 | 1 | 5.662714  | -0.23872  | -1.507423 |
| 29 | 6 | 6.094056  | -0.208864 | -0.496664 |
| 30 | 8 | 5.39427   | 0.076079  | 0.495171  |
| 31 | 7 | 7.40057   | -0.501954 | -0.460804 |
| 32 | 6 | 8.141512  | -0.823626 | -1.677361 |
| 33 | 1 | 8.955687  | -0.10649  | -1.823307 |
| 34 | 1 | 8.566449  | -1.829908 | -1.604474 |
| 35 | 1 | 7.474008  | -0.782356 | -2.539645 |
| 36 | 6 | 8.146842  | -0.510355 | 0.794381  |
| 37 | 1 | 7.471574  | -0.264455 | 1.612319  |
| 38 | 1 | 8.581449  | -1.501137 | 0.961849  |
| 39 | 1 | 8.955607  | 0.226508  | 0.751817  |
| 40 | 8 | -0.422085 | -1.774511 | -0.273924 |
| 41 | 1 | -1.070279 | -2.509584 | -0.458644 |
| 42 | 8 | -2.210314 | -3.675302 | -0.803541 |
| 43 | 8 | -6.330605 | 1.224095  | -0.013779 |
| 44 | 6 | -3.181446 | -3.406068 | -1.541012 |
| 45 | 7 | -4.177633 | -4.248285 | -1.837073 |
| 46 | 1 | -3.280577 | -2.418096 | -2.011039 |
| 47 | 6 | -5.276248 | -3.848776 | -2.713123 |
| 48 | 1 | -6.228636 | -3.923452 | -2.178758 |
| 49 | 1 | -5.133553 | -2.817736 | -3.040587 |
| 50 | 1 | -5.312352 | -4.500208 | -3.592124 |
| 51 | 6 | -4.215335 | -5.606741 | -1.301732 |
| 52 | 1 | -4.201978 | -6.330464 | -2.12309  |
| 53 | 1 | -3.348056 | -5.763122 | -0.662572 |
| 54 | 1 | -5.131393 | -5.750499 | -0.719922 |
| 55 | 6 | -5.301836 | 1.549532  | 0.597341  |
| 56 | 1 | -4.334983 | 1.661548  | 0.082538  |
| 57 | 7 | -5.220534 | 1.802609  | 1.92066   |

|    |   |           |           |          |
|----|---|-----------|-----------|----------|
| 58 | 6 | -6.388513 | 1.710755  | 2.787497 |
| 59 | 1 | -7.254023 | 1.430645  | 2.188259 |
| 60 | 1 | -6.223705 | 0.957053  | 3.565678 |
| 61 | 1 | -6.576043 | 2.675842  | 3.271268 |
| 62 | 6 | -3.954291 | 2.175972  | 2.54194  |
| 63 | 1 | -3.675254 | 1.442997  | 3.307322 |
| 64 | 1 | -3.170401 | 2.213816  | 1.783037 |
| 65 | 1 | -4.039734 | 3.159886  | 3.016626 |
| 66 | 1 | 3.275533  | -0.928467 | 2.214322 |

(I) bis-HPTA-IVc DMF complex.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.133191               | -0.09102  | -0.029203 |
| 2           | 6             | -0.166758               | -1.509189 | -1.283146 |
| 3           | 7             | 0.072328                | -0.410795 | -0.505757 |
| 4           | 6             | -1.476129               | 0.985378  | 0.917962  |
| 5           | 6             | -1.035864               | 2.316637  | 0.728986  |
| 6           | 6             | -2.273047               | 0.686904  | 2.037116  |
| 7           | 6             | -1.39282                | 3.30128   | 1.666571  |
| 8           | 6             | -2.629211               | 1.66729   | 2.96284   |
| 9           | 6             | -2.179968               | 2.978127  | 2.771413  |
| 10          | 1             | -1.052577               | 4.320448  | 1.511269  |
| 11          | 1             | -3.239699               | 1.410412  | 3.822478  |
| 12          | 1             | -2.443113               | 3.755716  | 3.482937  |
| 13          | 6             | 0.85446                 | -2.214689 | -2.086105 |
| 14          | 6             | 2.102424                | -2.606378 | -1.550192 |
| 15          | 6             | 0.573575                | -2.526382 | -3.427206 |
| 16          | 6             | 3.033017                | -3.273426 | -2.364209 |
| 17          | 6             | 1.494529                | -3.195222 | -4.23462  |
| 18          | 6             | 2.731144                | -3.563551 | -3.695049 |
| 19          | 1             | 3.986899                | -3.568387 | -1.937289 |
| 20          | 1             | 1.25361                 | -3.41748  | -5.269426 |
| 21          | 1             | 3.464932                | -4.080065 | -4.307523 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 22 | 7 | -2.048102 | -0.965854 | -0.5074   |
| 23 | 7 | -1.450274 | -1.879023 | -1.31087  |
| 24 | 1 | -3.071955 | -0.994797 | -0.36255  |
| 25 | 1 | -0.386167 | -2.22367  | -3.83453  |
| 26 | 8 | 2.363112  | -2.350472 | -0.241353 |
| 27 | 1 | -4.881963 | -2.933915 | 0.592254  |
| 28 | 6 | -5.433682 | -2.049839 | 0.24121   |
| 29 | 8 | -4.837879 | -1.061876 | -0.228711 |
| 30 | 7 | -6.763098 | -2.159892 | 0.374975  |
| 31 | 6 | -7.37344  | -3.360916 | 0.937525  |
| 32 | 1 | -7.946312 | -3.107802 | 1.835536  |
| 33 | 1 | -8.047538 | -3.819725 | 0.206925  |
| 34 | 1 | -6.597371 | -4.080529 | 1.203919  |
| 35 | 6 | -7.662856 | -1.08648  | -0.037319 |
| 36 | 1 | -7.074044 | -0.258861 | -0.429781 |
| 37 | 1 | -8.34687  | -1.449672 | -0.811424 |
| 38 | 1 | -8.251578 | -0.744193 | 0.820075  |
| 39 | 8 | -0.301127 | 2.613777  | -0.36819  |
| 40 | 8 | 4.795362  | -3.273966 | 0.540256  |
| 41 | 6 | 5.588873  | -3.18666  | 1.496466  |
| 42 | 1 | 6.654096  | -3.416274 | 1.354024  |
| 43 | 7 | 5.283532  | -2.834019 | 2.753061  |
| 44 | 6 | 3.92123   | -2.496871 | 3.157153  |
| 45 | 1 | 3.652423  | -3.073401 | 4.047337  |
| 46 | 1 | 3.848876  | -1.429798 | 3.393249  |
| 47 | 1 | 3.229876  | -2.735493 | 2.351373  |
| 48 | 6 | 6.317434  | -2.735186 | 3.780978  |
| 49 | 1 | 6.088386  | -3.41123  | 4.61078   |
| 50 | 1 | 7.286771  | -3.00626  | 3.359474  |
| 51 | 1 | 6.371035  | -1.711003 | 4.164304  |
| 52 | 1 | 3.248725  | -2.696769 | 0.023177  |
| 53 | 1 | -0.063877 | 3.58074   | -0.399029 |
| 54 | 8 | 0.371298  | 5.189189  | -0.555027 |
| 55 | 6 | 1.549158  | 5.491126  | -0.83795  |
| 56 | 1 | 2.313432  | 4.716073  | -0.987492 |
| 57 | 7 | 2.008161  | 6.739054  | -0.9875   |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 58 | 6 | 1.135838  | 7.899431  | -0.826614 |
| 59 | 1 | 1.118877  | 8.482395  | -1.753118 |
| 60 | 1 | 0.128884  | 7.559604  | -0.59011  |
| 61 | 1 | 1.508519  | 8.535313  | -0.01703  |
| 62 | 6 | 3.406956  | 6.999179  | -1.318021 |
| 63 | 1 | 3.873734  | 7.600706  | -0.531472 |
| 64 | 1 | 3.947229  | 6.055769  | -1.411049 |
| 65 | 1 | 3.4744    | 7.542961  | -2.265655 |
| 66 | 1 | -2.601631 | -0.337582 | 2.185472  |

Table S3. The optimized ground state energy of bis-HPTA DMF complexes in DMF.

| Bis-HPTA DMF complex | Relative energy (eV) |
|----------------------|----------------------|
| Bis-HPTA-III         | 0                    |
| Bis-HPTA-II          | 0.028                |
| Bis-HPTA-I           | 0.070                |
| Bis-HPTA-IVb         | 0.076                |
| Bis-HPTA-IIa         | 0.078                |
| Bis-HPTA-IIIa        | 0.079                |
| Bis-HPTA-IVa         | 0.090                |
| Bis-HPTA-Ia          | 0.104                |
| Bis-HPTA-Ib          | 0.126                |
| Bis-HPTA-Ic          | 0.169                |
| Bis-HPTA-IV          | 0.221                |
| Bis-HPTA-IVc         | 0.236                |

Table S4. The excitation energies of Bis-HPTA-III and Bis-HPTA-II DMF complexes in DMF using different functions and basis sets.

| Function     | Basis Set | Bis-HPTA-III | Bis-HPTA-II |
|--------------|-----------|--------------|-------------|
| Experimental |           | 3.80         | 3.86        |

|        |                |      |      |
|--------|----------------|------|------|
| B3LYP  | STO-3G         | 4.36 | 4.53 |
| B3LYP  | 321 + G        | 4.25 | 4.31 |
| B3LYP  | 6-31 + G (d,p) | 4.14 | 4.18 |
| B3LYP  | SDD            | 4.22 | 4.30 |
| B3LYP  | DGDZVP         | 4.15 | 4.20 |
| B3PW91 | STO-3G         | 4.36 | 4.55 |
| B3PW91 | 321 + G        | 4.27 | 4.33 |
| B3PW91 | 6-31 + G (d,p) | 4.16 | 4.21 |
| B3PW91 | SDD            | 4.25 | 4.33 |
| B3PW91 | DGDZVP         | 4.17 | 4.22 |
| B1B95  | STO-3G         | 4.66 | 4.78 |
| B1B95  | 321 + G        | 4.4  | 4.45 |
| B1B95  | 6-31 + G (d,p) | 4.29 | 4.33 |
| B1B95  | SDD            | 4.39 | 4.45 |
| B1B95  | DGDZVP         | 4.3  | 4.34 |
| M06    | STO-3G         | 4.38 | 4.62 |
| M06    | 321 + G        | 4.27 | 4.31 |
| M06    | 6-31 + G (d,p) | 4.2  | 4.23 |
| M06    | CCPVTZ         | 4.18 | 4.22 |
| M06    | SDD            | 4.3  | 4.35 |
| M06    | DGDZVP         | 4.21 | 4.25 |
| M06-2X | STO-3G         | 5.16 | 4.83 |
| M06-2X | 321 + G        | 4.71 | 4.75 |
| M06-2X | 6-31 + G (d,p) | 4.57 | 4.6  |
| M06-2X | CCPVTZ         | 4.57 | 4.6  |
| M06-2X | SDD            | 4.69 | 4.74 |
| M06-2X | DGDZVP         | 4.59 | 4.62 |

Table S5. The emission energy of the anion in DMF.

| Function | Energy |
|----------|--------|
|----------|--------|

|              |      |
|--------------|------|
| Experimental | 3.02 |
| B3LYP        | 2.94 |
| M06-2X       | 3.42 |

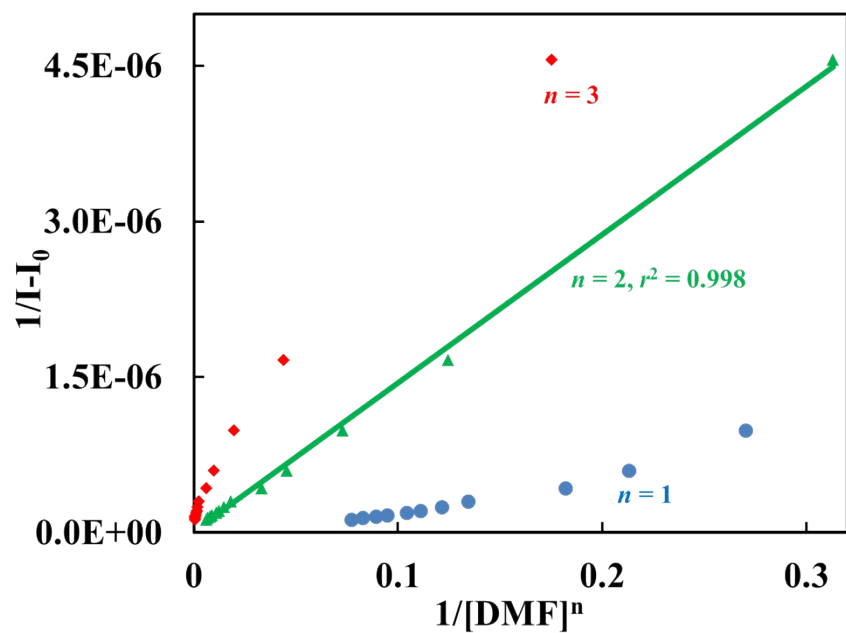


Figure S4. Benesi-Hildebrand plot using intensity at 313 nm of excitation spectra,  $\lambda_{em} = 410$  nm ( $r$  - regression).

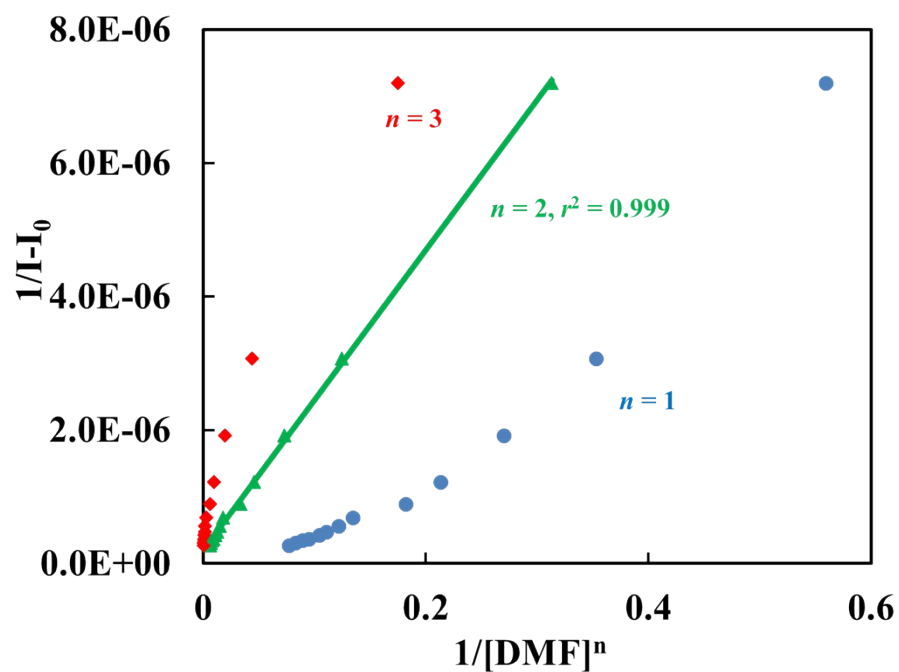


Figure S5. Benesi-Hildebrand plot using intensity at 323 nm of excitation spectra,  $\lambda_{\text{em}} = 480$  nm ( $r$  - regression).

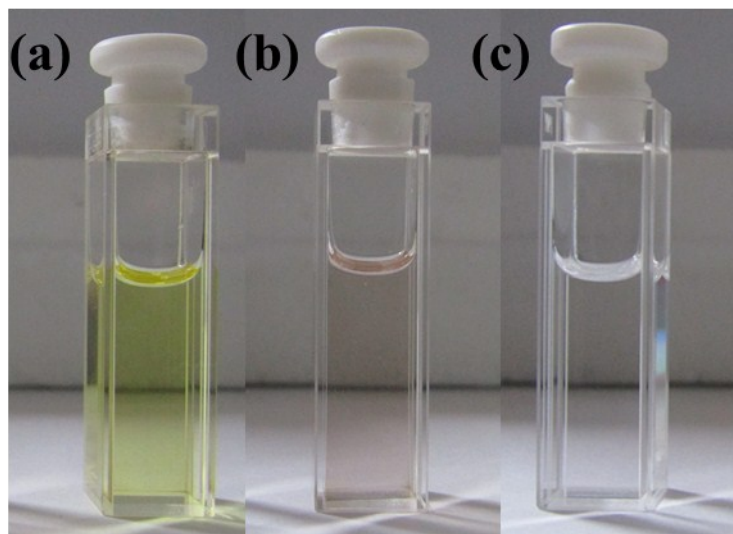


Figure S6. Images of (a) 0.5 mM silver nanoparticles solution in DMF, (b) bis-HPTA with 0.5 mM silver particles solution in DMF, (c) bis-HPTA solution in DMF.

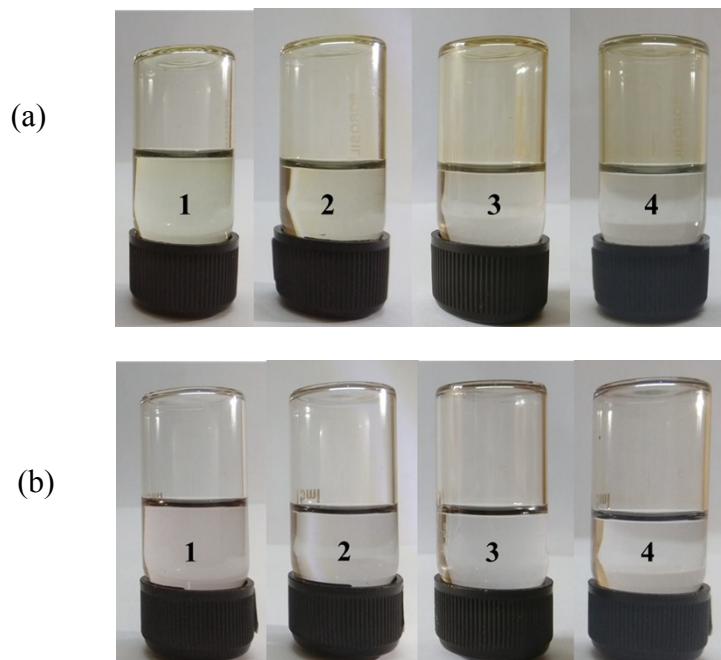


Figure S7. Images at different times after preparation of the solution (1) 5 min, (2) 5 hrs., (3) 12 hrs., (4) 24 hrs of (a) 0.5 mM silver nanoparticles solution in DMF (silver sticks at the side on the inverted vial and the colour deepens with time), (b) bis-HPTA with 0.5 mM silver particles solution in DMF (no silver sticks at the side on the inverted vial).

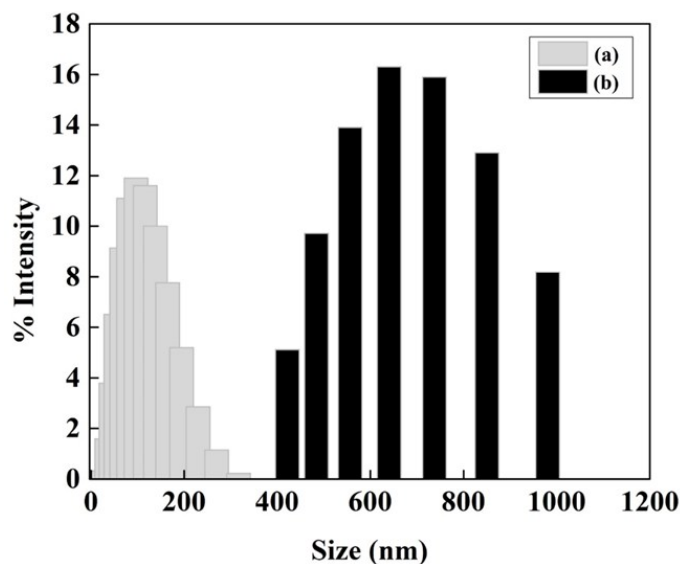


Figure S8. DLS plot of silver particles (a) in the absence and (b) in the presence of bis-HPTA.

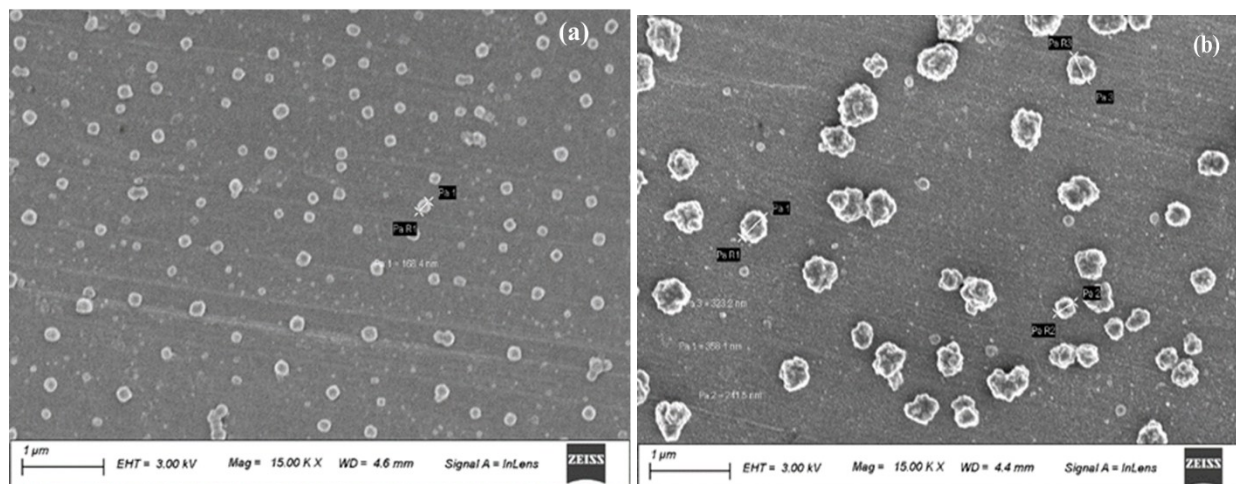


Figure S9. FESEM images of silver particles (a) in absence of bis-HPTA, (b) in the presence of bis-HPTA.

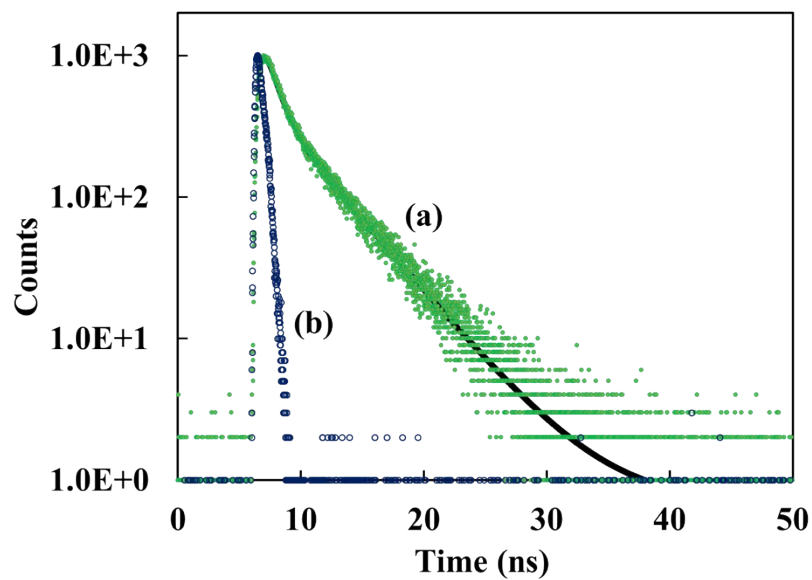


Figure S10. Fluorescence decays of (a) bis-HPTA in the presence of 0.05 mM silver particle in DMF recorded at 450 nm (b) the instrument response function,  $\lambda_{\text{ex}} = 308$  nm.

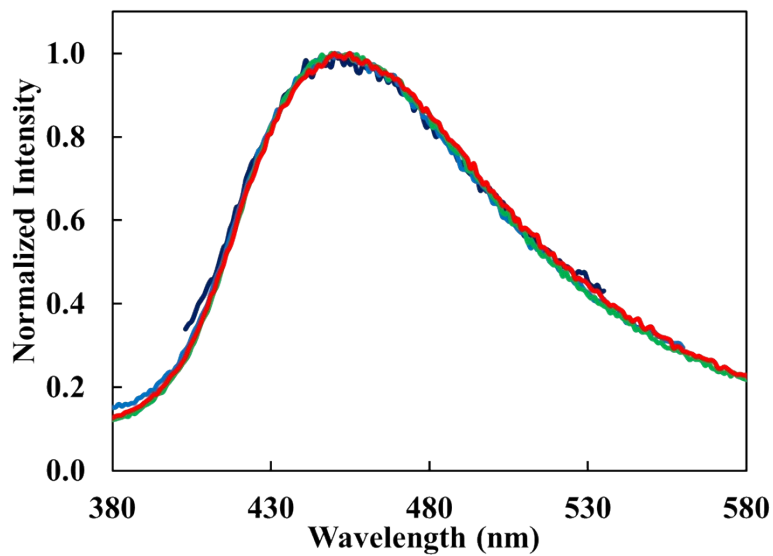


Figure S11. Normalized emission spectra of bis-HPTA in presence of (0.5 mM) silver particle.  $\lambda_{\text{ex}}$  = 290 nm, 300 nm, 310 nm, 320 nm.

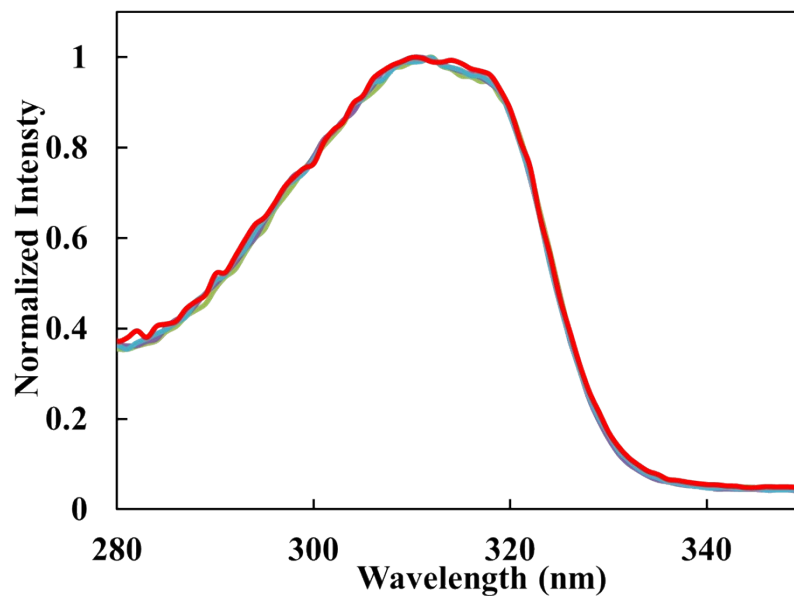
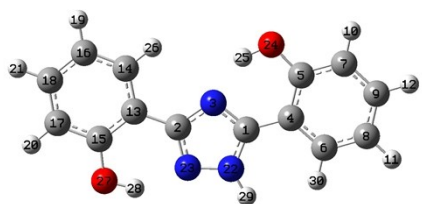


Figure S12. Normalized excitation spectra of bis-HPTA in presence of (0.5 mM) silver particle.  $\lambda_{\text{em}}$  = 430 nm, 450 nm, 480 nm, 500 nm.

Table S6. The optimized Cartesian coordinates of optimized bis-HPTA.

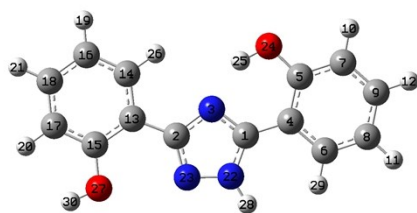
(a) bis-HPTA-I.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.123671               | -0.595629 | -0.00001  |
| 2           | 6             | 1.015478                | -0.439764 | 0.000029  |
| 3           | 7             | -0.131157               | 0.303794  | 0.000221  |
| 4           | 6             | -2.542928               | -0.261487 | 0.00013   |
| 5           | 6             | -2.935378               | 1.102898  | -0.000299 |
| 6           | 6             | -3.541965               | -1.2555   | 0.000665  |
| 7           | 6             | -4.299285               | 1.431681  | -0.000376 |
| 8           | 6             | -4.890427               | -0.921486 | 0.000602  |
| 9           | 6             | -5.264997               | 0.430959  | 0.000051  |
| 10          | 1             | -4.57635                | 2.480955  | -0.000739 |

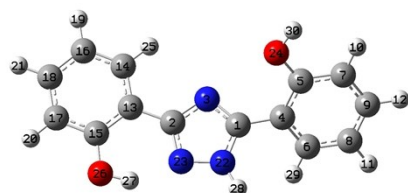
|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 11 | 1 | -5.643456 | -1.702192 | 0.001017  |
| 12 | 1 | -6.316156 | 0.70327   | 0.000004  |
| 13 | 6 | 2.370619  | 0.113688  | 0.000105  |
| 14 | 6 | 2.566418  | 1.507349  | 0.0003    |
| 15 | 6 | 3.506428  | -0.732942 | -0.000067 |
| 16 | 6 | 3.844194  | 2.057507  | 0.000351  |
| 17 | 6 | 4.792126  | -0.174393 | 0.00001   |
| 18 | 6 | 4.959624  | 1.207881  | 0.000221  |
| 19 | 1 | 3.972492  | 3.135     | 0.000491  |
| 20 | 1 | 5.646332  | -0.84411  | -0.000084 |
| 21 | 1 | 5.962598  | 1.624289  | 0.000272  |
| 22 | 7 | -0.578096 | -1.833064 | -0.000362 |
| 23 | 7 | 0.776806  | -1.751662 | -0.000665 |
| 24 | 8 | -2.043494 | 2.121915  | -0.000604 |
| 25 | 1 | -1.126474 | 1.743618  | -0.000089 |
| 26 | 1 | 1.694597  | 2.152909  | 0.000406  |
| 27 | 8 | 3.417499  | -2.090529 | -0.000193 |
| 28 | 1 | 2.471495  | -2.360073 | -0.000053 |
| 29 | 1 | -1.02638  | -2.738687 | -0.000625 |
| 30 | 1 | -3.26103  | -2.30412  | 0.001145  |

(b) bis-HPTA-Ia.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.137491               | -0.644689 | -0.000263 |
| 2           | 6             | 1.01066                 | -0.548762 | -0.000591 |
| 3           | 7             | -0.124375               | 0.226234  | 0.000446  |
| 4           | 6             | -2.549776               | -0.27756  | 0.000107  |
| 5           | 6             | -2.909352               | 1.095453  | 0.000552  |
| 6           | 6             | -3.572508               | -1.24636  | -0.000095 |
| 7           | 6             | -4.26426                | 1.458507  | 0.000504  |
| 8           | 6             | -4.913114               | -0.87924  | 0.000073  |
| 9           | 6             | -5.254812               | 0.481568  | 0.000311  |
| 10          | 1             | -4.515553               | 2.514346  | 0.000755  |
| 11          | 1             | -5.68497                | -1.641469 | -0.000048 |
| 12          | 1             | -6.299018               | 0.779613  | 0.000379  |

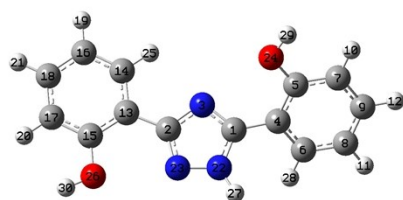
(c) bis-HPTA-Ib.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.0766                  | -0.44056  | 0.047724  |
| 2           | 6             | -1.049484               | -0.357309 | 0.035997  |
| 3           | 7             | 0.067716                | 0.400051  | -0.173902 |
| 4           | 6             | 2.519182                | -0.186237 | -0.080234 |
| 5           | 6             | 3.117128                | 0.990732  | 0.41955   |
| 6           | 6             | 3.337594                | -1.143571 | -0.706722 |
| 7           | 6             | 4.496779                | 1.186956  | 0.28023   |
| 8           | 6             | 4.710741                | -0.949299 | -0.842648 |
| 9           | 6             | 5.287346                | 0.224038  | -0.346355 |
| 10          | 1             | 4.947596                | 2.094891  | 0.67235   |
| 11          | 1             | 5.319904                | -1.698433 | -1.337095 |
| 12          | 1             | 6.354926                | 0.394646  | -0.445927 |
| 13          | 6             | -2.423687               | 0.136487  | -0.093979 |
| 14          | 6             | -2.661305               | 1.474306  | -0.459318 |

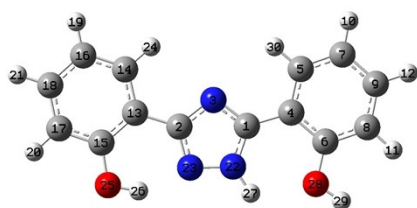
|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 15 | 6 | -3.534331 | -0.709522 | 0.144628  |
| 16 | 6 | -3.955286 | 1.97061   | -0.587061 |
| 17 | 6 | -4.836299 | -0.206565 | 0.014832  |
| 18 | 6 | -5.045253 | 1.12195   | -0.347719 |
| 19 | 1 | -4.115616 | 3.006063  | -0.869817 |
| 20 | 1 | -5.670201 | -0.875361 | 0.203776  |
| 21 | 1 | -6.060244 | 1.49633   | -0.443731 |
| 22 | 7 | 0.574694  | -1.656239 | 0.37835   |
| 23 | 7 | -0.777789 | -1.621833 | 0.376576  |
| 24 | 8 | 2.325112  | 1.902723  | 1.052694  |
| 25 | 1 | -1.805889 | 2.1164    | -0.640604 |
| 26 | 8 | -3.403278 | -2.016611 | 0.50247   |
| 27 | 1 | -2.44749  | -2.245917 | 0.559707  |
| 28 | 1 | 1.066346  | -2.497865 | 0.648738  |
| 29 | 1 | 2.880557  | -2.041265 | -1.112213 |
| 30 | 1 | 2.86474   | 2.635661  | 1.382788  |

(d) bis-HPTA-Ic.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.087425                | -0.487097 | 0.06146   |
| 2           | 6             | -1.045728               | -0.462752 | 0.067004  |
| 3           | 7             | 0.058036                | 0.32543   | -0.149221 |
| 4           | 6             | 2.523989                | -0.200962 | -0.076394 |
| 5           | 6             | 3.105254                | 0.980788  | 0.431283  |
| 6           | 6             | 3.356041                | -1.13485  | -0.719848 |
| 7           | 6             | 4.47958                 | 1.205194  | 0.282828  |
| 8           | 6             | 4.724655                | -0.91374  | -0.8647   |
| 9           | 6             | 5.283664                | 0.264599  | -0.360701 |
| 10          | 1             | 4.915734                | 2.117621  | 0.681257  |
| 11          | 1             | 5.343466                | -1.646322 | -1.371987 |
| 12          | 1             | 6.346971                | 0.456629  | -0.467085 |
| 13          | 6             | -2.409666               | 0.079177  | -0.074699 |
| 14          | 6             | -2.551963               | 1.436757  | -0.424362 |
| 15          | 6             | -3.590523               | -0.673517 | 0.118485  |
| 16          | 6             | -3.799363               | 2.035604  | -0.579375 |

(e) bis-HPTA-II.

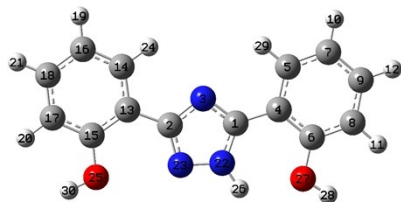


|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 17 | 6 | -4.847205 | -0.071751 | -0.038535 |
| 18 | 6 | -4.955934 | 1.273341  | -0.384596 |
| 19 | 1 | -3.868204 | 3.084548  | -0.849338 |
| 20 | 1 | -5.74086  | -0.672229 | 0.114237  |
| 21 | 1 | -5.93903  | 1.719614  | -0.50058  |
| 22 | 7 | 0.610384  | -1.712783 | 0.390826  |
| 23 | 7 | -0.743829 | -1.720784 | 0.402666  |
| 24 | 8 | 2.302463  | 1.871988  | 1.082268  |
| 25 | 1 | -1.649006 | 2.017527  | -0.573061 |
| 26 | 8 | -3.493723 | -1.993305 | 0.459896  |
| 27 | 1 | 1.12466   | -2.543848 | 0.650984  |
| 28 | 1 | 2.912556  | -2.036949 | -1.130778 |
| 29 | 1 | 2.832913  | 2.610906  | 1.413836  |
| 30 | 1 | -4.38262  | -2.364768 | 0.558207  |

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.053121                | -0.203343 | -0.000009 |
| 2           | 6             | -1.075727               | -0.224327 | 0.000004  |
| 3           | 7             | -0.003003               | 0.615892  | 0.000027  |
| 4           | 6             | 2.455775                | 0.218685  | -0.000005 |
| 5           | 6             | 2.753498                | 1.594272  | -0.000312 |
| 6           | 6             | 3.529001                | -0.69716  | 0.000179  |
| 7           | 6             | 4.068216                | 2.0498    | -0.000351 |
| 8           | 6             | 4.851431                | -0.242872 | 0.000141  |
| 9           | 6             | 5.119635                | 1.125187  | -0.000125 |
| 10          | 1             | 4.273519                | 3.115131  | -0.000561 |
| 11          | 1             | 5.663887                | -0.964386 | 0.000318  |
| 12          | 1             | 6.150321                | 1.466056  | -0.000155 |
| 13          | 6             | -2.475824               | 0.211104  | 0.000072  |
| 14          | 6             | -2.790083               | 1.582529  | 0.000322  |
| 15          | 6             | -3.536295               | -0.728042 | -0.000157 |
| 16          | 6             | -4.110495               | 2.022698  | 0.000341  |
| 17          | 6             | -4.865062               | -0.281413 | -0.000145 |
| 18          | 6             | -5.150053               | 1.081966  | 0.000101  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 19 | 1 | -4.329991 | 3.085555  | 0.000535  |
| 20 | 1 | -5.659388 | -1.021298 | -0.000321 |
| 21 | 1 | -6.184942 | 1.411562  | 0.000116  |
| 22 | 7 | 0.615395  | -1.485158 | -0.000096 |
| 23 | 7 | -0.73641  | -1.519268 | -0.000032 |
| 24 | 1 | -1.9729   | 2.296129  | 0.000502  |
| 25 | 8 | -3.330602 | -2.073806 | -0.000422 |
| 26 | 1 | -2.362303 | -2.256189 | -0.000376 |
| 27 | 1 | 1.17583   | -2.327846 | 0.000031  |
| 28 | 8 | 3.229122  | -2.034424 | 0.000465  |
| 29 | 1 | 4.035672  | -2.570184 | 0.000474  |
| 30 | 1 | 1.927425  | 2.296555  | -0.00049  |

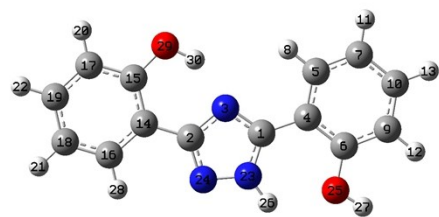
(f) bis-HPTA-IIa.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.063513               | -0.258436 | -0.000893 |
| 2           | 6             | 1.06944                 | -0.341877 | -0.001242 |
| 3           | 7             | 0.011766                | 0.529046  | 0.000278  |
| 4           | 6             | -2.456                  | 0.199483  | 0.000482  |
| 5           | 6             | -2.719736               | 1.581882  | 0.004737  |
| 6           | 6             | -3.553251               | -0.687237 | -0.002198 |
| 7           | 6             | -4.022331               | 2.072108  | 0.006317  |
| 8           | 6             | -4.863575               | -0.19871  | -0.000257 |
| 9           | 6             | -5.097624               | 1.175686  | 0.00387   |
| 10          | 1             | -4.199383               | 3.142578  | 0.00951   |
| 11          | 1             | -5.694088               | -0.899309 | -0.001917 |
| 12          | 1             | -6.119307               | 1.54271   | 0.005231  |
| 13          | 6             | 2.461476                | 0.144724  | -0.001245 |
| 14          | 6             | 2.677655                | 1.536976  | -0.006538 |
| 15          | 6             | 3.599734                | -0.693663 | 0.003978  |
| 16          | 6             | 3.955638                | 2.08959   | -0.006813 |
| 17          | 6             | 4.887501                | -0.138226 | 0.00383   |
| 18          | 6             | 5.069127                | 1.243056  | -0.001531 |
| 19          | 1             | 4.08125                 | 3.167611  | -0.0111   |
| 20          | 1             | 5.748042                | -0.803144 | 0.008116  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 21 | 1 | 6.075126  | 1.651762  | -0.001594 |
| 22 | 7 | -0.651049 | -1.5487   | -0.003009 |
| 23 | 7 | 0.700171  | -1.627404 | -0.002967 |
| 24 | 1 | 1.807162  | 2.182698  | -0.010525 |
| 25 | 8 | 3.431084  | -2.050193 | 0.009337  |
| 26 | 1 | -1.230573 | -2.377797 | -0.00452  |
| 27 | 8 | -3.290113 | -2.033077 | -0.00657  |
| 28 | 1 | -4.112066 | -2.544907 | -0.010882 |
| 29 | 1 | -1.875603 | 2.262476  | 0.006752  |
| 30 | 1 | 4.298208  | -2.48124  | 0.013702  |

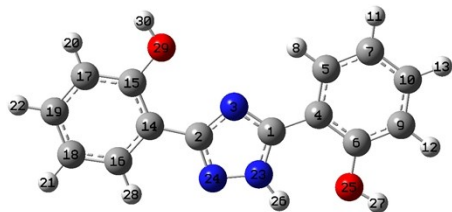
(g) bis-HPTA-III.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 0.996875                | -0.425405 | -0.000003 |
| 2           | 6             | -1.135605               | -0.643984 | -0.000017 |
| 3           | 7             | -0.133993               | 0.290315  | 0.000001  |
| 4           | 6             | 2.355282                | 0.118008  | 0.000006  |
| 5           | 6             | 2.536538                | 1.513846  | 0.000023  |
| 6           | 6             | 3.502083                | -0.704205 | -0.000002 |
| 7           | 6             | 3.808369                | 2.077992  | 0.000031  |
| 8           | 1             | 1.657717                | 2.148776  | 0.000029  |
| 9           | 6             | 4.781686                | -0.14066  | 0.000007  |
| 10          | 6             | 4.933809                | 1.245086  | 0.000023  |
| 11          | 1             | 3.923012                | 3.15678   | 0.000044  |
| 12          | 1             | 5.651829                | -0.791809 | 0.000001  |
| 13          | 1             | 5.931983                | 1.671687  | 0.000003  |
| 14          | 6             | -2.555009               | -0.274673 | -0.000009 |
| 15          | 6             | -2.946694               | 1.086826  | -0.000021 |
| 16          | 6             | -3.555493               | -1.264731 | 0.000021  |
| 17          | 6             | -4.309564               | 1.420426  | 0.000002  |
| 18          | 6             | -4.905815               | -0.92964  | 0.000043  |
| 19          | 6             | -5.279902               | 0.422313  | 0.000034  |
| 20          | 1             | -4.583999               | 2.470788  | -0.000009 |
| 21          | 1             | -5.660367               | -1.709665 | 0.000068  |
| 22          | 1             | -6.330506               | 0.697847  | 0.000005  |

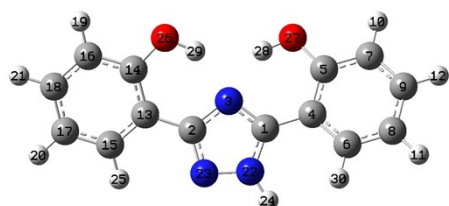
|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 23 | 7 | 0.658289  | -1.733835 | -0.000021 |
| 24 | 7 | -0.686137 | -1.899666 | -0.000012 |
| 25 | 8 | 3.314388  | -2.061166 | -0.000017 |
| 26 | 1 | 1.291358  | -2.523361 | -0.000031 |
| 27 | 1 | 4.162845  | -2.527406 | -0.000022 |
| 28 | 1 | -3.251819 | -2.306605 | 0.000032  |
| 29 | 8 | -2.0497   | 2.109087  | -0.000067 |
| 30 | 1 | -1.136018 | 1.724702  | -0.000129 |

(h) bis-HPTA-IIIa.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.03133                | -0.382102 | 0.000003  |
| 2           | 6             | 1.095217                | -0.534392 | 0.000007  |
| 3           | 7             | 0.072254                | 0.370218  | -0.000009 |
| 4           | 6             | -2.405848               | 0.126303  | -0.000009 |
| 5           | 6             | -2.618953               | 1.517431  | -0.000041 |
| 6           | 6             | -3.534926               | -0.719404 | 0.000012  |
| 7           | 6             | -3.903043               | 2.054554  | -0.000053 |
| 8           | 1             | -1.750405               | 2.166524  | -0.000057 |
| 9           | 6             | -4.826768               | -0.184025 | 0         |
| 10          | 6             | -5.010477               | 1.198174  | -0.000032 |
| 11          | 1             | -4.040895               | 3.130818  | -0.000079 |
| 12          | 1             | -5.682248               | -0.854281 | 0.000018  |
| 13          | 1             | -6.017975               | 1.602486  | -0.000041 |
| 14          | 6             | 2.537394                | -0.217021 | -0.000003 |
| 15          | 6             | 3.062904                | 1.095159  | 0.000034  |
| 16          | 6             | 3.457519                | -1.285792 | -0.000052 |
| 17          | 6             | 4.451632                | 1.300212  | 0.000018  |
| 18          | 6             | 4.833917                | -1.08281  | -0.000065 |
| 19          | 6             | 5.334436                | 0.224024  | -0.000031 |
| 20          | 1             | 4.832404                | 2.318825  | 0.000046  |
| 21          | 1             | 5.508432                | -1.933057 | -0.000104 |
| 22          | 1             | 6.404703                | 0.407236  | -0.000042 |
| 23          | 7             | -0.665534               | -1.685725 | 0.000026  |
| 24          | 7             | 0.678514                | -1.808904 | 0.00003   |

(i) bis-HPTA-IV.

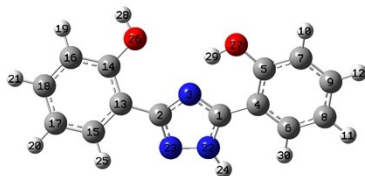


|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 25 | 8 | -3.319991 | -2.074058 | 0.000044  |
| 26 | 1 | -1.274103 | -2.493906 | 0.000042  |
| 27 | 1 | -4.159889 | -2.555522 | 0.000059  |
| 28 | 1 | 3.063237  | -2.295674 | -0.000081 |
| 29 | 8 | 2.212463  | 2.165528  | 0.000088  |
| 30 | 1 | 2.730269  | 2.983796  | 0.000119  |

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.070569                | -0.736291 | 0.033438  |
| 2           | 6             | -1.080644               | -0.781401 | -0.026363 |
| 3           | 7             | -0.001338               | 0.070861  | 0.016869  |
| 4           | 6             | 2.467238                | -0.311437 | 0.050499  |
| 5           | 6             | 2.810358                | 1.013636  | -0.315451 |
| 6           | 6             | 3.498776                | -1.204605 | 0.403825  |
| 7           | 6             | 4.155643                | 1.4058    | -0.333889 |
| 8           | 6             | 4.830914                | -0.808742 | 0.3887    |
| 9           | 6             | 5.155665                | 0.503293  | 0.014472  |
| 10          | 1             | 4.392586                | 2.424518  | -0.623115 |
| 11          | 1             | 5.608794                | -1.510232 | 0.670462  |
| 12          | 1             | 6.192891                | 0.823894  | -0.000057 |
| 13          | 6             | -2.4751                 | -0.324422 | -0.03749  |
| 14          | 6             | -2.817755               | 1.002399  | 0.312902  |
| 15          | 6             | -3.508486               | -1.218154 | -0.378867 |
| 16          | 6             | -4.161659               | 1.401709  | 0.316521  |
| 17          | 6             | -4.840939               | -0.819264 | -0.376197 |
| 18          | 6             | -5.164768               | 0.499382  | -0.02559  |
| 19          | 1             | -4.395606               | 2.425185  | 0.592038  |
| 20          | 1             | -5.620202               | -1.524072 | -0.647398 |
| 21          | 1             | -6.200875               | 0.824635  | -0.021292 |
| 22          | 7             | 0.627163                | -2.010046 | -0.005093 |
| 23          | 7             | -0.728554               | -2.063483 | -0.035411 |
| 24          | 1             | 1.160834                | -2.867894 | -0.040333 |
| 25          | 1             | -3.243645               | -2.234342 | -0.651864 |
| 26          | 8             | -1.893227               | 1.936744  | 0.671906  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 27 | 8 | 1.885999  | 1.942551  | -0.671824 |
| 28 | 1 | 0.989047  | 1.559348  | -0.574685 |
| 29 | 1 | -0.998011 | 1.548034  | 0.590317  |
| 30 | 1 | 3.252255  | -2.216162 | 0.711659  |

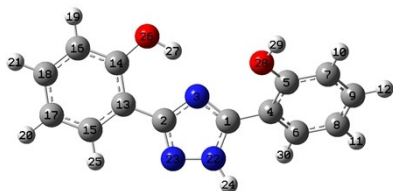
(j) bis-HPTA-IVa.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.105453               | -0.761329 | 0.094928  |
| 2           | 6             | 1.039465                | -0.750563 | 0.107424  |
| 3           | 7             | -0.055239               | 0.053435  | -0.056764 |
| 4           | 6             | -2.496508               | -0.331706 | 0.006893  |
| 5           | 6             | -2.779605               | 1.037801  | -0.240256 |
| 6           | 6             | -3.569776               | -1.230502 | 0.162299  |
| 7           | 6             | -4.113472               | 1.464497  | -0.325718 |
| 8           | 6             | -4.88855                | -0.799447 | 0.075934  |
| 9           | 6             | -5.15556                | 0.555883  | -0.169944 |
| 10          | 1             | -4.307452               | 2.515378  | -0.515492 |
| 11          | 1             | -5.700866               | -1.508024 | 0.198057  |
| 12          | 1             | -6.182032               | 0.903386  | -0.239644 |
| 13          | 6             | 2.441308                | -0.316033 | -0.016873 |
| 14          | 6             | 2.87203                 | 0.986468  | 0.315886  |
| 15          | 6             | 3.402557                | -1.236906 | -0.473026 |
| 16          | 6             | 4.221812                | 1.337869  | 0.179409  |
| 17          | 6             | 4.74569                 | -0.890986 | -0.602842 |
| 18          | 6             | 5.153685                | 0.406782  | -0.276325 |
| 19          | 1             | 4.53573                 | 2.34536   | 0.440714  |
| 20          | 1             | 5.463334                | -1.621077 | -0.962636 |
| 21          | 1             | 6.194979                | 0.697992  | -0.375932 |
| 22          | 7             | -0.63875                | -2.006623 | 0.337788  |
| 23          | 7             | 0.718996                | -2.020329 | 0.355463  |
| 24          | 1             | -1.148605               | -2.861051 | 0.514064  |
| 25          | 1             | 3.071537                | -2.236303 | -0.734862 |
| 26          | 8             | 1.955175                | 1.882735  | 0.789956  |
| 27          | 8             | -1.807061               | 1.967025  | -0.398071 |
| 28          | 1             | 2.398951                | 2.712369  | 1.018088  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 29 | 1 | -0.92107  | 1.518354  | -0.311913 |
| 30 | 1 | -3.370198 | -2.280814 | 0.352337  |

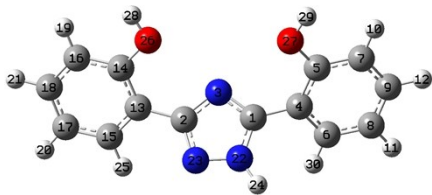
(k) bis-HPTA-IVb.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.023312               | -0.66561  | -0.103291 |
| 2           | 6             | 1.116572                | -0.766158 | -0.131877 |
| 3           | 7             | 0.062728                | 0.085805  | 0.081622  |
| 4           | 6             | -2.434079               | -0.28695  | 0.041602  |
| 5           | 6             | -2.920143               | 0.962445  | -0.401722 |
| 6           | 6             | -3.338769               | -1.191974 | 0.627201  |
| 7           | 6             | -4.275934               | 1.278474  | -0.250689 |
| 8           | 6             | -4.688009               | -0.878126 | 0.773492  |
| 9           | 6             | -5.153246               | 0.364854  | 0.332106  |
| 10          | 1             | -4.638787               | 2.24185   | -0.59909  |
| 11          | 1             | -5.364635               | -1.58904  | 1.23548   |
| 12          | 1             | -6.200722               | 0.628287  | 0.441904  |
| 13          | 6             | 2.510296                | -0.324826 | -0.01926  |
| 14          | 6             | 2.814545                | 1.021076  | 0.303594  |
| 15          | 6             | 3.570864                | -1.225847 | -0.229499 |
| 16          | 6             | 4.154032                | 1.426796  | 0.405408  |
| 17          | 6             | 4.89732                 | -0.818856 | -0.127144 |
| 18          | 6             | 5.185299                | 0.516331  | 0.192426  |
| 19          | 1             | 4.36182                 | 2.463063  | 0.653418  |
| 20          | 1             | 5.699618                | -1.530534 | -0.293422 |
| 21          | 1             | 6.216479                | 0.847192  | 0.275443  |
| 22          | 7             | -0.613993               | -1.916461 | -0.41668  |
| 23          | 7             | 0.73856                 | -2.005884 | -0.442202 |
| 24          | 1             | -1.178549               | -2.71915  | -0.661504 |
| 25          | 1             | 3.33366                 | -2.255881 | -0.475618 |
| 26          | 8             | 1.855916                | 1.959802  | 0.523243  |
| 27          | 1             | 0.965917                | 1.531615  | 0.421991  |
| 28          | 8             | -2.04547                | 1.826441  | -0.991368 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 29 | 1 | -2.512943 | 2.623261  | -1.281441 |
| 30 | 1 | -2.969116 | -2.144601 | 0.994592  |

(I) bis-HPTA-IVc.

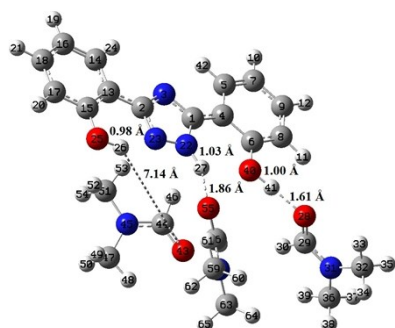


| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.053551                | -0.54092  | 0.243209  |
| 2           | 6             | -1.072786               | -0.586521 | 0.290896  |
| 3           | 7             | -0.011467               | 0.120689  | -0.204765 |
| 4           | 6             | 2.475462                | -0.274766 | -0.027026 |
| 5           | 6             | 3.022728                | 1.02322   | 0.059172  |
| 6           | 6             | 3.32598                 | -1.340545 | -0.371799 |
| 7           | 6             | 4.383025                | 1.228808  | -0.202967 |
| 8           | 6             | 4.680969                | -1.137281 | -0.628636 |
| 9           | 6             | 5.206116                | 0.155824  | -0.544777 |
| 10          | 1             | 4.793883                | 2.232471  | -0.130317 |
| 11          | 1             | 5.314838                | -1.97475  | -0.900393 |
| 12          | 1             | 6.258003                | 0.334666  | -0.745737 |
| 13          | 6             | -2.49128                | -0.291419 | 0.007059  |
| 14          | 6             | -3.014878               | 1.018357  | 0.022437  |
| 15          | 6             | -3.366784               | -1.353035 | -0.280073 |
| 16          | 6             | -4.369325               | 1.239963  | -0.25913  |
| 17          | 6             | -4.716978               | -1.137021 | -0.554385 |
| 18          | 6             | -5.21569                | 0.169255  | -0.547471 |
| 19          | 1             | -4.757642               | 2.255301  | -0.241533 |
| 20          | 1             | -5.368158               | -1.975454 | -0.779601 |
| 21          | 1             | -6.262439               | 0.359953  | -0.764644 |
| 22          | 7             | 0.631176                | -1.599707 | 0.977725  |
| 23          | 7             | -0.720886               | -1.644963 | 1.025005  |
| 24          | 1             | 1.181847                | -2.268357 | 1.499993  |
| 25          | 1             | -2.963694               | -2.360515 | -0.294712 |
| 26          | 8             | -2.178617               | 2.051503  | 0.344616  |
| 27          | 8             | 2.20026                 | 2.049055  | 0.42431   |
| 28          | 1             | -2.674961               | 2.882425  | 0.357684  |

|    |   |          |           |           |
|----|---|----------|-----------|-----------|
| 29 | 1 | 2.705493 | 2.872773  | 0.483386  |
| 30 | 1 | 2.907265 | -2.338635 | -0.460344 |

Table S7. The optimized Cartesian coordinates of excited state optimized bis-HPTA-II and bis-HPTA-III DMF complexes.

(a) bis-HPTA-II-DMF complex.

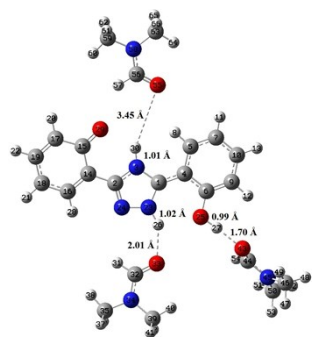


| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | 1.348748                | 1.490882  | -0.655314 |
| 2           | 6             | 3.206022                | 0.405983  | -0.695971 |
| 3           | 7             | 2.704463                | 1.646963  | -0.500689 |
| 4           | 6             | 0.400734                | 2.522753  | -0.540932 |
| 5           | 6             | 0.859354                | 3.870614  | -0.269467 |
| 6           | 6             | -1.035447               | 2.336986  | -0.685325 |
| 7           | 6             | -0.036721               | 4.920781  | -0.172568 |
| 8           | 6             | -1.914415               | 3.414491  | -0.585649 |
| 9           | 6             | -1.42742                | 4.714785  | -0.331181 |
| 10          | 1             | 0.33531                 | 5.922335  | 0.027321  |
| 11          | 1             | -2.977852               | 3.233506  | -0.703983 |
| 12          | 1             | -2.1198                 | 5.547117  | -0.25385  |
| 13          | 6             | 4.595005                | 0.033814  | -0.639621 |
| 14          | 6             | 5.574368                | 1.022975  | -0.355293 |
| 15          | 6             | 5.038275                | -1.314515 | -0.862282 |
| 16          | 6             | 6.919427                | 0.701034  | -0.291844 |
| 17          | 6             | 6.40384                 | -1.624435 | -0.79426  |
| 18          | 6             | 7.336251                | -0.629847 | -0.512044 |
| 19          | 1             | 7.653651                | 1.469729  | -0.073281 |
| 20          | 1             | 6.708281                | -2.65145  | -0.966542 |
| 21          | 1             | 8.39084                 | -0.882773 | -0.462423 |
| 22          | 7             | 1.111387                | 0.132102  | -0.946688 |
| 23          | 7             | 2.251824                | -0.532215 | -0.967724 |
| 24          | 1             | 5.235433                | 2.039166  | -0.189333 |
| 25          | 8             | 4.189641                | -2.324159 | -1.140434 |
| 26          | 1             | 3.263319                | -1.980171 | -1.160104 |
| 27          | 1             | 0.23569                 | -0.381243 | -1.129144 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 28 | 8 | -4.043621 | 0.783175  | -1.223217 |
| 29 | 6 | -4.801411 | 0.572545  | -0.251248 |
| 30 | 1 | -4.415042 | 0.560784  | 0.776699  |
| 31 | 7 | -6.11531  | 0.346679  | -0.34095  |
| 32 | 6 | -6.802625 | 0.327522  | -1.630228 |
| 33 | 1 | -6.076447 | 0.486898  | -2.425457 |
| 34 | 1 | -7.296707 | -0.638924 | -1.77094  |
| 35 | 1 | -7.559351 | 1.118146  | -1.659382 |
| 36 | 6 | -6.930063 | 0.117792  | 0.850074  |
| 37 | 1 | -7.708947 | 0.883217  | 0.924615  |
| 38 | 1 | -7.405703 | -0.866457 | 0.795553  |
| 39 | 1 | -6.303303 | 0.16077   | 1.742107  |
| 40 | 8 | -1.460284 | 1.080652  | -0.91255  |
| 41 | 1 | -2.460497 | 1.017998  | -1.003978 |
| 42 | 1 | 1.923458  | 4.033591  | -0.151873 |
| 43 | 8 | -1.91321  | -0.428099 | 3.510767  |
| 44 | 6 | -0.734924 | -0.04652  | 3.527385  |
| 45 | 7 | 0.327249  | -0.78189  | 3.916257  |
| 46 | 1 | -0.456037 | 0.970836  | 3.208383  |
| 47 | 6 | 0.171944  | -2.156999 | 4.375472  |
| 48 | 1 | -0.87896  | -2.435825 | 4.309854  |
| 49 | 1 | 0.768949  | -2.831156 | 3.751791  |
| 50 | 1 | 0.510414  | -2.249809 | 5.413475  |
| 51 | 6 | 1.678203  | -0.232797 | 3.904395  |
| 52 | 1 | 2.324891  | -0.826449 | 3.249263  |
| 53 | 1 | 1.655497  | 0.795461  | 3.538661  |
| 54 | 1 | 2.101994  | -0.240047 | 4.91468   |
| 55 | 8 | -0.660591 | -1.952065 | -1.581053 |
| 56 | 6 | -1.639281 | -2.389123 | -0.951441 |
| 57 | 1 | -2.076927 | -1.825282 | -0.114822 |
| 58 | 7 | -2.263585 | -3.553343 | -1.195748 |
| 59 | 6 | -1.827977 | -4.441361 | -2.268927 |
| 60 | 1 | -2.644952 | -4.59563  | -2.981705 |
| 61 | 1 | -0.978218 | -3.991241 | -2.779938 |
| 62 | 1 | -1.535088 | -5.412388 | -1.855658 |
| 63 | 6 | -3.403687 | -3.987027 | -0.394594 |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 64 | 1 | -4.287098 | -4.113632 | -1.029266 |
| 65 | 1 | -3.181794 | -4.941952 | 0.093428  |
| 66 | 1 | -3.621876 | -3.24123  | 0.371715  |

(b) bis-HPTA-III-DMF complex.



| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -0.272535               | -0.207465 | -0.005759 |
| 2           | 6             | -1.377532               | 1.74178   | 0.074098  |
| 3           | 7             | -1.529261               | 0.380069  | 0.068897  |
| 4           | 6             | -0.002774               | -1.58647  | -0.046612 |
| 5           | 6             | -1.066061               | -2.557612 | 0.002555  |
| 6           | 6             | 1.339376                | -2.103446 | -0.14144  |
| 7           | 6             | -0.800101               | -3.921269 | -0.034484 |
| 8           | 1             | -2.099201               | -2.232097 | 0.070433  |
| 9           | 6             | 1.580449                | -3.467589 | -0.177445 |
| 10          | 6             | 0.516025                | -4.398628 | -0.122939 |
| 11          | 1             | -1.63081                | -4.621086 | 0.006445  |
| 12          | 1             | 2.608021                | -3.812172 | -0.251651 |
| 13          | 1             | 0.723921                | -5.463115 | -0.15196  |
| 14          | 6             | -2.496257               | 2.697229  | 0.130938  |
| 15          | 6             | -3.88442                | 2.229826  | 0.164631  |
| 16          | 6             | -2.237927               | 4.058278  | 0.148755  |
| 17          | 6             | -4.926744               | 3.236823  | 0.21387   |
| 18          | 6             | -3.281976               | 4.998279  | 0.196036  |
| 19          | 6             | -4.628764               | 4.580534  | 0.228404  |
| 20          | 1             | -5.949702               | 2.877327  | 0.238175  |
| 21          | 1             | -3.043276               | 6.055793  | 0.207872  |
| 22          | 1             | -5.422113               | 5.319676  | 0.264759  |
| 23          | 7             | 0.575801                | 0.890295  | -0.006112 |
| 24          | 7             | -0.117853               | 2.083514  | 0.022627  |
| 25          | 8             | 2.345804                | -1.177812 | -0.198858 |
| 26          | 1             | 1.587679                | 0.913507  | -0.118435 |
| 27          | 1             | 3.236179                | -1.607538 | -0.280528 |
| 28          | 1             | -1.210149               | 4.402392  | 0.124435  |
| 29          | 8             | -4.183091               | 1.00026   | 0.150304  |

|    |   |           |           |           |
|----|---|-----------|-----------|-----------|
| 30 | 1 | -2.437786 | -0.065351 | 0.082116  |
| 31 | 1 | 2.247752  | 3.728993  | -0.008063 |
| 32 | 6 | 3.212153  | 3.225831  | -0.173523 |
| 33 | 8 | 3.281649  | 1.989409  | -0.264349 |
| 34 | 7 | 4.252235  | 4.075946  | -0.261408 |
| 35 | 6 | 4.066974  | 5.517488  | -0.136367 |
| 36 | 1 | 4.644531  | 5.903014  | 0.710727  |
| 37 | 1 | 4.40069   | 6.024273  | -1.048225 |
| 38 | 1 | 3.010946  | 5.741442  | 0.025434  |
| 39 | 6 | 5.611762  | 3.595981  | -0.483238 |
| 40 | 1 | 5.595532  | 2.510147  | -0.566364 |
| 41 | 1 | 6.016199  | 4.027372  | -1.405291 |
| 42 | 1 | 6.255823  | 3.889552  | 0.352866  |
| 43 | 8 | 4.815464  | -2.215412 | -0.47987  |
| 44 | 6 | 5.660555  | -2.115779 | 0.43169   |
| 45 | 7 | 6.920419  | -2.565659 | 0.366736  |
| 46 | 6 | 7.431217  | -3.23624  | -0.82581  |
| 47 | 1 | 8.295122  | -2.689845 | -1.217909 |
| 48 | 1 | 7.743284  | -4.255494 | -0.575487 |
| 49 | 1 | 6.646872  | -3.269319 | -1.580263 |
| 50 | 6 | 7.842367  | -2.409314 | 1.488369  |
| 51 | 1 | 7.339897  | -1.901004 | 2.313014  |
| 52 | 1 | 8.186651  | -3.389987 | 1.832309  |
| 53 | 1 | 8.711489  | -1.81793  | 1.182647  |
| 54 | 1 | 5.412468  | -1.63146  | 1.386638  |
| 55 | 8 | -4.677121 | -2.696631 | 0.114526  |
| 56 | 6 | -5.729504 | -2.045888 | 0.042103  |
| 57 | 1 | -5.72153  | -0.945653 | 0.074633  |
| 58 | 7 | -6.968517 | -2.568791 | -0.081893 |
| 59 | 6 | -8.148094 | -1.715548 | -0.157488 |
| 60 | 1 | -7.84932  | -0.667247 | -0.097779 |
| 61 | 1 | -8.678057 | -1.878705 | -1.102538 |
| 62 | 1 | -8.832683 | -1.935568 | 0.669235  |
| 63 | 6 | -7.184721 | -4.008928 | -0.146767 |
| 64 | 1 | -6.221671 | -4.514725 | -0.08832  |
| 65 | 1 | -7.819179 | -4.334355 | 0.685228  |

Table S8. The optimized Cartesian coordinates of excited state optimized anion.

| Atom Number | Atomic Number | Coordinates (Angstroms) |           |           |
|-------------|---------------|-------------------------|-----------|-----------|
|             |               | X                       | Y         | Z         |
| 1           | 6             | -1.067124               | -0.207537 | -0.000002 |
| 2           | 6             | 1.082489                | -0.233335 | -0.000002 |
| 3           | 7             | -0.022966               | 0.614902  | -0.000001 |
| 4           | 6             | -2.474177               | 0.202814  | 0         |
| 5           | 6             | -2.794553               | 1.554899  | 0.000005  |
| 6           | 6             | -3.556685               | -0.789807 | -0.000003 |
| 7           | 6             | -4.128548               | 1.985525  | 0.000008  |
| 8           | 6             | -4.920778               | -0.294058 | 0.000001  |
| 9           | 6             | -5.19259                | 1.052708  | 0.000006  |
| 10          | 1             | -4.345083               | 3.047984  | 0.000012  |
| 11          | 1             | -5.709879               | -1.038193 | -0.000001 |
| 12          | 1             | -6.218127               | 1.40715   | 0.000009  |
| 13          | 6             | 2.434164                | 0.202879  | -0.000001 |
| 14          | 6             | 2.785436                | 1.608632  | -0.000004 |
| 15          | 6             | 3.540066                | -0.72681  | 0.000002  |
| 16          | 6             | 4.111639                | 2.024789  | -0.000003 |
| 17          | 1             | 1.982763                | 2.338479  | -0.000006 |
| 18          | 6             | 4.852522                | -0.295451 | 0.000003  |
| 19          | 6             | 5.170785                | 1.097844  | 0.000001  |
| 20          | 1             | 4.329128                | 3.091674  | -0.000005 |
| 21          | 1             | 5.640134                | -1.045061 | 0.000006  |
| 22          | 1             | 6.205728                | 1.423964  | 0.000001  |
| 23          | 7             | -0.660155               | -1.491791 | -0.000005 |
| 24          | 7             | 0.701518                | -1.561458 | -0.000005 |
| 25          | 8             | 3.308411                | -2.091502 | 0.000006  |
| 26          | 1             | -1.262331               | -2.304994 | -0.000008 |
| 27          | 1             | 2.334683                | -2.243151 | 0.000006  |
| 28          | 8             | -3.327363               | -2.03216  | -0.000007 |
| 29          | 1             | -1.990064               | 2.281299  | 0.000007  |

