Supporting Information

A fluorescent di-zinc(II) complex of bis-calix[4]arene conjugate as chemosensing-ensemble for the selective recognition of ATP

V.V. Sreenivasu Mummidivarapu,a Rakesh Kumar Pathak,a Vijaya Kumar Hinge,b Jayaraman Dessingoua and Chebrolu Pulla Raoa,b*

aDepartment of Chemistry, bDepartment of Biosciences & Bioengineering, Indian Institute of Technology Bombay, Powai, Mumbai 400 076, India. Email: cprao@iitb.ac.in, cprao@chem.iitb.ac.in

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S1. Characterization of $\mathbf{L}$

Figure S2. $^1\text{H}$ NMR spectrum (CDCl$_3$, 400 MHz) of $\mathbf{L}$

Figure S3. $^{13}\text{C}$ NMR spectrum (CDCl$_3$, 100 MHz) of $\mathbf{L}$
Figure S4. ESI MS of L.

Figure S5. HRMS spectrum of L
S6. Characterization of [Zn\textsubscript{2}L]

**Figure S7.** \textsuperscript{1}H NMR spectrum (CDCl\textsubscript{3}, 400 MHz) of [Zn\textsubscript{2}L]

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Figure S9. ESI MS of [Zn₂L].

Figure S10. HRMS spectrum of [Zn₂L].
Figure S12. Fluorescence spectral traces for the titration of L with other metal ions.
S13. Determination of the association constant by fluorescence titration

![Graph](image)

**Figure S14.** The binding constant of L with Zn$^{2+}$ has been derived based on the Benesi – Hildebrand equation using fluorescence emission data

S15. Determination of minimum concentration of Zn$^{2+}$ by L

![Graph](image)

**Figure S16.** Determination of minimum concentration of Zn$^{2+}$ that can be detected by L carried out by maintaining the ratio of L:Zn$^{2+}$ as 1:2

S17. Determination of the association constant by absorption titration

![Graph](image)

**Figure S18.** The binding constant of L with Zn$^{2+}$ has been derived based on the Benesi – Hildebrand equation using absorption titration
S19. Fluorescence studies of $[\text{Zn}_2\text{L}]$ with anions
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**S21.** Dilution experiment by maintaining the ratio of \([\text{Zn}_2\text{L}]\):ATP as 1:2

**Figure S22.** Minimum concentration of ATP that can be detected by \([\text{Zn}_2\text{L}]\).
S23. Absorption studies of [Zn_2L] with anions

![Graphs showing absorption studies of different anions with [Zn_2L].]
Figure S24. Absorption spectral traces for the titration of $[\text{Zn}_2\text{L}]$ with other anions.
S25. PM3 optimized structure of L′ and the molecular mechanics minimized structure of [Zn₂L′].

Figure S26. Stereo view representation of (a) L′, (b) [Zn₂L′].
S27. The metric data of Zn$^{2+}$ coordination sphere of MM minimized [(Zn)$_2$L'X] complexes

Table S01. The metric data {bond distances (Å)} of Zn$^{2+}$ coordination sphere of MM minimized structures of [(Zn)$_2$L'X] complexes.

| Distances (Å°) | [(Zn)$_2$L'PPi]$^{4+}$ | [(Zn)$_2$L'ADP]$^{2+}$ | [(Zn)$_2$L'ATP]$^{2+}$ |
|---------------|-------------------------|-------------------------|-------------------------|
| O1 – Zn$^a$   | 1.908                   | 1.878                   | 1.874                   |
| O2 – Zn$^a$   | 1.974                   | 1.875                   | 1.850                   |
| O3 – Zn$^a$   | 1.8513                  | 1.832                   | 1.781                   |
| O4 – Zn$^a$   | 1.841                   | 1.836                   | 1.841                   |
| N1 – Zn$^a$   | 2.023                   | 1.977                   | 1.959                   |
| N2 – Zn$^a$   | 2.035                   | 2.001                   | 1.957                   |
| O5 – Zn$^b$   | 1.951                   | 1.852                   | 1.874                   |
| O6 – Zn$^b$   | 1.973                   | 1.799                   | 1.791                   |
| O7 – Zn$^b$   | 1.852                   | 1.816                   | 1.785                   |
| O8 – Zn$^b$   | 1.828                   | 1.873                   | 1.861                   |
| N3 – Zn$^b$   | 2.038                   | 1.961                   | 2.018                   |
| N4 – Zn$^b$   | 1.949                   | 2.004                   | 1.949                   |
Table S02. The calculated metric data \{bond distances (Å)\} of \(\text{Zn}_a\) coordination sphere of MM minimized structures of \([(\text{Zn})_2L'X]\) complexes.

| Angle (°) | \([(\text{Zn})_2L'PPi]^{4-}\) | \([(\text{Zn})_2L'ADP]^{2-}\) | \([(\text{Zn})_2L'ATP]^{2-}\) |
|-----------|----------------|----------------|----------------|
| O1 – Zn\(_a\) - O2 | 163.4 | 158.4 | 161.6 |
| N1 – Zn\(_a\) - O3 | 152.7 | 150.5 | 151.1 |
| N2 – Zn\(_a\) - O4 | 150.9 | 154.9 | 155.2 |
| O1 – Zn\(_a\) - N1 | 101.1 | 76.6 | 79.4 |
| O1 – Zn\(_a\) - N2 | 64.6 | 86.2 | 88.9 |
| O1 – Zn\(_a\) - O3 | 87.0 | 81.5 | 82.2 |
| O1 – Zn\(_a\) - O4 | 103.4 | 118.0 | 114.4 |
| O2 – Zn\(_a\) - O3 | 109.3 | 111.7 | 109.6 |
| O2 – Zn\(_a\) - O4 | 80.26 | 80.2 | 81.0 |
| O3 – Zn\(_a\) - O4 | 87.5 | 89.2 | 86.7 |
| N1 – Zn\(_a\) - N2 | 108.4 | 109.6 | 113.1 |
| N1 – Zn\(_a\) - O2 | 79.4 | 95.2 | 94.0 |
| N1 – Zn\(_a\) - O4 | 82.2 | 83.8 | 80.8 |
| N2 – Zn\(_a\) - O2 | 99.2 | 83.8 | 77.7 |
| N2 – Zn\(_a\) - O3 | 92.6 | 88.1 |

Table S03. The calculated metric data \{bond distances (Å)\} of \(\text{Zn}_b\) coordination sphere of MM minimized structures of \([(\text{Zn})_2L'X]\) complexes.

| Angle (°) | \([(\text{Zn})_2L'PPi]^{4-}\) | \([(\text{Zn})_2L'ADP]^{2-}\) | \([(\text{Zn})_2L'ATP]^{2-}\) |
|-----------|----------------|----------------|----------------|
| O5 – Zn\(_b\) - O8 | 156.1 | 141.8 | 140.1 |
| N3 – Zn\(_b\) - O6 | 149.8 | 140.9 | 137.1 |
| N4 – Zn\(_b\) - O7 | 155.0 | 141.8 | 136.7 |
| O5 – Zn\(_b\) - N3 | 97.4 | 86.0 | 72.9 |
| O5 – Zn\(_b\) - N4 | 106.2 | 88.4 | 127.9 |
| O5 – Zn\(_b\) - O6 | 87.4 | 65.9 | 82.2 |
| O5 – Zn\(_b\) - O7 | 74.6 | 126.2 | 92.2 |
| O6 – Zn\(_b\) - O7 | 113.2 | 98.0 | 99.3 |
| O6 – Zn\(_b\) - O8 | 77.5 | 90.9 | 130.1 |
| O7 – Zn\(_b\) - O8 | 94.1 | 84.9 | 63.4 |
| N3 – Zn\(_b\) - N4 | 62.9 | 92.8 | 93.5 |
| N3 – Zn\(_b\) - O7 | 95.1 | 76.4 | 115.7 |
| N3 – Zn\(_b\) - O8 | 102.2 | 126. | 89.0 |
| N4 – Zn\(_b\) - O6 | 90.8 | 112.0 | 74.7 |
| N4 – Zn\(_b\) - O8 | 94.7 | 71.9 | 87.4 |
Table S04. The range and its average values of trans angles are given for Zn$^{2+}$ coordination sphere of [(Zn)$_2$L′X] complexes.

| Angle (°) | [(Zn)$_2$L′PPi]$^{4+}$ Range (average) | [(Zn)$_2$L′ADP]$^{2-}$ Range (average) | [(Zn)$_2$L′ATP]$^{3-}$ Range (average) |
|-----------|----------------------------------------|----------------------------------------|----------------------------------------|
| Zn$_a$ Trans angles | 151-163 (156) | 151-158 (155) | 151-162 (156) |
| Zn$_a$ other angles | 65-109 (91) | 77-118 (92) | 78-114 (91) |
| Zn$_b$ Trans angles | 150-156 (154) | 141-142 (141.5) | 137-140 (137.9) |
| Zn$_b$ other angles | 63-113 (91) | 66-126 (93) | 137-130 (94) |
S28. Cartesian coordinates for PM3 optimized structure of $[L']$.

| Z  | X       | Y       | Z       | X       | Y       | Z       | X       |
|----|---------|---------|---------|---------|---------|---------|---------|
| 8  | 6.43875 | -1.52477| 2.232743| 11.73281| -2.32824| -2.61309|
| 8  | 5.411696| 0.453263|-0.12072 | 6       | -9.43259| -1.34526| 1.188343|
| 8  | 7.736145| -2.61756| -0.3944  | 6       | -8.65875| -1.41877| 2.471728|
| 8  | -5.79428| -0.99239| 2.305056 | 6       | -9.34669| 1.57624 | 3.326393|
| 8  | 0.80646 | -1.91664| 2.318767 | 6       | -8.16126| -0.44164| 2.661843|
| 8  | -1.40348| 2.982174| 2.349037 | 6       | -6.27249| -2.30109| 2.290435|
| 8  | 1.887083| -1.57836| 5.514241 | 6       | -7.65439| -2.5345 | 2.42433 |
| 8  | 3.132597| 1.151026| 4.747121 | 6       | -8.10581| -3.85342| 2.480888|
| 7  | 4.77953 | -4.46821| 3.240682 | 6       | -9.17969| -4.04784| 2.591866|
| 7  | 3.766117| -5.02411| 2.706214 | 6       | -7.21181| -4.91331| 2.390537|
| 7  | 3.109584| -4.08519| 1.949363 | 6       | -5.86306| -4.67124| 2.167295|
| 7  | -1.15269| -1.3185 | 5.423566 | 6       | -5.15455| -5.51099| 2.071047|
| 7  | 1.151821| 2.650303| 2.987327 | 6       | -5.38056| -3.3649 | 2.065479|
| 7  | -4.62554| 2.970996| 3.27988  | 6       | 9.093507| -2.74182| 2.078002|
| 7  | -5.7003 | 2.986089| 4.314085 | 6       | 9.176071| -3.26736| 2.831078|
| 7  | -6.08177| 1.783961| 4.314549 | 6       | 8.154766| -3.32699| 2.007061|
| 6  | 7.55536 | -0.75534| 2.550219 | 6       | 5.892504| -2.18406| 3.383545|
| 6  | 8.837516| -1.33525| 2.539609 | 6       | 5.435499| -1.42483| 4.062319|
| 6  | 9.928248| -0.5499 | 2.917994 | 6       | 6.683406| -2.71827| 3.944896|
| 6  | 10.9296 | -0.99823| 2.934263 | 6       | 4.841231| -3.10749| 2.887781|
| 6  | 9.761945| 0.789029| 3.24572  | 6       | 3.76206 | -2.85287| 2.057351|
| 6  | 8.508732| 1.378035| 3.146337 | 6       | 3.44385 | -1.92919| 1.569704|
| 6  | 8.389211| 2.450631| 3.342894 | 6       | 1.820515| -4.33184| 1.2625  |
| 6  | 7.393472| 0.623924| 2.777143 | 6       | 1.871943| -5.31998| 0.758245|
| 6  | 6.083852| 1.33692 | 2.594362 | 6       | 0.20348 | -3.06343| 2.757653|
| 6  | 5.870908| 1.946132| 3.495924 | 6       | 0.657833| -4.27727| 2.207889|
| 6  | 5.225533| 0.622949| 2.526572 | 6       | 0.003756| -5.45926| 2.547821|
| 6  | 5.910363| 1.714733| 0.081981 | 6       | 0.337824| -6.41844| 2.115655|
| 6  | 6.135069| 2.214118| 1.38005  | 6       | -1.07308| -5.46578| 3.436943|
| 6  | 6.45648 | 3.563247| 1.532047 | 6       | -1.49047| -4.2604 | 4.001642|
| 6  | 6.620542| 3.971551| 2.536705 | 6       | -2.33679| -4.26729| 4.708712|
| 6  | 6.577565| 4.39273 | 0.424669 | 6       | -0.86027| -3.06095| 3.678609|
| 6  | 6.423197| 3.876194| -0.85594 | 6       | -1.3667 | -1.8025 | 4.254136|
| 6  | 6.564558| 4.529202| -1.7258  | 6       | -0.36188| -1.88614| 6.507221|
| 6  | -3.76327| -3.46548| 0.21551  | 1       | -0.97879| -2.6657 | 6.997254|
| 6  | -3.94685 | -3.15431| 1.673319 | 1       | -0.25836| -1.05548| 7.238988|
| 6  | -3.61142| -2.12054| 1.895397 | 6       | 1.011009| -2.47312| 6.162437|
| 6  | -3.2939 | -3.81181| 2.290563 | 1       | 1.473464| -2.89024| 7.078521|
| 6  | 9.096405| -2.56915 | -0.46275 | 6       | 0.942094| -3.28454| 5.413177|
| 6  | 9.797579| -2.71346| 0.752616 | 6       | 2.459605| -0.58376| 6.353272|
| 6  | 11.18902| -2.78601| 0.712717 | 6       | 2.871569| -1.04623| 7.271749|
|   |       |       |       |   |       |       |       |
|---|-------|-------|-------|---|-------|-------|-------|
| 1 | -9.73449 | -2.33246 | -3.66672 | 6 | -5.41191 | 2.47017 | -2.93349 |
| 6 | -7.81993 | -3.20271 | -4.14571 | 6 | -4.5027 | 2.66957 | -0.33081 |
| 6 | -3.67171 | 5.597231 | -0.29398 | 1 | 5.454032 | -0.33081 | -4.44354 |
| 1 | -3.93277 | 4.119696 | 0.085289 | 1 | 6.454682 | -1.8183 | -4.54076 |
| 6 | -1.27252 | 4.683499 | -1.57486 | 1 | -12.3277 | -2.50325 | -0.18387 |
| 6 | -2.45144 | 5.430413 | -1.35453 | 1 | -7.57565 | -5.94262 | 2.472279 |
| 6 | -2.47103 | 6.780962 | -1.68168 | 1 | -8.25756 | -4.09024 | -6.14047 |
| 1 | -3.38658 | 7.376976 | -1.5229 | 1 | -2.913 | -6.08941 | -1.79265 |
| 6 | -1.34802 | 7.418053 | -2.22 | 1 | 10.6246 | 1.387822 | 3.55479 |
| 6 | -0.18591 | 6.680545 | -2.41703 | 1 | 6.815848 | 5.452542 | 0.560355 |
| 1 | 0.701995 | 7.189667 | -2.82877 | 1 | 12.96769 | -2.75403 | -0.50473 |
| 6 | -0.12828 | 5.317573 | -2.11006 | 1 | 10.54477 | 2.294916 | -3.5287 |
| 6 | 1.120567 | 4.604175 | -2.38457 | 6 | -1.7766 | 6.477532 | 6.810627 |
| 6 | 2.386292 | 2.537816 | -2.42292 | 6 | -0.77375 | 6.129117 | 7.911906 |
| 1 | 2.361191 | 1.696565 | -1.70252 | 6 | -3.18172 | 6.435072 | 7.41394 |
| 6 | 2.343059 | 1.890706 | -3.85535 | 1 | -3.9524 | 6.604009 | 6.644015 |
| 1 | 1.300345 | 1.836055 | -4.217 | 1 | -3.39127 | 5.461706 | 7.876361 |
| 1 | 2.857433 | 1.00149 | -3.89536 | 1 | -3.30412 | 7.205185 | 8.186218 |
| 6 | 2.819775 | 2.756247 | -6.07135 | 1 | -1.00901 | 5.163755 | 8.378351 |
| 1 | 3.81788 | 2.985921 | -6.48529 | 1 | -0.77409 | 6.890399 | 8.702445 |
| 1 | 2.565333 | 1.715852 | -6.35228 | 1 | 0.251004 | 6.0586 | 7.512002 |
| 6 | 1.784514 | 3.766177 | -6.60448 | 6 | -1.48954 | 7.88949 | 6.292765 |
| 1 | 2.135312 | 4.196699 | -7.55904 | 1 | -0.47989 | 7.959601 | 5.867746 |
| 1 | 1.618405 | 4.600171 | -5.89464 | 1 | -2.20163 | 8.176892 | 5.508252 |
| 6 | -0.40286 | 3.04556 | -5.97925 | 1 | -1.56395 | 8.632944 | 7.097485 |
| 1 | 0.065038 | 2.762912 | -5.00918 | 6 | -1.80904 | -6.7559 | 3.747446 |
| 1 | -0.87675 | 4.036624 | -5.84338 | 6 | -2.95355 | -6.90008 | 2.740256 |
| 6 | -1.44218 | 2.010986 | -6.42908 | 6 | -2.38638 | -6.73495 | 5.16389 |
| 1 | -2.44051 | 2.293578 | -6.03062 | 1 | -1.59262 | -6.74774 | 5.92205 |
| 1 | -1.53531 | 1.97487 | -7.53276 | 1 | -2.99092 | -5.82931 | 5.336661 |
| 6 | -1.7536 | -0.08685 | -5.27716 | 1 | -3.0299 | -7.60645 | 5.533942 |
| 6 | -0.3128 | -1.48451 | -3.77321 | 1 | -3.7534 | -6.15701 | 2.912406 |
| 6 | -1.20983 | -1.3916 | -4.85389 | 1 | -3.41481 | -7.89448 | 2.799369 |
| 6 | -1.59716 | -2.54861 | -5.51837 | 1 | -2.60446 | -6.75209 | 1.70416 |
| 1 | -2.32056 | -2.49889 | -6.3489 | 6 | -0.87511 | -7.96213 | 3.630556 |
| 6 | -1.09717 | -3.79841 | -5.13768 | 1 | -0.08673 | -7.93448 | 4.39428 |
| 6 | -0.15282 | -3.87009 | -4.11701 | 1 | -1.42498 | -8.904 | 3.753805 |
| 1 | 0.272255 | -4.85295 | -3.85177 | 1 | -0.37692 | -7.98801 | 2.647737 |
| 6 | 0.245525 | -2.72655 | -3.42409 | 6 | -1.57561 | -5.0457 | -5.85524 |
| 6 | 1.230525 | -2.85273 | -2.30547 | 6 | -3.06872 | -4.91937 | -6.16837 |
| 1 | 1.097049 | -3.8212 | -1.77744 | 6 | -1.36787 | -6.29821 | -5.0025 |
| 1 | 1.073134 | -2.05117 | -1.54649 | 1 | -0.32729 | -6.37062 | -4.64646 |
| 6 | 3.312275 | -1.59028 | -3.14873 | 1 | -2.01522 | -6.29177 | -4.11317 |
| 1 | 2.896181 | -0.57316 | -3.16056 | 1 | -1.59323 | -7.2077 | -5.57356 |
| 6 | 4.582464 | -2.03225 | -3.48367 | 1 | -3.66273 | -4.83185 | -5.24142 |
| 6 | 5.769149 | -1.23882 | -3.89242 | 1 | -3.43577 | -5.78969 | -6.72555 |
|---|---|---|---|---|---|---|---|
| 6 | -0.78516 | -5.18201 | -7.15745 | 1 | -3.27063 | -4.01798 | -6.77009 |
| 6 | 0.287717 | -5.30261 | -6.95963 | 1 | 7.398874 | -2.60002 | -1.28695 |
| 1 | -1.11776 | -6.05428 | -7.73556 | 1 | 5.993022 | -0.15072 | 0.328538 |
| 1 | -0.90906 | -4.29479 | -7.79246 | 1 | 1.707186 | -3.56925 | 0.462511 |
| 6 | -1.38616 | 8.902375 | -2.52942 | 1 | -3.08407 | 8.88828 | -3.90494 |
| 6 | -0.41846 | 9.257431 | -3.65965 | 1 | -0.50097 | 2.643284 | 2.256227 |
| 1 | -0.73704 | 8.818174 | -4.61399 | 1 | -0.44558 | 2.984767 | -1.44921 |
| 1 | -0.35373 | 10.34426 | -3.79801 | 1 | 0.745001 | -1.25358 | 3.003983 |
| 1 | 0.596846 | 8.883268 | -3.44952 | 1 | 0.391166 | -0.5543 | -2.2864 |
| 6 | -2.79056 | 9.340654 | -2.94869 | 1 | 1.950379 | 5.177763 | -2.83007 |
| 1 | -3.54265 | 9.040613 | -2.20065 | 1 | 1.844081 | 3.79343 | 4.623309 |
| 1 | -2.84712 | 10.43068 | -3.06321 | 1 | -2.76927 | 0.161776 | -4.91848 |
| 6 | -0.97819 | 9.653622 | -1.25923 | 1 | -2.04355 | -1.21149 | 3.613372 |
| 1 | -1.66132 | 9.430373 | -0.42938 | 1 | 3.331356 | 3.092862 | -2.23029 |
| 1 | 0.034686 | 9.375326 | -0.94052 | 1 | -4.90134 | -0.84521 | -0.9905 |
| 1 | -0.99056 | 10.74034 | -1.4165 | 1 | -7.48908 | 0.104354 | 1.025001 |

S29. Cartesian coordinates for MM minimized structure of \([\text{Zn}_2\text{L}']\)

| Z | X   | Y   | Z   | X   | Y   | Z   | X   |
|---|-----|-----|-----|-----|-----|-----|-----|
| 8 | 6.778 | -1.513 | 0.38 | 6 | -6.993 | -3.394 | -4.739 |
| 8 | -3.732 | 0.192 | 1.329 | 6 | -6.524 | -2.024 | -4.476 |
| 8 | 1.375 | -2.103 | 2.592 | 6 | -5.033 | -1.753 | -4.433 |
| 8 | 1.067 | 0.961 | 2.262 | 6 | -3.957 | -1.991 | -2.028 |
| 8 | -0.531 | -0.032 | 6.606 | 6 | -4.363 | -2.562 | -3.337 |
| 8 | 1.844 | -0.523 | 7.724 | 6 | -4.061 | -3.977 | -3.611 |
| 7 | 4.542 | -4.854 | 4.327 | 6 | -3.62 | -4.869 | -2.541 |
| 7 | 3.58 | -5.217 | 3.425 | 6 | -3.342 | -4.328 | -1.213 |
| 7 | 3.552 | -4.329 | 2.388 | 6 | 4.879 | 3.254 | 0.164 |
| 7 | -0.866 | -0.725 | 3.999 | 6 | 4.79 | 3.061 | -1.332 |
| 7 | 2.151 | -0.045 | 4.827 | 6 | -7.811 | -0.568 | 0.198 |
| 7 | -0.628 | 2.98 | 0.467 | 6 | -9.005 | -1.089 | -0.499 |
| 7 | -1.249 | 4.055 | 1.041 | 6 | -10.023 | -1.83 | 0.259 |
| 7 | -2.488 | 3.706 | 1.5 | 6 | -9.882 | -2.009 | 1.703 |
| 6 | 7.032 | -0.95 | 3.5 | 6 | -8.767 | -1.382 | 2.412 |
| 6 | 8.314 | -1.568 | 3.089 | 6 | 8.239 | -1.782 | -1.48 |
| 6 | 9.503 | -0.702 | 3.031 | 6 | 7.26 | -1.277 | -2.519 |
| 6 | 9.333 | 0.744 | 2.892 | 6 | 5.967 | 1.029 | -2.47 |
| 6 | 7.987 | 1.32 | 2.881 | 6 | 7.218 | 0.238 | -2.579 |
| 6 | 6.814 | 0.478 | 3.18 | 6 | 8.495 | 0.974 | -2.608 |
| 6 | 5.457 | 1.105 | 3.421 | 6 | 8.552 | 2.376 | -2.193 |
| 6 | 4.808 | 2.099 | 1.083 | 6 | 7.334 | 3.052 | -1.75 |
| 6 | 5.183 | 2.277 | 2.504 | 6 | 6.037 | 2.367 | -1.843 |
| 6 | 5.38 | 3.638 | 3.03 | 6 | -9.25 | -0.767 | -1.957 |
|   | 5.38 | 4.789 | 2.128 |   | -7.046 | 0.828 | -5.206 |
|---|---|---|---|---|---|---|---|
| 6 | 5.123 | 4.6 | 0.702 | 6 | -6.285 | 1.965 | -4.586 |
| 6 | -3.462 | -2.886 | -0.96 | 6 | -5.776 | 1.983 | -3.218 |
| 6 | -2.854 | -2.322 | 0.305 | 6 | -5.336 | 3.84 | -1.566 |
| 6 | 7.848 | -1.943 | -0.061 | 6 | -2.779 | 3.95 | -2.082 |
| 6 | 8.759 | -2.631 | 0.877 | 6 | -3.992 | 4.528 | -1.466 |
| 6 | 10.07 | -3.104 | 0.41 | 6 | -3.924 | 5.833 | -0.799 |
| 6 | 10.469 | -2.915 | -0.984 | 6 | -2.696 | 6.643 | -0.833 |
| 6 | 9.548 | -2.284 | -1.929 | 6 | -1.613 | 6.185 | -1.719 |
| 6 | -7.732 | -0.638 | 1.676 | 6 | -1.602 | 4.83 | -2.3 |
| 6 | -6.71 | 0.152 | 2.468 | 6 | -0.356 | 4.452 | -3 |
| 6 | -4.36 | -0.779 | 1.771 | 6 | 1.339 | 2.723 | -3.606 |
| 6 | -5.479 | -0.689 | 2.738 | 6 | 1.52 | 1.916 | -4.912 |
| 6 | -5.614 | -1.778 | 3.722 | 6 | 0.966 | 1.893 | -7.224 |
| 6 | -5.096 | -3.106 | 3.389 | 6 | -0.12 | 2.409 | -8.202 |
| 6 | -4.347 | -3.296 | 2.147 | 6 | -2.02 | 2.975 | -6.831 |
| 6 | -3.914 | -2.129 | 1.136 | 6 | -2.905 | 2.212 | -5.818 |
| 6 | 8.351 | -2.869 | 2.315 | 6 | -1.973 | -0.058 | -5.314 |
| 6 | 6.094 | -2.819 | 4.664 | 6 | -0.891 | -0.811 | -3.027 |
| 6 | 5.186 | -3.692 | 3.844 | 6 | -1.295 | -1.038 | -4.44 |
| 6 | 4.541 | -3.343 | 2.58 | 6 | -1.049 | -2.358 | -5.048 |
| 6 | 2.547 | -4.312 | 1.345 | 6 | -0.611 | -3.517 | -4.251 |
| 6 | 0.649 | -3.1 | 2.632 | 6 | -0.514 | -3.322 | -2.798 |
| 6 | 1.158 | -4.301 | 1.944 | 6 | -0.409 | -1.967 | -2.243 |
| 6 | 0.346 | -5.523 | 1.893 | 6 | 0.425 | -1.791 | -0.993 |
| 6 | -0.857 | -5.671 | 2.73 | 6 | 2.629 | -0.776 | -1.657 |
| 6 | -1.327 | -4.479 | 3.456 | 6 | 3.661 | -1.276 | -2.561 |
| 6 | -0.66 | -3.171 | 3.332 | 6 | 4.386 | -0.424 | -3.561 |
| 6 | -1.403 | -2.021 | 3.89 | 6 | 1.72 | 6.299 | 3.912 |
| 6 | -1.638 | 0.403 | 4.495 | 6 | 1.764 | 6.449 | 5.465 |
| 6 | -1.784 | 0.364 | 6.035 | 6 | 0.313 | 6.773 | 3.432 |
| 6 | -0.536 | 0.019 | 8.041 | 6 | 2.82 | 7.223 | 3.308 |
| 6 | 0.707 | -0.731 | 8.584 | 6 | -1.547 | -7.035 | 2.844 |
| 6 | 1.994 | -1.585 | 6.759 | 6 | -2.112 | -7.446 | 1.45 |
| 6 | 2.849 | -1.077 | 5.576 | 6 | -2.733 | -7.035 | 3.859 |
| 6 | 2.45 | 1.326 | 4.965 | 6 | -0.514 | -8.1 | 3.328 |
| 6 | 1.519 | 2.052 | 2.619 | 6 | -0.121 | -4.792 | -4.943 |
| 6 | 2.014 | 2.345 | 3.987 | 6 | -1.247 | -5.376 | -5.85 |
| 6 | 2.19 | 3.751 | 4.388 | 6 | 0.296 | -5.905 | -3.932 |
| 6 | 1.944 | 4.857 | 3.448 | 6 | 1.126 | -4.442 | -5.813 |
| 6 | 1.81 | 4.509 | 2.022 | 6 | -2.597 | 7.923 | 0.003 |
| 6 | 1.493 | 3.134 | 1.617 | 6 | -1.168 | 8.55 | -0.026 |
| 6 | 0.811 | 2.913 | 0.284 | 6 | -3.602 | 8.977 | -0.553 |
| 6 | -1.487 | 1.859 | 0.533 | 6 | -2.942 | 7.601 | 1.491 |
| 6 | -2.677 | 2.334 | 1.232 | 3 | 0.941 | -0.493 | 3.412 |
| 6 | -3.902 | 1.551 | 1.6 | 3 | -1.467 | 1.859 | -3.283 |
| 8  | -7.681 | 0.071 | -4.215 | 1  | 10.455 | -1.125 | 2.886 |
| 8  | -3.97  | -0.782 | -1.788 | 1  | 7.878  | 2.355  | 2.735 |
| 8  | -6.905 | -0.099 | -0.495 | 1  | 5.418  | 1.439  | 4.46  |
| 8  | 4.852  | 0.709 | -2.899 | 1  | 4.676  | 0.357  | 3.284 |
| 8  | -2.836 | 2.76  | -2.402 | 1  | 5.605  | 3.783  | 4.046 |
| 8  | -0.921 | 0.282 | -2.454 | 1  | 5.158  | 5.429  | 0.057 |
| 8  | 0.861  | 2.608 | -5.983 | 1  | -2.358 | -1.376 | 0.085 |
| 8  | -1.429 | 2.026 | -7.741 | 1  | -2.096 | -3.01  | 0.683 |
| 7  | -6.403 | 3.317 | -4.987 | 1  | 10.73  | -3.577 | 1.077 |
| 7  | -5.964 | 4.113 | -3.962 | 1  | 9.83   | -2.193 | 2.937 |
| 7  | 7.577  | 3.341 | -2.905 | 1  | -7.146 | 0.454  | 3.423 |
| 7  | -0.041 | 3.135 | -3.392 | 1  | -6.459 | 1.062  | 1.929 |
| 7  | -2.11  | 1.308 | -5     | 1  | -6.272 | -1.672 | 4.535 |
| 7  | 1.831  | -1.894 | -1.338 | 1  | -4.026 | -4.26  | 1.88  |
| 7  | 2.364  | -3.001 | -1.942 | 1  | 9.055  | -3.547 | 2.8   |
| 7  | 3.453  | -2.666 | -2.697 | 1  | 7.372  | -3.344 | 2.309 |
| 6  | -7.499 | -1.1  | -3.861 | 1  | 5.694  | -2.762 | 5.679 |
| 6  | -8.423 | -1.662 | -2.854 | 1  | 7.084  | -3.272 | 4.72  |
| 6  | -8.719 | -3.105 | -2.908 | 1  | 4.483  | -2.37  | 2.196 |
| 6  | -8.073 | -3.947 | -3.919 | 1  | 2.677  | -5.192 | 0.712 |
| 1  | 0.688  | -6.336 | 1.322  | 1  | 1.089  | 0.922  | 4.78  |
| 1  | -2.189 | -4.539 | 4.053  | 1  | 2.585  | 1.822  | -5.128 |
| 1  | -2.632 | 0.392  | 4.047  | 1  | 1.955  | 2.056  | -7.657 |
| 1  | -1.139 | 1.33   | 4.205  | 1  | 0.812  | 0.822  | -7.075 |
| 1  | -2.078 | 1.353  | 6.392  | 1  | 0.043  | 1.932  | -9.171 |
| 1  | -2.556 | -0.36  | 6.304  | 1  | -0.04  | 3.49   | -8.334 |
| 1  | -1.435 | -0.448 | 8.449  | 1  | -1.276 | 3.549  | -6.28 |
| 1  | -0.497 | 1.063  | 8.361  | 1  | -2.64  | 3.67   | 7.401 |
| 1  | 0.946  | -0.332 | 9.572  | 1  | -3.407 | 2.932  | -5.171 |
| 1  | 0.484  | -1.794 | 8.693  | 1  | -3.668 | 1.65   | -6.362 |
| 1  | 1.032  | -1.926 | 6.373  | 1  | -1.191 | -2.471 | -6.084 |
| 1  | 2.501  | -2.429 | 7.232  | 1  | -0.326 | -4.138 | -2.164 |
| 1  | 3.065  | -1.911 | 4.906  | 1  | 0.176  | -2.574 | -0.277 |
| 1  | 3.796  | -0.69  | 5.958  | 1  | 0.224  | -0.826 | -0.528 |
| 1  | 2.518  | 3.957  | 5.365  | 1  | 2.265  | 0.204  | -1.682 |
| 1  | 1.761  | 5.274  | 1.302  | 1  | 3.678  | -0.112 | -4.329 |
| 1  | 1.119  | 3.685  | -0.423 | 1  | 5.183  | -0.981 | -4.049 |
| 1  | 1.097  | 1.943  | -0.123 | 1  | -10.616 | -2.536 | 2.241 |
| 1  | -1.158 | 0.866  | 0.553  | 1  | -5.316 | -3.928 | 4.005 |
| 1  | -4.109 | 1.71   | 2.66   | 1  | -8.336 | -4.96  | -4.007 |
| 1  | -4.731 | 1.937  | 1.01   | 1  | -3.45  | -5.886 | -2.74 |
| 1  | -9.452 | -3.519 | -2.28  | 1  | 10.169 | 1.359  | 2.73  |
| 1  | -6.454 | -4.025 | -5.383 | 1  | 5.614  | 5.744  | 2.496 |
| 1  | -4.6   | -2.031 | -5.397 | 1  | 11.406 | -3.259 | -1.313 |
| 1  | -4.848 | -0.692 | -4.286 | 1  | 9.475  | 2.877  | -2.156 |
| 1  | -4.204 | -4.368 | -4.576 | 1  | 0.259  | 6.768  | 2.344 |
| 1   | -2.944 | -4.96 | -0.475 | 1  | -0.459 | 6.109 | 3.826 |
|-----|--------|-------|--------|----|--------|-------|-------|
| 1   | 4.694  | 4.027 | -1.832 | 1  | 0.115  | 7.788 | 3.782 |
| 1   | 3.898  | 2.476 | -1.558 | 1  | 1.01   | 5.81  | 5.929 |
| 1   | -10.864| -2.226| -0.232 | 1  | 1.561  | 7.484 | 5.748 |
| 1   | -8.723 | -1.45 | 3.46   | 1  | 2.749  | 6.176 | 5.846 |
| 1   | 7.542  | -1.655| -3.504 | 1  | 3.803  | 6.91  | 3.662 |
| 1   | 6.282  | -1.682| -2.271 | 1  | 2.808  | 7.179 | 2.218 |
| 1   | 9.387  | 0.477 | -2.857 | 1  | 2.652  | 8.257 | 3.614 |
| 1   | 7.39   | 4.035 | -1.382 | 1  | -2.382 | -6.754| 4.854 |
| 1   | -10.306| -0.907| -2.196 | 1  | -3.508 | -6.336| 3.541 |
| 1   | -9.003 | 0.281 | -2.133 | 1  | -3.176 | -8.032| 3.919 |
| 1   | -6.37  | 0.228 | -5.813 | 1  | -2.853 | -6.716| 1.12  |
| 1   | -7.818 | 1.237 | -5.861 | 1  | -2.591 | -8.425| 1.511 |
| 1   | -6.03  | 1.264 | -2.503 | 1  | -1.314 | -7.497| 0.708 |
| 1   | -6.133 | 4.54  | -1.309 | 1  | -0.077 | -7.79 | 4.28  |
| 1   | -5.363 | 3.015 | -0.854 | 1  | -1.004 | -9.066| 3.466 |
| 1   | -4.774 | 6.195 | -0.299 | 1  | 0.287  | -8.224| 2.598 |
| 1   | -0.796 | 6.816 | -1.911 | 1  | 1.121  | -5.562| -3.304|
| 1   | 1.658  | 2.111 | -2.762 | 1  | -0.549 | -6.178| -3.297|
| 1   | 0.625  | -6.797| -4.469 | 1  | -3.979 | 7.277 | 1.587 |
| 1   | -2.121 | -5.624| -5.247 | 1  | -2.292 | 6.806 | 1.86  |
| 1   | -0.897 | -6.284| -6.346 | 1  | -2.801 | 8.487 | 2.112 |
| 1   | -1.541 | -4.659| -6.617 | 1  | -4.24  | -0.137| -2.408|
| 1   | 1.908  | -4.006| -5.187 | 1  | -6.111 | 0.246 | -0.139|
| 1   | 1.519  | -5.342| -6.289 | 1  | 6.148  | -1.06 | -0.146|
| 1   | 0.862  | -3.726| -6.593 | 1  | 4.349  | 0.239 | 1.144 |
| 1   | -0.92  | 8.891 | -1.033 | 1  | 2.678  | -3.425| 0.725 |
| 1   | -1.12  | 9.409 | 0.646  | 1  | -3.379 | 9.189 | -1.601|
| 1   | -0.425 | 7.818 | 0.295  | 1  | 0.388  | 5.189 | -3.112|
| 1   | -4.626 | 8.607 | -0.481 | 1  | 2.991  | 1.638 | 5.813 |
| 1   | -3.528 | 9.905 | 0.016  | 1  | -2.332 | -0.389| -6.247|
| 1   | 1.985  | 3.603 | -3.652 | 1  | -2.367 | -2.189| 4.275 |
| 8    | 6.149  | -1.52 | 4.153  |     |        |       |       |
| 8    | 4.428  | 1.017 | 0.626  |     |        |       |       |
S30. Cartesian coordinates for MM minimized structure of [Zn2L′PPi]+

| Z | X     | Y     | Z     | X     | Y     | Z     | X     |
|---|-------|-------|-------|-------|-------|-------|-------|
| 30| -1.30997 | -2.4801 | 2.06842 | 6 | -5.29999 | 0.388151 | -4.47118 |
| 8 | 5.559882 | -3.01122 | 0.799962 | 1 | -5.03441 | -0.5577 | -4.92535 |
| 8 | 5.987501 | 0.120233 | 0.256955 | 6 | -4.67483 | 0.809399 | -3.28425 |
| 8 | 8.02878 | -2.10952 | -0.90747 | 6 | -3.67585 | -0.11425 | -2.61346 |
| 8 | -8.33397 | -0.81216 | 1.174788 | 1 | -2.81556 | -0.24113 | -3.3026 |
| 8 | -1.27193 | -2.29812 | 0.102865 | 1 | -3.24366 | 0.320728 | -1.68818 |
| 8 | -2.39976 | -0.86154 | 2.10929 | 6 | -5.37202 | -1.61472 | -1.36171 |
| 8 | -4.19007 | -4.59272 | 4.255872 | 6 | -4.31479 | -1.46074 | -2.36085 |
| 8 | -2.17996 | -4.6009 | 6.329903 | 6 | -3.92457 | 2.57146 | -3.07305 |
| 7 | 2.690951 | -5.22355 | 0.197149 | 1 | -3.12485 | -2.48701 | -3.79609 |
| 7 | 1.618486 | -4.87529 | -0.61025 | 6 | -4.5896 | -3.78901 | -2.95289 |
| 7 | 1.873106 | -3.71361 | -1.04453 | 6 | -5.65255 | -3.92736 | -2.06714 |
| 7 | -2.83679 | -3.8295 | 2.094825 | 1 | -6.16693 | -4.87867 | -2.01111 |
| 7 | -1.64492 | -3.40515 | 3.751106 | 6 | 6.315502 | 2.252283 | 1.288537 |
| 7 | -5.32461 | 1.80709 | 2.073811 | 6 | 7.015263 | 2.753685 | 0.043193 |
| 7 | -5.92905 | 2.908665 | 1.934802 | 1 | 7.078351 | 3.864006 | 0.045732 |
| 7 | -7.27625 | 2.583068 | 1.826407 | 6 | 6.393067 | 2.49702 | -0.83777 |
| 6 | 6.393837 | -2.77203 | 1.880621 | 6 | -8.43029 | 2.617225 | -1.32343 |
| 6 | 7.652417 | -3.41889 | 1.984188 | 6 | -8.11347 | 3.79363 | -2.1197 |
| 6 | 8.44523 | -3.20967 | 3.122255 | 6 | -9.13483 | 4.629415 | -2.48532 |
| 6 | 9.397037 | -3.7159 | 3.228126 | 1 | -8.91698 | 5.495586 | -3.0977 |
| 6 | 8.03625 | -2.33114 | 4.120931 | 6 | -10.4457 | 4.414889 | -2.05759 |
| 6 | 6.842491 | -1.62911 | 3.986497 | 6 | -10.7558 | 3.31115 | -1.26148 |
| 6 | 6.559813 | -0.92228 | 4.757107 | 1 | -11.7808 | 3.165201 | -0.94397 |
| 6 | 6.021104 | -1.82088 | 2.863729 | 6 | 10.46348 | -1.86957 | -1.0627 |
| 6 | 4.776482 | -0.97241 | 2.734004 | 6 | 10.39201 | -0.58654 | -1.86635 |
| 6 | 4.177204 | -1.09657 | 3.661856 | 1 | 11.37154 | -0.37125 | -2.34715 |
| 6 | 4.114643 | -1.31462 | 1.915242 | 1 | 9.694782 | -0.71564 | -2.71456 |
| 6 | 5.811592 | 0.934662 | 1.352474 | 6 | 8.748119 | 1.186971 | -1.0123 |
| 6 | 5.156639 | 0.482706 | 2.531977 | 6 | 10.03312 | 0.593077 | -0.98524 |
| 6 | 4.948275 | 1.388402 | 3.584924 | 6 | 11.00055 | 1.089974 | -0.09752 |
| 6 | 4.449513 | 1.07217 | 4.492675 | 1 | 11.99424 | 0.65953 | -0.07545 |
| 6 | 5.421811 | 2.696314 | 3.501199 | 6 | 10.69112 | 2.125951 | 0.782386 |
| 6 | 6.113695 | 3.122888 | 2.362262 | 6 | 9.406484 | 2.66616 | 0.805651 |
| 6 | 6.488331 | 4.138152 | 2.333709 | 1 | 9.174948 | 3.446228 | 1.520685 |
| 6 | -6.06536 | -2.84533 | -1.27896 | 6 | 8.417352 | 2.191373 | -0.06897 |
| 6 | -7.27292 | -3.0036 | -0.3761 | 6 | -6.6891 | 3.999605 | -2.56964 |
| 6 | -6.97422 | -2.74507 | 0.66101 | 1 | -6.63774 | 4.876343 | -3.25112 |
| 6 | -7.61196 | -4.06192 | -0.34357 | 6 | -6.0987 | 4.263269 | -1.66779 |
| 6 | 9.29891 | -2.52754 | -0.57737 | 6 | -3.36075 | 3.468866 | -2.09101 |
| 6 | 9.428498 | -3.64633 | 0.271331 | 1 | -2.55241 | 2.919976 | -2.62226 |
6 10.70335 -4.1524 0.564954 1 -3.78917 4.228582 -2.78631
1 10.81715 -5.01761 1.206213 6 -2.76168 4.198487 -0.9304
6 11.84251 -3.53599 0.050947 6 -2.05231 3.64717 0.057853
6 11.72644 -2.39902 -0.74763 1 -1.84331 2.590807 0.163436
1 12.629 -1.9202 -1.10692 6 -0.88988 4.365542 2.120788
6 -9.7578 2.398089 -0.88792 1 -1.3561 4.987064 2.914569
6 -10.1331 1.195285 -0.03714 6 -2.76168 4.198487 -0.9304
1 -11.2008 1.219072 0.28137 6 1.355164 4.05606 2.451864
6 -9.45926 0.816462 6 0.582811 4.69321 1.969763
1 -8.87588 -0.12864 1 0.568206 6.159881 3.620812
6 -9.3078 -0.74849 1 0.568206 6.159881 3.620812
6 -10.3815 -1.99498 6 2.547813 5.967969 2.835052
1 -11.101 2.202051 -2.45458 6 0.371195 5.2522 1.807856
6 -9.97489 -2.66848 1 4.247249 5.469061 1.692131
6 -8.99579 -2.1215 6 2.794438 4.350381 1.005721
1 -8.66339 -2.68952 6 3.441542 3.663287 -0.04379
6 -8.42324 -0.86779 6 3.778112 3.662849 -2.25223
1 8.203844 -0.87707 6 3.43814 4.697824 -2.30773
1 8.448665 -5.28952 1 3.798368 3.933033 -3.7014
1 7.462842 -0.70643 1 2.97819 2.494389 -3.91771
6 4.772444 -1.81724 1 4.752942 2.671849 -3.86711
1 4.395849 -2.13283 6 2.51961 5.048927 -4.4605
1 5.368921 -0.91735 6 2.242348 5.576353 -5.39735
6 3.565659 -0.192447 1 1.66884 4.453988 -4.02959
6 3.07322 -0.59535 6 2.67829 6.044559 -3.25678
1 3.49466 -0.77511 1 3.331926 6.905286 -3.51093
6 0.925759 -1.85345 1 3.165941 5.311417 -2.55932
1 1.308541 -2.89016 6 0.772914 5.491608 -1.95917
6 -1.30051 -0.7398 1 1.44508 5.270206 -1.12394
6 -0.44149 -1.85754 1 -0.14376 5.930153 -1.51818
1 -0.64196 -2.76196 6 0.388034 4.215466 -2.76436
1 0.036471 -3.59843 1 -0.61216 4.39687 -3.2247
6 -1.60667 -2.51444 1 1.138943 4.240702 -3.59325
6 -2.31285 -1.29393 6 0.176222 1.970938 -2.90781
1 -2.99393 -0.97433 6 1.723978 0.303111 -3.39742
6 -2.12271 -0.45208 6 0.481482 0.852824 -3.6853
1 -2.63905 -0.83735 6 -0.32585 0.389812 -4.72588
6 -4.25094 -3.59843 1 -1.27758 0.879414 -4.87061
1 -4.90349 -1.74916 6 0.087799 -0.63115 -5.5189
1 -4.34373 -1.81724 6 1.382512 -1.16296 -5.30282
6 -4.85222 -3.55915 1 1.746162 -1.95859 -5.93863
1 -4.78204 -4.08145 6 2.209567 -0.7039 -4.25885
1 -5.93486 -3.47043 6 3.531202 -1.39173 -4.0311
1 -4.49892 -5.63470 6 3.687275 -2.22099 -4.75483
1 -5.4781 5.807069 1 3.514911 -1.85603 -3.02671
1 -4.55013 -3.51243 6 5.516725 -0.23139 -3.14301
| 6 | -3.41621 | -5.2897 | 6.424148 | 1 | 5.467444 | -0.64236 | -2.14608 |
| 1 | -3.71859 | -5.29286 | 7.492809 | 6 | 6.442806 | 0.588892 | -3.69045 |
| 1 | -3.36729 | -6.36198 | 6.121955 | 6 | 7.628763 | 1.200842 | -3.01636 |
| 6 | -1.30838 | -5.19184 | 5.379481 | 1 | 7.46467 | 2.298804 | -2.93755 |
| 1 | -1.81174 | -5.86837 | 4.66542 | 1 | 8.530921 | 1.009337 | -3.63565 |
| 6 | -0.529 | -5.76799 | 5.922134 | 30 | 1.723527 | 1.916068 | -0.8882 |
| 6 | -0.63066 | -4.0993 | 4.549136 | 1 | -11.2258 | 5.108748 | -2.34344 |
| 1 | 0.08812 | -4.59849 | 3.868888 | 1 | -10.3947 | -1.82642 | -3.63918 |
| 1 | -0.05573 | -3.40554 | 5.205816 | 1 | 1.723527 | 1.916068 | -0.8882 |
| 6 | -2.13352 | -2.29653 | 4.420221 | 1 | -4.29611 | -4.62684 | -3.56632 |
| 6 | -2.8358 | -0.31606 | 3.335153 | 1 | 8.661325 | -2.17235 | 4.990234 |
| 6 | -2.6476 | -0.99927 | 4.545739 | 1 | 5.270132 | 3.375974 | 4.328658 |
| 6 | -3.01459 | -0.46097 | 5.777494 | 1 | 12.82228 | -3.92946 | 0.289421 |
| 1 | -2.84329 | -1.05891 | 6.661096 | 1 | 11.44391 | 2.495321 | 1.466796 |
| 6 | -3.59781 | 0.8207 | 5.844922 | 15 | 0.330757 | 0.731421 |
| 6 | -3.82322 | 1.501168 | 4.629314 | 15 | 0.983176 | -2.14079 | 2.212259 |
| 1 | -4.2985 | 2.473422 | 4.636723 | 8 | 1.694127 | -1.31802 | 0.831515 |
| 6 | -3.4746 | 0.940231 | 3.386678 | 8 | 2.462654 | 1.409018 | 0.73246 |
| 6 | -3.86983 | 1.685416 | 2.142341 | 8 | -0.20859 | 0.989767 | 1.674111 |
| 1 | -3.41249 | 2.694852 | 2.176239 | 8 | 0.118917 | -3.52182 | 1.60291 |
| 6 | -3.50953 | 1.170809 | 1.227053 | 8 | -0.25769 | -1.21432 | 2.93887 |
| 6 | -6.17967 | 0.767433 | 2.082494 | 8 | 0.624634 | 0.444262 | -0.75759 |
| 1 | -5.8963 | -0.27583 | 2.151078 | 8 | 2.008293 | -2.76713 | 3.493566 |
| 6 | -7.38824 | 1.250621 | 1.918628 | 6 | -4.01531 | 1.478969 | 7.176 |
| 6 | -8.60931 | 0.467339 | 1.68017 | 6 | -3.69024 | 0.606666 | 8.412663 |
| 1 | -9.07547 | 0.375403 | 2.652564 | 6 | -5.53836 | 1.734038 | 7.168642 |
| 1 | -9.12769 | 0.850323 | 1.199331 | 1 | -5.83042 | 2.446731 | 6.369352 |
| 8 | -4.3409 | 2.557959 | -1.6328 | 8 | -6.08834 | 0.782076 | 7.004577 |
| 8 | -5.77443 | -0.59635 | -0.52523 | 8 | -5.87011 | 2.167024 | 8.137304 |
| 8 | -7.44027 | 1.731965 | -0.99189 | 8 | -4.24007 | -0.35861 | 8.373002 |
| 8 | 7.747197 | 0.597345 | -1.7479 | 8 | -3.993 | 1.122469 | 9.349865 |
| 8 | 0.777521 | 3.263326 | 0.077555 | 8 | -2.59892 | 0.406073 | 8.479325 |
| 8 | 2.485485 | 0.803248 | -2.33007 | 6 | -3.26998 | 2.821573 | 7.341685 |
| 8 | 3.716202 | 4.280342 | -4.63184 | 8 | -2.17081 | 2.661014 | 7.304084 |
| 8 | 1.395417 | 6.479328 | -2.78948 | 8 | -3.54344 | 3.54296 | 6.543685 |
| 7 | -2.82045 | 5.34447 | -0.75673 | 8 | -3.5208 | 3.294526 | 8.315952 |
| 7 | -2.10072 | 5.789946 | 0.406317 | 6 | -1.74186 | -6.80914 | -3.48295 |
| 7 | -1.62632 | 4.566216 | 0.872269 | 6 | -1.91492 | -6.30307 | -4.93541 |
| 7 | 3.53016 | 2.79695 | -1.1244 | 6 | -2.95634 | -7.71062 | -3.15476 |
| 7 | 0.351891 | 2.962452 | -1.96933 | 6 | -2.82497 | -8.22091 | -2.17654 |
| 7 | 4.655085 | -0.4687 | -4.13782 | 6 | -3.89403 | -7.11461 | -3.13368 |
| 7 | 4.998082 | 0.115256 | -5.20927 | 6 | -3.07527 | -8.50763 | -3.92061 |
| 7 | 6.061858 | 0.760398 | -4.96555 | 6 | -2.78116 | -5.61505 | -5.0138 |
| 7 | -5.01812 | 2.0693 | -2.73671 | 6 | -2.08481 | -7.15283 | -5.63157 |
| 6 | -6.10523 | 2.798274 | -3.28472 | 6 | -1.01314 | -5.76776 | -5.29725 |
| 6 | -6.71154 | 2.348094 | -4.46673 | 6 | -0.46566 | -7.67115 | -3.39856 |
S31. Cartesian coordinates for MM minimized structure of [Zn$_2$L'ADP]$^{2-}$.

|  | X     | Y   | Z     | X     | Y   | Z     | X     | Y   | Z     |
|---|-------|-----|-------|-------|-----|-------|-------|-----|-------|
| 30| 1.66  | 2.593| 1.961 | 6     | 1.314|       | 1     | 3.873|       |
| 8 | -6.204| 1.326| 1.201 | 1     | 1.557|       | -4.377|       | 0.905 |
| 8 | -6.28 | -0.782| -1.421| 1     | 1.359|       | -2.8  |       | 0.141 |
| 8 | -7.602| 2.133| -1.457| 6     | -0.7 |       | -3.854|       | -1.521|
| 8 | 9.056 | 0.366| 1.82  | 6     | -0.082|       | -4.241|       | -0.509|
| 8 | 0.849 | 3.603| 0.607  | 6     | -0.846|       | -5.247|       | 0.278 |
| 8 | 3.066 | 1.425| 2.265 | 1     | -0.315|       | -5.762|       | 1.068 |
| 8 | 4.701 | 4.452| 3.316 | 6     | -2.148|       | -5.518|       | 0.006 |
| 8 | 3.143 | 4.666| 5.805 | 6     | -2.801|       | -4.756|       | -1.105|
| 7 | -3.714| 3.135| 3.221 | 1     | -3.842|       | -4.95  |       | -1.348|
| 7 | -2.701| 3.87  | 2.611 | 6     | -2.121|       | -3.832|       | -1.807|
| 7 | -2.823| 3.753| 1.301 | 6     | -2.732|       | -3.103|       | -2.814|
| 7 | 2.992 | 3.943| 1.311 | 6     | -2.869|       | -1.446|       | -4.441|
| 7 | 1.88  | 3.132| 3.834 | 1     | -3.741|       | 0.978  |       | -3.998|
| 7 | 5.427 | -1.591| 1.84  | 6     | -2.482|       | -1.055|       | -5.829|
| 7 | 5.915 | -2.798| 1.621 | 1     | -1.643|       | -0.328|       | -5.765|
| 7 | 7.294 | -2.76 | 1.815 | 1     | -3.352|       | -0.561|       | -6.314|
| 6 | -7.442| 0.757| 1.452 | 6     | -1.449|       | -1.842|       | -7.751|
| 6 | -8.607| 1.564| 1.454 | 1     | -1.575|       | -0.773|       | -8.048|
| 6 | -9.845| 0.992| 1.79  | 1     | -1.867|       | -2.443|       | -8.586|
| 1  | -10.739| 1.602| 1.821  | 6     | 0.037|       | -2.171|       | -7.623|
| 6 | -9.946 | -0.368 | 2.062 | 1 | 0.162 | -3.281 | -7.605 |
|---|---|---|---|---|---|---|---|
| 6 | -8.821 | -1.183 | 1.97 | 1 | 0.552 | -1.818 | -8.541 |
| 1 | -8.929 | -2.246 | 2.147 | 6 | 0.869 | -2.404 | -5.462 |
| 6 | -7.568 | -0.641 | 1.637 | 1 | -0.068 | -2.834 | -5.061 |
| 6 | -6.403 | -1.588 | 1.46 | 1 | 1.508 | -3.244 | -5.822 |
| 1 | -6.307 | -2.171 | 2.4 | 6 | 1.652 | -1.715 | -4.351 |
| 1 | -5.433 | -1.064 | 1.34 | 1 | 2.603 | -1.35 | -4.802 |
| 6 | -6.659 | -2.061 | -1.066 | 6 | 1.954 | -2.468 | -3.608 |
| 6 | -6.656 | -2.516 | 0.285 | 6 | 1.544 | 0.565 | -3.586 |
| 6 | -7.011 | -3.848 | 0.555 | 6 | -0.518 | 1.727 | -3.2 |
| 1 | -7.025 | -4.219 | 1.572 | 6 | 0.873 | 1.732 | -3.277 |
| 6 | -7.386 | -4.71 | -0.473 | 6 | 1.583 | 2.95 | -3.257 |
| 6 | -7.425 | -4.258 | -1.788 | 1 | 2.658 | 2.899 | -3.35 |
| 1 | -7.738 | -4.941 | -2.568 | 6 | 0.948 | 4.148 | -3.206 |
| 6 | 7.206 | 2.351 | -1.188 | 6 | -0.458 | 4.148 | -3.09 |
| 6 | 8.122 | 2.399 | 0.018 | 1 | -0.99 | 5.087 | -3.015 |
| 1 | 7.557 | 2.026 | 0.896 | 6 | -1.195 | 2.954 | -3.088 |
| 1 | 8.419 | 3.444 | 0.252 | 6 | -2.677 | 3.022 | -2.848 |
| 6 | -8.851 | 2.714 | -1.458 | 1 | -3.026 | 4.073 | -2.758 |
| 6 | -9.349 | 3.213 | -0.235 | 1 | -2.886 | 2.523 | -1.879 |
| 6 | -10.586 | 3.874 | -0.206 | 6 | -4.511 | 1.589 | -3.685 |
| 1 | -10.977 | 4.27 | 0.723 | 1 | -4.836 | 1.237 | -2.714 |
| 6 | -11.34 | 4.013 | -1.37 | 6 | -5.104 | 1.383 | -4.857 |
| 6 | -10.879 | 3.481 | -2.573 | 6 | -6.376 | 0.624 | -5.069 |
| 1 | -11.499 | 3.577 | -3.455 | 1 | -6.141 | -0.336 | -5.58 |
| 6 | 10.91 | 2.905 | -0.387 | 1 | -7.047 | 1.229 | -5.718 |
| 6 | 11.045 | -1.806 | 0.661 | 30 | -0.727 | -1.001 | -2.589 |
| 1 | 12.032 | -1.841 | 1.174 | 1 | 12.927 | -5.208 | -1.896 |
| 1 | 10.248 | -1.788 | 1.425 | 1 | 11.92 | 1.481 | -2.52 |
| 6 | 9.712 | 0.483 | 0.572 | 1 | 9.414 | -0.774 | -5.905 |
| 6 | 10.84 | -0.418 | 0.079 | 1 | 6.029 | 4.402 | -3.636 |
| 6 | 11.625 | 0.004 | -0.997 | 1 | -10.906 | -0.8 | 2.313 |
| 1 | 12.452 | -0.603 | -1.342 | 1 | -7.662 | -5.732 | -0.245 |
| 6 | 11.314 | 1.179 | -1.675 | 1 | -12.296 | 4.519 | -1.335 |
| 6 | 10.198 | 1.939 | -1.324 | 1 | -11.758 | -1.711 | -3.751 |
| 1 | 9.961 | 2.812 | -1.92 | 15 | -1.098 | -0.461 | -0.355 |
| 6 | 9.38 | 1.591 | -0.236 | 15 | 0.048 | 1.015 | 1.658 |
| 6 | -8.572 | 3.02 | 1.048 | 8 | -1.037 | 1.145 | 0.302 |
| 1 | -9.004 | 3.627 | 1.873 | 8 | -2.24 | -0.552 | -1.649 |
| 1 | -7.535 | 3.389 | 0.9 | 8 | -1.286 | -1.848 | 0.703 |
| 6 | -5.638 | 1.725 | 2.435 | 8 | -0.018 | 2.456 | 2.644 |
| 1 | -5.326 | 0.831 | 3.017 | 8 | 1.63 | 1.122 | 0.925 |
| 1 | -6.358 | 2.322 | 3.043 | 8 | 0.277 | -0.648 | -1.097 |
| 6 | -4.426 | 2.585 | 2.219 | 8 | 0.091 | -0.442 | 2.672 |
| 6 | -3.889 | 2.958 | 1.054 | 6 | 2.804 | -2.591 | 6.381 |
| 1 | -4.242 | 2.685 | 0.068 | 6 | 2.183 | -2.114 | 7.717 |
|   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1 | 9.725 | -1.57 | 1.85 | 1 | -4.129 | -4.991 | 1.726 |
| 2 | 5.977 | -2.924 | -2.334 | 1 | -4.988 | 5.82 | 0.384 |
| 3 | 6.837 | 0.014 | -0.834 | 1 | -4.826 | -6.642 | 1.953 |
| 4 | 8.521 | -2.507 | -0.883 | 1 | 6.187 | -0.687 | -1.076 |
| 5 | -6.945 | 0.393 | -3.799 | 1 | 8.669 | -1.75 | -0.283 |
| 6 | -0.004 | -2.715 | -2.33 | 1 | -7.157 | 2.362 | -2.308 |
| 7 | -1.209 | 0.571 | -3.492 | 1 | -5.738 | -0.38 | -0.702 |
| 8 | -2.131 | -2.206 | -6.564 | 1 | -1.461 | 3.55 | -0.286 |
| 9 | 0.606 | -1.495 | -6.512 | 1 | -1.313 | -7.68 | 1.748 |
| 10 | 3.602 | -5.495 | -2.392 | 1 | 3.508 | 6.004 | 1.446 |
| 11 | 2.357 | -5.554 | -1.5 | 1 | 1.59 | 2.259 | 5.824 |
| 12 | 7.317 | -4.258 | -1.039 | 1 | -3.771 | -3.313 | -3.063 |
| 13 | -1.959 | -2.174 | -3.597 | 1 | 2.589 | 0.642 | -3.867 |
| 14 | 0.9 | -0.626 | -3.692 | 6 | -3.363 | -2.575 | 3.84 |
| 15 | -3.445 | 2.373 | -3.898 | 8 | -2.103 | -2.136 | 3.39 |
| 16 | -3.415 | 2.663 | -5.188 | 6 | -2.027 | -0.771 | 3.719 |
| 17 | -4.415 | 2.052 | -5.803 | 6 | -2.77 | -0.584 | 5.039 |
| 18 | 6.891 | -2.347 | -3.398 | 8 | -3.34 | 0.697 | 5.109 |
| 19 | 8.094 | -3.026 | -3.714 | 6 | -3.811 | -1.688 | 5.01 |
| 20 | 8.985 | -2.454 | -4.635 | 8 | -5.097 | -1.174 | 4.776 |
| 21 | 9.902 | -2.967 | -4.899 | 6 | -0.584 | -0.346 | 3.808 |
| 22 | 8.717 | -1.208 | -5.199 | 7 | -3.284 | -3.978 | 4.239 |
| 23 | 7.573 | -0.503 | -4.83 | 6 | -2.288 | -4.557 | 5.099 |
| 24 | 7.401 | 0.478 | -5.256 | 7 | -2.741 | -5.645 | 5.769 |
| 25 | 6.664 | -1.045 | -3.906 | 6 | -4.026 | -5.787 | 5.407 |
| 26 | 5.466 | -0.216 | -3.486 | 6 | -4.393 | -4.812 | 4.538 |
| 27 | 4.864 | -0.021 | -4.399 | 7 | -5.66 | -4.697 | 4.072 |
| 28 | 4.788 | -0.759 | -2.796 | 6 | -6.586 | -5.613 | 4.485 |
| 29 | 6.633 | 1.131 | -1.617 | 7 | -6.234 | -6.614 | 5.355 |
| 30 | 5.907 | 1.088 | -2.843 | 6 | -4.959 | -6.721 | 5.835 |
| 31 | 5.676 | 2.286 | -3.54 | 7 | -4.603 | -7.755 | 6.753 |
| 32 | 5.121 | 2.284 | -4.471 | 1 | -4.073 | -2.492 | 2.99 |
| 33 | 6.194 | 3.492 | -3.075 | 1 | -2.529 | -0.18 | 2.917 |
| 34 | 6.961 | 3.526 | -1.914 | 1 | -3.79 | -2.236 | 5.983 |
| 35 | 7.383 | 4.47 | -1.592 | 1 | -2.08 | -0.75 | 5.901 |
| 36 | -7.081 | -2.934 | -2.096 | 1 | -1.294 | -4.153 | 5.226 |
| 37 | -7.161 | -2.463 | -3.532 | 1 | -7.603 | -5.549 | 4.123 |
| 38 | -7.253 | -3.325 | -4.229 | 1 | -5.734 | -1.912 | 4.964 |
| 39 | -6.204 | -1.969 | -3.797 | 1 | -3.642 | 0.82 | 6.047 |
| 40 | 9.711 | -3.158 | -1.125 | 1 | -0.128 | -0.977 | 4.561 |
| 41 | 9.716 | -4.113 | -2.165 | 1 | -0.573 | 0.648 | 4.239 |
| 42 | 10.879 | -4.849 | -2.43 | 1 | -4.822 | -8.669 | 6.297 |
| 43 | 10.895 | -5.586 | -3.224 | 1 | -5.228 | -7.664 | 7.586 |
| 44 | 12.033 | -4.636 | -1.682 | 1 | -2.258 | -1.857 | 1.099 |
| 45 | 12.052 | -3.67 | -0.677 | 6 | -8.354 | -1.552 | -3.736 |
| 46 | 12.976 | -3.507 | -0.136 | 6 | 8.483 | -4.317 | -3.023 |
S32. Cartesian coordinates for MM minimized structure of [Zn$_2$L’ATP]$^{2-}$

| Z | X  | Y  | Z  | X  | Y  | Z  | X  |
|---|----|----|----|----|----|----|----|
| 30 | 1.8131 | -2.3326 | -2.3164 | 6 | 7.6111 | -0.2696 | 4.9106 |
| 8 | -5.8979 | -1.7566 | -1.3614 | 1 | 7.4061 | -1.2946 | 5.1956 |
| 8 | -5.8899 | -0.9096 | 1.9826 | 6 | 6.6921 | 0.4454 | 4.1236 |
| 8 | -7.9339 | -2.9636 | 0.5296 | 6 | 5.4421 | -0.2566 | 3.6346 |
| 8 | 9.0611 | -0.4166 | -2.1874 | 1 | 4.8711 | -0.5836 | 4.5306 |
| 8 | 1.2071 | -3.5926 | -1.0674 | 1 | 4.7591 | 0.4134 | 3.0746 |
| 8 | 3.0831 | -0.9816 | -2.4814 | 6 | 6.4731 | -1.2976 | 5.2226 |
| 8 | 5.3961 | -4.1226 | -4.0454 | 6 | 5.8051 | -1.4466 | 2.7686 |
| 8 | 3.5451 | -3.6316 | -6.1264 | 6 | 5.5831 | -2.7386 | 3.2736 |
| 7 | -3.9609 | -3.9586 | -3.2844 | 1 | 5.0681 | -2.8826 | 4.2156 |
| 7 | -2.9039 | -4.7286 | -2.8054 | 6 | 6.0651 | -3.8586 | 2.5976 |
| 7 | -2.4139 | -4.1086 | -1.6574 | 6 | 6.7951 | -3.7066 | 1.4206 |
| 7 | 3.3001 | -3.6596 | -2.0094 | 1 | 7.1951 | -4.5876 | 0.9346 |
| 7 | 1.8621 | -2.4956 | -4.2574 | 6 | -6.2939 | 1.0144 | 3.3776 |
| 7 | 5.4561 | 1.7724 | -1.8064 | 6 | -6.7979 | 0.1044 | 4.4736 |
| 7 | 6.1471 | 2.9754 | -1.6904 | 1 | -6.8339 | 0.6384 | 5.4486 |
| 7 | 7.4601 | 2.7434 | -2.0924 | 1 | -6.0639 | -0.7066 | 4.6056 |
| 6 | -6.8399 | -0.7226 | -1.4184 | 6 | 9.6401 | 2.9734 | 1.4976 |
| 6 | -8.1519 | -0.9876 | -1.8754 | 6 | 9.7731 | 3.6634 | 2.7226 |
| 6 | -9.0589 | 0.0734 | -2.0234 | 6 | 10.9961 | 4.2644 | 3.0526 |
| 1 | -10.0609 | -0.1096 | -2.3894 | 1 | 11.1121 | 4.8014 | 3.9856 |
| 6 | -8.6859 | 1.3734 | -1.6904 | 6 | 12.0831 | 4.1754 | 2.1846 |
| 6 | -7.4199 | 1.6244 | -1.1664 | 6 | 11.9701 | 3.4704 | 0.9876 |
| 1 | -7.1649 | 2.6373 | -0.8804 | 1 | 12.8381 | 3.3944 | 0.3446 |
| 6 | -6.4959 | 0.5804 | -0.9914 | 6 | -10.2889 | -3.3576 | 1.1656 |
| 6 | -5.1789 | 0.8824 | -0.3054 | 6 | -9.9889 | -3.4586 | 2.6506 |
| 1 | -4.6539 | 1.6704 | -0.8854 | 1 | -10.8559 | -3.8926 | 3.1956 |
| 1 | -4.4799 | 0.0224 | -0.3044 | 1 | -9.1629 | -4.1776 | 2.8246 |
| 6 | -5.8669 | 0.4814 | 2.1416 | 6 | -8.4389 | -1.7426 | 3.7466 |
| 6 | -5.4409 | 1.3604 | 1.1076 | 6 | -9.7129 | -2.0906 | 3.2416 |
|   | -5.4029 | 2.7434 | 1.3586 | 6 | -10.7529 | -1.1486 | 3.2816 |
|---|---|---|---|---|---|---|---|
| 1 | -5.0909 | 3.4344 | 0.5846 | 1 | -11.7419 | -1.4106 | 3.9266 |
| 6 | -5.8269 | 3.2564 | 2.5816 | 6 | -10.5239 | 0.1384 | 3.7596 |
| 6 | -6.2659 | 2.4004 | 3.5876 | 6 | -9.2489 | 0.5144 | 4.1756 |
| 1 | -6.5949 | 2.8204 | 4.5296 | 1 | -9.0819 | 1.5354 | 4.4966 |
| 6 | 7.0231 | -2.4306 | 0.8856 | 6 | -8.1869 | -0.4036 | 4.1486 |
| 6 | 7.8891 | -2.2786 | -0.3464 | 6 | 8.6101 | 3.7484 | 3.6866 |
| 1 | 7.2791 | -1.7996 | -1.1364 | 1 | 8.8671 | 4.3654 | 4.5746 |
| 1 | 8.2071 | -3.2706 | -0.7354 | 1 | 7.7741 | 4.2704 | 3.1746 |
| 6 | -9.2909 | -3.0446 | 0.2006 | 6 | 5.0921 | 3.2044 | 3.8966 |
| 6 | -9.6599 | -2.8156 | -1.1434 | 1 | 4.5781 | 2.4734 | 4.5596 |
| 6 | -10.9979 | -2.9736 | -1.5324 | 1 | 5.6001 | 3.9644 | 4.5306 |
| 1 | -11.2939 | -2.8106 | -2.5614 | 6 | 4.0591 | 3.8664 | 3.0476 |
| 6 | -11.9669 | -3.3306 | -0.5984 | 6 | 3.3011 | 3.2594 | 2.1266 |
| 6 | -11.6199 | -3.5126 | 0.7396 | 1 | 3.3711 | 2.2184 | 1.8346 |
| 1 | -12.4009 | -3.7546 | 1.4506 | 6 | 1.3761 | 3.8044 | 0.6876 |
| 6 | 10.7621 | 2.8464 | 0.6336 | 1 | 1.5631 | 4.4114 | -0.2244 |
| 6 | 10.7111 | 2.0234 | -0.6414 | 1 | 1.4111 | 2.7384 | 0.3746 |
| 1 | 9.8781 | 2.4254 | -1.2304 | 6 | -0.5829 | 3.3154 | 2.1626 |
| 1 | 11.6321 | 2.1704 | -1.2464 | 6 | 0.0191 | 4.1264 | 1.2676 |
| 6 | 9.4581 | -0.3366 | -0.8334 | 6 | -0.6779 | 5.3524 | 0.8096 |
| 6 | 10.5811 | 0.5414 | -0.3394 | 1 | -0.1669 | 5.9664 | 0.0846 |
| 6 | 11.4611 | 0.0004 | 0.6116 | 6 | -1.8859 | 5.6974 | 1.2066 |
| 1 | 12.3311 | 0.5594 | 0.9346 | 6 | -2.5199 | 4.7774 | 2.2916 |
| 6 | 11.1671 | -1.1956 | 1.2566 | 1 | -3.4909 | 5.0324 | 2.6926 |
| 6 | 9.9901 | -1.8826 | 0.9766 | 6 | -1.9189 | 3.6344 | 2.6726 |
| 1 | 9.7651 | -2.7796 | 1.5416 | 6 | -2.5069 | 2.8154 | 3.5466 |
| 6 | 9.1281 | -1.4606 | -0.0464 | 6 | -2.8769 | 0.7334 | 4.7186 |
| 6 | -8.6249 | -2.3946 | -2.1634 | 1 | -3.3179 | -0.1096 | 4.1476 |
| 1 | -9.0439 | -2.4226 | -3.1934 | 6 | -2.2229 | 0.2684 | 6.0086 |
| 1 | -7.7909 | -3.1266 | -2.1494 | 1 | -1.2869 | -0.2826 | 5.7746 |
| 6 | -5.1169 | -1.8466 | -2.5534 | 1 | -2.9309 | -0.4236 | 6.5166 |
| 1 | -4.5769 | -0.8896 | -2.7324 | 6 | -1.2449 | 0.9914 | 7.9846 |
| 1 | -5.7699 | -2.0566 | -3.4304 | 1 | -1.2919 | -0.1016 | 8.2106 |
| 6 | -4.1069 | -2.9386 | -2.4134 | 1 | -1.6829 | 1.5094 | 8.8636 |
| 6 | -3.2079 | -3.0386 | -1.4334 | 6 | 0.2121 | 1.4274 | 7.8526 |
| 1 | -3.1419 | -2.3866 | -0.5734 | 1 | 0.2611 | 2.5424 | 7.8096 |
| 6 | -1.4779 | -4.6926 | -0.7024 | 1 | 0.7491 | 1.1294 | 8.7776 |
| 1 | -2.0269 | -5.3936 | -0.0394 | 6 | 1.0141 | 1.6644 | 5.6826 |
| 6 | 0.9101 | -4.8606 | -1.5674 | 1 | 0.0471 | 2.0584 | 5.3146 |
| 6 | -0.3649 | -5.4336 | -1.3964 | 1 | 1.6431 | 2.5264 | 6.0046 |
| 6 | -0.5869 | -6.7496 | -1.8234 | 6 | 1.7661 | 0.9684 | 4.5546 |
| 1 | -1.5709 | -7.1806 | -1.6894 | 1 | 2.6851 | 0.5264 | 5.0066 |
| 6 | 0.4561 | -7.5176 | -2.3784 | 6 | 1.2141 | 1.7204 | 3.8366 |
| 6 | 1.7221 | -6.9016 | -2.4944 | 6 | 1.5421 | -1.2546 | 3.6546 |
| 1 | 2.5661 | -7.4416 | -2.9004 | 6 | -0.5079 | -2.2676 | 3.0686 |
|    |   6 | 1.9151 | -5.5636 | -2.1024 | 6 | 0.8731 | -2.3206 | 3.2126 |
|----|----|--------|---------|---------|---|--------|---------|--------|
|    | 6  | 3.1241 | -5.0026 | -2.1814 | 6 | 1.5451 | -3.5476 | 3.0306 |
|    | 6  | 4.6891 | -3.1836 | -1.9234 | 1 | 2.6161 | -3.5746 | 3.1866 |
|    | 1  | 5.3241 | -3.9276 | -1.3914 | 6 | 0.8871 | -4.6916 | 2.7126 |
|    | 1  | 4.7311 | -2.2646 | -1.3044 | 6 | -0.5199 | -4.6316 | 2.5606 |
|    | 6  | 5.2851 | -2.9186 | -3.3144 | 1 | -1.0949 | -5.5096 | 2.3096 |
|    | 1  | 4.6491 | -2.1916 | -3.8604 | 6 | -1.2179 | -3.4276 | 2.7346 |
|    | 1  | 6.2961 | -2.4756 | -3.1824 | 6 | -2.6959 | -3.3656 | 2.4616 |
|    | 6  | 5.8341 | -3.8616 | -5.3704 | 1 | -2.9769 | -4.1396 | 1.7166 |
|    | 1  | 6.7551 | -4.4546 | -5.5534 | 1 | -2.9619 | -2.3846 | 2.0116 |
|    | 1  | 6.1011 | -2.7956 | -5.5724 | 6 | -4.8069 | -3.8146 | 3.6266 |
|    | 6  | 4.7691 | -4.3016 | -6.3764 | 1 | -5.3209 | -4.2036 | 2.7566 |
|    | 1  | 5.1151 | -4.0166 | -7.3934 | 6 | -5.4039 | -3.3276 | 4.7156 |
|    | 1  | 4.6901 | -5.4156 | -6.3804 | 6 | -6.8849 | -3.2006 | 4.8766 |
|    | 6  | 2.6151 | -4.5096 | -5.5224 | 1 | -7.1319 | -2.5626 | 5.7546 |
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|    | 1  | 2.2231 | -5.2186 | -6.2844 | 30 | -0.6519 | 0.5384 | 2.7766 |
|    | 6  | 1.4341 | -3.7316 | -4.9324 | 1 | 13.0231 | 4.6434 | 2.4486 |
|    | 1  | 0.8711 | -4.3746 | -4.2334 | 1 | 11.8311 | -1.5646 | 2.0276 |
|    | 1  | 0.7201 | -3.4926 | -5.7514 | 1 | 9.5111 | -0.2456 | 5.9146 |
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|    | 6  | 2.8991 | 0.1064  | -3.3324 | 1 | -9.3909 | 2.1854 | -1.8114 |
|    | 6  | 2.2991 | -0.0556 | -4.5884 | 1 | -5.8249 | 4.3254 | 2.7496 |
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|    | 1  | 1.6721 | 0.9174  | -6.3864 | 1 | -11.3319| 0.8584 | 3.7786 |
|    | 6  | 2.4991 | 2.3634  | -4.9964 | 15 | -0.9639 | 0.2624 | 0.4506 |
|    | 6  | 3.1281 | 2.4884  | -3.7434 | 15 | 0.0971  | -0.9946 | -1.7534 |
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|    | 6  | 3.3371 | 1.3774  | -2.9174 | 8  | -2.1399 | 0.2794 | 1.7206 |
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|    | 6  | 3.6041 | 2.4794  | -1.0864 | 8  | 0.0961  | -2.3746 | -2.8274 |
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|    | 6  | 6.3341 | 0.8594  | -2.2694 | 8  | 0.3131  | 0.3294 | 1.2936 |
|    | 6  | 6.0871 | -0.1666 | -2.4964 | 8  | -0.0989 | 0.4894 | -2.6644 |
|    | 6  | 7.5291 | 1.4374  | -2.4254 | 6  | 2.2221  | 3.6294 | -5.8354 |
|    | 6  | 8.7571 | 0.7534  | -2.9484 | 6  | 1.5181  | 3.3284 | -7.1804 |
|    | 1  | 9.6331 | 1.4184  | -3.0564 | 6  | 3.5541  | 4.3434 | -6.1524 |
|    | 1  | 8.5251 | 0.4214  | -3.9824 | 1  | 4.0591  | 4.6974 | -5.2924 |
| 8  | 8  | 6.0401 | 2.5414  | 3.0626 | 1  | 4.2441  | 3.6534 | -6.6854 |
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| 8  | 8  | 8.3881 | 2.4294  | 1.1846 | 1  | 2.1491  | 2.6724 | -7.8194 |
| 8  | 8  | -7.4079 | -2.6816 | 3.6506 | 1  | 1.3351  | 4.2664 | -7.7484 |
| 8  | 8  | 0.1001 | 2.2504  | 2.7326 | 1  | 0.5321  | 2.8434 | -7.0124 |
| 8  | 8  | -1.1839 | -1.1156 | 3.4496 | 6  | 1.3051  | 4.5804 | -5.0344 |
| 8  | 8  | -1.9769 | 1.3834  | 6.8376 | 1  | 0.3571  | 4.0654 | -4.7614 |
| 8  | 8  | 0.8281 | 0.7694  | 6.7586 | 1  | 1.7921  | 4.9284 | -4.0994 |
|   |    |   |    |   |    |    |    |    |
|---|---|---|---|---|---|---|---|---|
| 7 | 3.6841 | 5.1544 | 3.1736 | 1 | 1.0521 | 5.4834 | -5.6324 |
| 7 | 2.6351 | 5.3224 | 2.2766 | 6 | 0.1871 | -8.9746 | -2.8064 |
| 7 | 2.4271 | 4.0924 | 1.6556 | 6 | -0.2619 | -9.7946 | -1.5774 |
| 7 | -1.9749 | 1.5224 | 3.8766 | 6 | 1.4311 | -9.6706 | -3.4084 |
| 7 | 0.9501 | -0.0396 | 3.8466 | 1 | 1.7871 | -9.1316 | -4.3134 |
| 7 | -3.4799 | -3.5676 | 3.6736 | 1 | 2.2551 | -9.7246 | -2.6634 |
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| 7 | -4.4949 | -2.7366 | 5.5136 | 1 | 0.5111 | -9.7476 | -0.7746 |
| 6 | 6.9681 | 1.7934 | 3.7966 | 1 | -0.4189 | -10.8606 | -1.8504 |
| 6 | 8.2081 | 2.3684 | 4.1596 | 1 | -1.2169 | -9.4146 | -1.1584 |
| 6 | 9.1121 | 1.6244 | 4.9346 | 6 | -0.9259 | -8.9996 | -3.8764 |
| 1 | 10.0611 | 2.0544 | 5.2306 | 1 | -0.6379 | -8.3746 | -4.7484 |
| 6 | 8.8071 | 0.3194 | 5.3176 | 1 | -1.1069 | -10.0366 | -4.2344 |
| 6 | -6.1209 | 4.2854 | -4.1034 | 1 | -1.8879 | -8.6166 | -3.4764 |
| 8 | -7.2889 | 3.8894 | -3.4304 | 6 | 1.6771 | -6.0156 | 2.5796 |
| 6 | -3.3639 | 1.8564 | -4.4084 | 6 | 2.2591 | -6.3986 | 3.9566 |
| 8 | -2.5419 | 1.3394 | -3.4264 | 6 | 2.8371 | -5.8486 | 1.5706 |
| 15 | -1.3909 | 0.3084 | -3.7734 | 1 | 2.4511 | -5.4686 | 0.6086 |
| 8 | -1.9939 | -1.0786 | -3.7774 | 1 | 3.6051 | -5.1396 | 1.9346 |
| 8 | -0.8669 | 0.6014 | -5.1604 | 1 | 3.3501 | -6.8176 | 1.3856 |
| 7 | -4.2309 | 5.7634 | -3.6194 | 1 | 2.9711 | -5.6296 | 4.3226 |
| 6 | -2.8199 | 5.7674 | -3.8844 | 1 | 2.8071 | -7.3646 | 3.8976 |
| 7 | -2.2889 | 7.0074 | -3.7884 | 1 | 1.4441 | -6.5026 | 4.7046 |
| 6 | -3.3059 | 7.8124 | -3.4404 | 6 | 0.8051 | -7.1966 | 2.0856 |
| 6 | -4.4279 | 7.1374 | -3.3134 | 1 | 0.3461 | -6.9616 | 1.1006 |
| 7 | -5.5869 | 7.7194 | -2.9134 | 1 | 1.4171 | -8.1156 | 1.9596 |
| 6 | -5.5839 | 9.0574 | -2.6424 | 1 | 0.0051 | -7.4356 | 2.8186 |
| 7 | -4.4289 | 9.7804 | -2.7694 | 6 | -2.6369 | 6.9774 | 0.8866 |
| 6 | -3.2699 | 9.1784 | -3.1674 | 6 | -2.9309 | 7.8364 | 2.1356 |
| 7 | -2.0619 | 9.9324 | -3.2744 | 1 | -1.9859 | 8.0824 | 2.6666 |
| 1 | -5.4839 | 4.9504 | -2.1304 | 1 | -3.4299 | 8.7884 | 1.8506 |
| 1 | -5.1529 | 1.7394 | -3.2124 | 1 | 3.6039 | 7.3124 | 2.8456 |
| 1 | -6.3479 | 5.1164 | -4.8124 | 6 | -1.8429 | 7.8604 | -0.1084 |
| 1 | -4.9179 | 3.4974 | -5.7034 | 1 | 1.6399 | 7.3104 | -1.0514 |
| 1 | -2.2349 | 4.8844 | -4.1024 | 1 | -2.4199 | 8.7734 | -0.3704 |
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| 1 | -3.7109 | 1.0424 | -5.0854 | 1 | 6.0441 | 0.6824 | 1.2726 |
| 1 | -2.0589 | 10.9524 | -3.0494 | 1 | 8.3311 | 1.9394 | 0.3086 |
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| 1 | 0.093 | 0.5985 | -5.147 | 1 | -5.4569 | -1.2626 | 1.1446 |
| 1 | -0.122 | 2.07 | -0.5829 | 1 | -1.0609 | -3.8906 | -0.0624 |
| 1 | 2.5851 | -1.3866 | 3.9226 | 1 | -0.8799 | 8.1894 | 0.3376 |
| 6 | -5.0279 | 4.6504 | -3.1004 | 1 | 3.9841 | -5.6326 | -2.3904 |

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|   |      |      |      | 1   |      |      |
|---|------|------|------|-----|------|------|
| 8 | -4.1999 | 3.5264 | -2.8794 | 1   | 1.5451 | -1.3716 | -6.0884 |
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