**NBO Analysis Data of NiL complex ($L^{2-}$ is double deprotonated form of 3,10-dithio-6,7,13,14-tetramethyl-1,2,4,5,8,9,11,12-octaazacyclotetradecatetraene-1,5,7,12)**

**DFT B3PW91/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 132.3 кДж/моль**

**Alpha occupied eigenvalues (highest) = -5.6697477 eV**
**Alpha virtual eigenvalues (lowest) = -3.091056 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Ni | 1 | 0.37942 | 17.99148 | 9.61737 | 0.01174 | 27.62058 |
| N | 2 | -0.31645 | 1.99918 | 5.28260 | 0.03466 | 7.31645 |
| N | 3 | -0.18726 | 1.99907 | 5.15745 | 0.03074 | 7.18726 |
| N | 4 | -0.31649 | 1.99918 | 5.28264 | 0.03466 | 7.31649 |
| N | 5 | -0.18726 | 1.99907 | 5.15745 | 0.03075 | 7.18726 |
| N | 6 | -0.39196 | 1.99939 | 5.37012 | 0.02245 | 7.39196 |
| N | 7 | -0.39199 | 1.99939 | 5.37015 | 0.02245 | 7.39199 |
| H | 8 | 0.41893 | 0.00000 | 0.57800 | 0.00307 | 0.58107 |
| H | 9 | 0.41895 | 0.00000 | 0.57798 | 0.00307 | 0.58105 |
| C | 10 | 0.18589 | 1.99941 | 3.78055 | 0.03414 | 5.81411 |
| C | 11 | 0.18591 | 1.99941 | 3.78054 | 0.03414 | 5.81409 |
| S | 12 | -0.14926 | 9.99902 | 6.12918 | 0.02106 | 16.14926 |
| S | 13 | -0.14929 | 9.99902 | 6.12921 | 0.02106 | 16.14929 |
| N | 14 | -0.14289 | 1.99930 | 5.12059 | 0.02300 | 7.14289 |
| N | 15 | -0.14286 | 1.99930 | 5.12056 | 0.02300 | 7.14286 |
| C | 16 | 0.20388 | 1.99918 | 3.77647 | 0.02047 | 5.79612 |
| C | 17 | 0.20390 | 1.99918 | 3.77645 | 0.02047 | 5.79610 |
| C | 18 | 0.11132 | 1.99921 | 3.86598 | 0.02350 | 5.88868 |
| C | 19 | 0.11131 | 1.99921 | 3.86598 | 0.02350 | 5.88869 |
| C | 20 | -0.68313 | 1.99941 | 4.67541 | 0.00831 | 6.68313 |
| H | 21 | 0.23468 | 0.00000 | 0.76354 | 0.00178 | 0.76532 |
| H | 22 | 0.23466 | 0.00000 | 0.76356 | 0.00178 | 0.76534 |
| H | 23 | 0.25018 | 0.00000 | 0.74868 | 0.00114 | 0.74982 |
| C | 24 | -0.63903 | 1.99942 | 4.63163 | 0.00799 | 6.63903 |
| H | 25 | 0.21362 | 0.00000 | 0.78501 | 0.00137 | 0.78638 |
| H | 26 | 0.21362 | 0.00000 | 0.78501 | 0.00137 | 0.78638 |
| H | 27 | 0.25351 | 0.00000 | 0.74518 | 0.00131 | 0.74649 |
| C | 28 | -0.63904 | 1.99942 | 4.63163 | 0.00799 | 6.63904 |
| H | 29 | 0.21362 | 0.00000 | 0.78501 | 0.00137 | 0.78638 |
| H | 30 | 0.25351 | 0.00000 | 0.74517 | 0.00131 | 0.74649 |
| H | 31 | 0.21362 | 0.00000 | 0.78501 | 0.00137 | 0.78638 |
| C | 32 | -0.68312 | 1.99941 | 4.67540 | 0.00831 | 6.68312 |
| H | 33 | 0.23468 | 0.00000 | 0.76354 | 0.00178 | 0.76532 |
| H | 34 | 0.23466 | 0.00000 | 0.76356 | 0.00178 | 0.76534 |
| H | 35 | 0.25018 | 0.00000 | 0.74868 | 0.00114 | 0.74982 |
| * Total * | | -0.00000 | 73.97666 | 115.53529 | 0.48806 | 190.00000 |

**M06/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 148.7 кДж/моль**

**Alpha occupied eigenvalues (highest) = -5.888244 eV**
**Alpha virtual eigenvalues (lowest) = -2.8456218 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Ni | 1 | 0.38236 | 17.99170 | 9.61426 | 0.01167 | 27.61764 |
| N | 2 | -0.33535 | 1.99918 | 5.30298 | 0.03319 | 7.33535 |
| N | 3 | -0.19794 | 1.99906 | 5.16945 | 0.02943 | 7.19794 |
| N | 4 | -0.33539 | 1.99918 | 5.30303 | 0.03318 | 7.33539 |
| N | 5 | -0.19794 | 1.99906 | 5.16945 | 0.02943 | 7.19794 |
| N | 6 | -0.40747 | 1.99939 | 5.38632 | 0.02177 | 7.40747 |
| N | 7 | -0.40750 | 1.99939 | 5.38634 | 0.02177 | 7.40750 |
| H | 8 | 0.41423 | 0.00000 | 0.58283 | 0.00294 | 0.58577 |
| H | 9 | 0.41425 | 0.00000 | 0.58281 | 0.00294 | 0.58575 |
| C | 10 | 0.21038 | 1.99941 | 3.75606 | 0.03415 | 5.78962 |
| C | 11 | 0.21038 | 1.99941 | 3.75605 | 0.03415 | 5.78962 |
| S | 12 | -0.14902 | 9.99903 | 6.12940 | 0.02058 | 16.14902 |
| S | 13 | -0.14904 | 9.99903 | 6.12943 | 0.02058 | 16.14904 |
| N | 14 | -0.14646 | 1.99928 | 5.12375 | 0.02342 | 7.14646 |
| N | 15 | -0.14643 | 1.99929 | 5.12372 | 0.02342 | 7.14643 |
| C | 16 | 0.22884 | 1.99917 | 3.75193 | 0.02006 | 5.77116 |
| C | 17 | 0.22887 | 1.99917 | 3.75191 | 0.02006 | 5.77113 |
| C | 18 | 0.12195 | 1.99918 | 3.85654 | 0.02233 | 5.87805 |
| C | 19 | 0.12195 | 1.99918 | 3.85654 | 0.02233 | 5.87805 |
| C | 20 | -0.67040 | 1.99939 | 4.66275 | 0.00826 | 6.67040 |
| H | 21 | 0.23019 | 0.00000 | 0.76803 | 0.00178 | 0.76981 |
| H | 22 | 0.23017 | 0.00000 | 0.76805 | 0.00178 | 0.76983 |
| H | 23 | 0.24303 | 0.00000 | 0.75594 | 0.00103 | 0.75697 |
| C | 24 | -0.62323 | 1.99940 | 4.61605 | 0.00778 | 6.62323 |
| H | 25 | 0.20675 | 0.00000 | 0.79185 | 0.00140 | 0.79325 |
| H | 26 | 0.20676 | 0.00000 | 0.79185 | 0.00140 | 0.79324 |
| H | 27 | 0.24640 | 0.00000 | 0.75235 | 0.00125 | 0.75360 |
| C | 28 | -0.62324 | 1.99940 | 4.61606 | 0.00778 | 6.62324 |
| H | 29 | 0.20676 | 0.00000 | 0.79184 | 0.00140 | 0.79324 |
| H | 30 | 0.24641 | 0.00000 | 0.75234 | 0.00125 | 0.75359 |
| H | 31 | 0.20676 | 0.00000 | 0.79185 | 0.00140 | 0.79324 |
| C | 32 | -0.67040 | 1.99939 | 4.66275 | 0.00826 | 6.67040 |
| H | 33 | 0.23019 | 0.00000 | 0.76803 | 0.00178 | 0.76981 |
| H | 34 | 0.23017 | 0.00000 | 0.76805 | 0.00178 | 0.76983 |
| H | 35 | 0.24303 | 0.00000 | 0.75594 | 0.00103 | 0.75697 |
| * Total * | | -0.00000 | 73.97668 | 115.54653 | 0.47679 | 190.00000 |

**OPBE/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 101.6 кДж/моль**

**Alpha occupied eigenvalues (highest) = -4.7005275 eV**
**Alpha virtual eigenvalues (lowest) = -3.4847847 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Ni | 1 | 0.31367 | 17.99128 | 9.68066 | 0.01439 | 27.68633 |
| N | 2 | -0.26538 | 1.99921 | 5.23324 | 0.03293 | 7.26538 |
| N | 3 | -0.17255 | 1.99910 | 5.14287 | 0.03058 | 7.17255 |
| N | 4 | -0.26545 | 1.99921 | 5.23331 | 0.03292 | 7.26545 |
| N | 5 | -0.17254 | 1.99910 | 5.14286 | 0.03058 | 7.17254 |
| N | 6 | -0.36457 | 1.99940 | 5.34487 | 0.02031 | 7.36457 |
| N | 7 | -0.36459 | 1.99940 | 5.34489 | 0.02031 | 7.36459 |
| H | 8 | 0.42115 | 0.00000 | 0.57555 | 0.00331 | 0.57885 |
| H | 9 | 0.42117 | 0.00000 | 0.57552 | 0.00331 | 0.57883 |
| C | 10 | 0.13375 | 1.99942 | 3.83568 | 0.03116 | 5.86625 |
| C | 11 | 0.13379 | 1.99942 | 3.83563 | 0.03116 | 5.86621 |
| S | 12 | -0.12198 | 9.99901 | 6.10353 | 0.01944 | 16.12198 |
| S | 13 | -0.12206 | 9.99901 | 6.10361 | 0.01943 | 16.12206 |
| N | 14 | -0.12851 | 1.99933 | 5.10737 | 0.02181 | 7.12851 |
| N | 15 | -0.12847 | 1.99933 | 5.10734 | 0.02181 | 7.12847 |
| C | 16 | 0.16403 | 1.99919 | 3.81760 | 0.01918 | 5.83597 |
| C | 17 | 0.16404 | 1.99919 | 3.81759 | 0.01918 | 5.83596 |
| C | 18 | 0.09909 | 1.99921 | 3.88012 | 0.02158 | 5.90091 |
| C | 19 | 0.09909 | 1.99921 | 3.88012 | 0.02158 | 5.90091 |
| C | 20 | -0.70424 | 1.99940 | 4.69778 | 0.00705 | 6.70424 |
| H | 21 | 0.24029 | 0.00000 | 0.75789 | 0.00182 | 0.75971 |
| H | 22 | 0.24028 | 0.00000 | 0.75790 | 0.00182 | 0.75972 |
| H | 23 | 0.25924 | 0.00000 | 0.73956 | 0.00121 | 0.74076 |
| C | 24 | -0.66552 | 1.99942 | 4.65944 | 0.00667 | 6.66552 |
| H | 25 | 0.22384 | 0.00000 | 0.77477 | 0.00139 | 0.77616 |
| H | 26 | 0.22384 | 0.00000 | 0.77477 | 0.00139 | 0.77616 |
| H | 27 | 0.26044 | 0.00000 | 0.73814 | 0.00143 | 0.73956 |
| C | 28 | -0.66553 | 1.99942 | 4.65944 | 0.00667 | 6.66553 |
| H | 29 | 0.22385 | 0.00000 | 0.77477 | 0.00139 | 0.77615 |
| H | 30 | 0.26044 | 0.00000 | 0.73813 | 0.00143 | 0.73956 |
| H | 31 | 0.22384 | 0.00000 | 0.77477 | 0.00139 | 0.77616 |
| C | 32 | -0.70423 | 1.99940 | 4.69777 | 0.00705 | 6.70423 |
| H | 33 | 0.24028 | 0.00000 | 0.75789 | 0.00182 | 0.75972 |
| H | 34 | 0.24027 | 0.00000 | 0.75791 | 0.00182 | 0.75973 |
| H | 35 | 0.25922 | 0.00000 | 0.73957 | 0.00121 | 0.74078 |
| * Total * | | -0.00000 | 73.97666 | 115.56284 | 0.46049 | 190.00000 |

**NBO Analysis Data of CuL complex ($L^{2-}$ is double deprotonated form of 3,10-dithio-6,7,13,14-tetramethyl-1,2,4,5,8,9,11,12-octaazacyclotetradecatetraene-1,5,7,12)**

**DFT B3PW91/TZVP level**

**ΔE(multipl.=2) = 0.0 кДж/моль**
**ΔE(multipl.=4) = 144.7 кДж/моль**

**Alpha occupied eigenvalues (highest) = -5.8327356 eV**
**Alpha virtual eigenvalues (lowest) = -3.0589482 eV**
**Beta occupied eigenvalues (highest) = -5.7891996 eV**
**Beta virtual eigenvalues (lowest) = -3.0439827 eV**

**<S**2> = 0.7500**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Cu | 1 | 0.72967 | 17.99418 | 10.26765 | 0.00850 | 28.27033 |
| N | 2 | -0.41057 | 1.99926 | 5.37391 | 0.03740 | 7.41057 |
| N | 3 | -0.25679 | 1.99917 | 5.22545 | 0.03217 | 7.25679 |
| N | 4 | -0.41057 | 1.99926 | 5.37391 | 0.03740 | 7.41057 |
| N | 5 | -0.25679 | 1.99917 | 5.22545 | 0.03217 | 7.25679 |
| N | 6 | -0.39158 | 1.99942 | 5.36907 | 0.02309 | 7.39158 |
| N | 7 | -0.39158 | 1.99942 | 5.36907 | 0.02309 | 7.39158 |
| H | 8 | 0.41419 | 0.00000 | 0.58254 | 0.00327 | 0.58581 |
| H | 9 | 0.41419 | 0.00000 | 0.58254 | 0.00327 | 0.58581 |
| C | 10 | 0.18775 | 1.99943 | 3.78004 | 0.03278 | 5.81225 |
| C | 11 | 0.18775 | 1.99943 | 3.78004 | 0.03278 | 5.81225 |
| S | 12 | -0.15300 | 9.99902 | 6.13314 | 0.02085 | 16.15300 |
| S | 13 | -0.15300 | 9.99902 | 6.13314 | 0.02085 | 16.15300 |
| N | 14 | -0.15319 | 1.99930 | 5.12955 | 0.02434 | 7.15319 |
| N | 15 | -0.15319 | 1.99930 | 5.12955 | 0.02434 | 7.15319 |
| C | 16 | 0.20539 | 1.99919 | 3.77425 | 0.02117 | 5.79461 |
| C | 17 | 0.20539 | 1.99919 | 3.77425 | 0.02117 | 5.79461 |
| C | 18 | 0.12140 | 1.99923 | 3.85582 | 0.02355 | 5.87860 |
| C | 19 | 0.12140 | 1.99923 | 3.85582 | 0.02355 | 5.87860 |
| C | 20 | -0.68618 | 1.99941 | 4.67831 | 0.00846 | 6.68618 |
| H | 21 | 0.23461 | 0.00000 | 0.76361 | 0.00178 | 0.76539 |
| H | 22 | 0.23453 | 0.00000 | 0.76369 | 0.00178 | 0.76547 |
| H | 23 | 0.24880 | 0.00000 | 0.75001 | 0.00119 | 0.75120 |
| C | 24 | -0.63951 | 1.99942 | 4.63209 | 0.00801 | 6.63951 |
| H | 25 | 0.21294 | 0.00000 | 0.78569 | 0.00137 | 0.78706 |
| H | 26 | 0.21294 | 0.00000 | 0.78569 | 0.00137 | 0.78706 |
| H | 27 | 0.25345 | 0.00000 | 0.74519 | 0.00136 | 0.74655 |
| C | 28 | -0.63951 | 1.99942 | 4.63209 | 0.00801 | 6.63951 |
| H | 29 | 0.21294 | 0.00000 | 0.78569 | 0.00137 | 0.78706 |
| H | 30 | 0.25345 | 0.00000 | 0.74519 | 0.00136 | 0.74655 |
| H | 31 | 0.21294 | 0.00000 | 0.78569 | 0.00137 | 0.78706 |
| C | 32 | -0.68618 | 1.99941 | 4.67831 | 0.00846 | 6.68618 |
| H | 33 | 0.23461 | 0.00000 | 0.76361 | 0.00178 | 0.76539 |
| H | 34 | 0.23453 | 0.00000 | 0.76369 | 0.00178 | 0.76547 |
| H | 35 | 0.24880 | 0.00000 | 0.75001 | 0.00119 | 0.75120 |
| * Total * | | -0.00000 | 73.97986 | 116.52379 | 0.49635 | 191.00000 |

**M06/TZVP level**

**ΔE(multipl.=2) = 0.0 кДж/моль**
**ΔE(multipl.=4) = 200.1 кДж/моль**

**Alpha occupied eigenvalues (highest) = -6.0000771 eV**
**Alpha virtual eigenvalues (lowest) = -2.8067115 eV**
**Beta occupied eigenvalues (highest) = -5.9862 eV**
**Beta virtual eigenvalues (lowest) = -2.7925623 eV**

**<S**2> = 0.7500**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Cu | 1 | 0.71114 | 17.99425 | 10.28591 | 0.00871 | 28.28886 |
| N | 2 | -0.42463 | 1.99925 | 5.38941 | 0.03598 | 7.42463 |
| N | 3 | -0.26202 | 1.99915 | 5.23179 | 0.03108 | 7.26202 |
| N | 4 | -0.42463 | 1.99925 | 5.38941 | 0.03598 | 7.42463 |
| N | 5 | -0.26202 | 1.99915 | 5.23179 | 0.03108 | 7.26202 |
| N | 6 | -0.40705 | 1.99942 | 5.38522 | 0.02240 | 7.40705 |
| N | 7 | -0.40705 | 1.99942 | 5.38522 | 0.02240 | 7.40705 |
| H | 8 | 0.40930 | 0.00000 | 0.58754 | 0.00316 | 0.59070 |
| H | 9 | 0.40930 | 0.00000 | 0.58754 | 0.00316 | 0.59070 |
| C | 10 | 0.21228 | 1.99942 | 3.75534 | 0.03296 | 5.78772 |
| C | 11 | 0.21228 | 1.99942 | 3.75534 | 0.03296 | 5.78772 |
| S | 12 | -0.15245 | 9.99903 | 6.13310 | 0.02032 | 16.15245 |
| S | 13 | -0.15245 | 9.99903 | 6.13310 | 0.02032 | 16.15245 |
| N | 14 | -0.15706 | 1.99928 | 5.13287 | 0.02491 | 7.15706 |
| N | 15 | -0.15706 | 1.99928 | 5.13287 | 0.02491 | 7.15706 |
| C | 16 | 0.22830 | 1.99917 | 3.75172 | 0.02081 | 5.77170 |
| C | 17 | 0.22830 | 1.99917 | 3.75172 | 0.02081 | 5.77170 |
| C | 18 | 0.13430 | 1.99920 | 3.84415 | 0.02235 | 5.86570 |
| C | 19 | 0.13430 | 1.99920 | 3.84415 | 0.02235 | 5.86570 |
| C | 20 | -0.67328 | 1.99939 | 4.66545 | 0.00844 | 6.67328 |
| H | 21 | 0.22990 | 0.00000 | 0.76832 | 0.00178 | 0.77010 |
| H | 22 | 0.22989 | 0.00000 | 0.76833 | 0.00178 | 0.77011 |
| H | 23 | 0.24171 | 0.00000 | 0.75722 | 0.00107 | 0.75829 |
| C | 24 | -0.62377 | 1.99940 | 4.61659 | 0.00778 | 6.62377 |
| H | 25 | 0.20633 | 0.00000 | 0.79228 | 0.00139 | 0.79367 |
| H | 26 | 0.20633 | 0.00000 | 0.79228 | 0.00139 | 0.79367 |
| H | 27 | 0.24635 | 0.00000 | 0.75236 | 0.00129 | 0.75365 |
| C | 28 | -0.62377 | 1.99940 | 4.61659 | 0.00778 | 6.62377 |
| H | 29 | 0.20633 | 0.00000 | 0.79228 | 0.00139 | 0.79367 |
| H | 30 | 0.24635 | 0.00000 | 0.75236 | 0.00129 | 0.75365 |
| H | 31 | 0.20633 | 0.00000 | 0.79228 | 0.00139 | 0.79367 |
| C | 32 | -0.67328 | 1.99939 | 4.66545 | 0.00844 | 6.67328 |
| H | 33 | 0.22992 | 0.00000 | 0.76830 | 0.00178 | 0.77008 |
| H | 34 | 0.22988 | 0.00000 | 0.76834 | 0.00178 | 0.77012 |
| H | 35 | 0.24171 | 0.00000 | 0.75722 | 0.00107 | 0.75829 |
| * Total * | | -0.00000 | 73.97968 | 116.53380 | 0.48652 | 191.00000 |

**OPBE/TZVP level**

**ΔE(multipl.=2) = 0.0 кДж/моль**
**ΔE(multipl.=4) = 120.7 кДж/моль**

**Alpha occupied eigenvalues (highest) = -4.1971425 eV**
**Alpha virtual eigenvalues (lowest) = -3.4787985 eV**
**Beta occupied eigenvalues (highest) = -4.9995654 eV**
**Beta virtual eigenvalues (lowest) = -3.4499559 eV**

**<S**2> = 0.7500**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population | | | |
|---|---|---|---|---|---|---|
| | | | Core | Valence | Rydberg | Total |
| Cu | 1 | 0.67173 | 17.99426 | 10.32433 | 0.00967 | 28.32827 |
| N | 2 | -0.36379 | 1.99929 | 5.32896 | 0.03554 | 7.36379 |
| N | 3 | -0.24518 | 1.99921 | 5.21408 | 0.03190 | 7.24518 |
| N | 4 | -0.36379 | 1.99929 | 5.32896 | 0.03554 | 7.36379 |
| N | 5 | -0.24519 | 1.99921 | 5.21409 | 0.03190 | 7.24519 |
| N | 6 | -0.36106 | 1.99943 | 5.34078 | 0.02085 | 7.36106 |
| N | 7 | -0.36106 | 1.99943 | 5.34078 | 0.02085 | 7.36106 |
| H | 8 | 0.41489 | 0.00000 | 0.58153 | 0.00358 | 0.58511 |
| H | 9 | 0.41489 | 0.00000 | 0.58153 | 0.00358 | 0.58511 |
| C | 10 | 0.13772 | 1.99944 | 3.83311 | 0.02973 | 5.86228 |
| C | 11 | 0.13772 | 1.99944 | 3.83311 | 0.02973 | 5.86228 |
| S | 12 | -0.12675 | 9.99901 | 6.10849 | 0.01924 | 16.12675 |
| S | 13 | -0.12675 | 9.99901 | 6.10849 | 0.01924 | 16.12675 |
| N | 14 | -0.13880 | 1.99933 | 5.11639 | 0.02308 | 7.13880 |
| N | 15 | -0.13880 | 1.99933 | 5.11639 | 0.02308 | 7.13880 |
| C | 16 | 0.16882 | 1.99920 | 3.81221 | 0.01978 | 5.83118 |
| C | 17 | 0.16882 | 1.99920 | 3.81221 | 0.01978 | 5.83118 |
| C | 18 | 0.10783 | 1.99924 | 3.87124 | 0.02169 | 5.89217 |
| C | 19 | 0.10783 | 1.99924 | 3.87124 | 0.02169 | 5.89217 |
| C | 20 | -0.70753 | 1.99941 | 4.70093 | 0.00719 | 6.70753 |
| H | 21 | 0.24026 | 0.00000 | 0.75794 | 0.00180 | 0.75974 |
| H | 22 | 0.24026 | 0.00000 | 0.75792 | 0.00181 | 0.75974 |
| H | 23 | 0.25727 | 0.00000 | 0.74144 | 0.00129 | 0.74273 |
| C | 24 | -0.66621 | 1.99942 | 4.66011 | 0.00668 | 6.66621 |
| H | 25 | 0.22305 | 0.00000 | 0.77556 | 0.00140 | 0.77695 |
| H | 26 | 0.22301 | 0.00000 | 0.77559 | 0.00140 | 0.77699 |
| H | 27 | 0.26034 | 0.00000 | 0.73815 | 0.00150 | 0.73966 |
| C | 28 | -0.66621 | 1.99942 | 4.66011 | 0.00668 | 6.66621 |
| H | 29 | 0.22301 | 0.00000 | 0.77559 | 0.00140 | 0.77699 |
| H | 30 | 0.26034 | 0.00000 | 0.73815 | 0.00150 | 0.73966 |
| H | 31 | 0.22305 | 0.00000 | 0.77555 | 0.00140 | 0.77695 |
| C | 32 | -0.70753 | 1.99941 | 4.70093 | 0.00719 | 6.70753 |
| H | 33 | 0.24025 | 0.00000 | 0.75795 | 0.00180 | 0.75975 |
| H | 34 | 0.24027 | 0.00000 | 0.75792 | 0.00181 | 0.75973 |
| H | 35 | 0.25727 | 0.00000 | 0.74144 | 0.00129 | 0.74273 |
| * Total * | | -0.00000 | 73.98022 | 116.55321 | 0.46658 | 191.00000 |

**NBO Analysis Data of ZnL complex ($L^{2-}$ is double deprotonated form of 3,10-dithio-6,7,13,14-tetramethyl-1,2,4,5,8,9,11,12-octaazacyclotetradecatetraene-1,5,7,12)**

**DFT B3PW91/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 146.7 кДж/моль**

**Alpha occupied eigenvalues (highest) = -5.8623945 eV**
**Alpha virtual eigenvalues (lowest) = -3.0096981 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Zn | 1 | 1.08887 | 17.99585 | 10.90968 | 0.00560 | 28.91113 |
| N | 2 | -0.50842 | 1.99930 | 5.47319 | 0.03594 | 7.50842 |
| N | 3 | -0.32125 | 1.99925 | 5.29207 | 0.02992 | 7.32125 |
| N | 4 | -0.50859 | 1.99930 | 5.47335 | 0.03594 | 7.50859 |
| N | 5 | -0.32140 | 1.99925 | 5.29221 | 0.02993 | 7.32140 |
| N | 6 | -0.39133 | 1.99944 | 5.36821 | 0.02368 | 7.39133 |
| N | 7 | -0.39145 | 1.99944 | 5.36835 | 0.02366 | 7.39145 |
| H | 8 | 0.41099 | 0.00000 | 0.58556 | 0.00345 | 0.58901 |
| H | 9 | 0.41097 | 0.00000 | 0.58558 | 0.00345 | 0.58903 |
| C | 10 | 0.18945 | 1.99942 | 3.77739 | 0.03373 | 5.81055 |
| C | 11 | 0.18957 | 1.99942 | 3.77727 | 0.03374 | 5.81043 |
| S | 12 | -0.15278 | 9.99901 | 6.13292 | 0.02085 | 16.15278 |
| S | 13 | -0.15288 | 9.99901 | 6.13303 | 0.02084 | 16.15288 |
| N | 14 | -0.17131 | 1.99931 | 5.14692 | 0.02508 | 7.17131 |
| N | 15 | -0.17125 | 1.99931 | 5.14687 | 0.02507 | 7.17125 |
| C | 16 | 0.20292 | 1.99919 | 3.77624 | 0.02165 | 5.79708 |
| C | 17 | 0.20297 | 1.99919 | 3.77619 | 0.02166 | 5.79703 |
| C | 18 | 0.13212 | 1.99924 | 3.84504 | 0.02360 | 5.86788 |
| C | 19 | 0.13204 | 1.99924 | 3.84513 | 0.02359 | 5.86796 |
| C | 20 | -0.68905 | 1.99941 | 4.68118 | 0.00846 | 6.68905 |
| H | 21 | 0.23419 | 0.00000 | 0.76404 | 0.00177 | 0.76581 |
| H | 22 | 0.23416 | 0.00000 | 0.76407 | 0.00177 | 0.76584 |
| H | 23 | 0.24757 | 0.00000 | 0.75120 | 0.00122 | 0.75243 |
| C | 24 | -0.63989 | 1.99942 | 4.63243 | 0.00804 | 6.63989 |
| H | 25 | 0.21231 | 0.00000 | 0.78632 | 0.00137 | 0.78769 |
| H | 26 | 0.21232 | 0.00000 | 0.78632 | 0.00137 | 0.78768 |
| H | 27 | 0.25377 | 0.00000 | 0.74485 | 0.00139 | 0.74623 |
| C | 28 | -0.63991 | 1.99942 | 4.63246 | 0.00804 | 6.63991 |
| H | 29 | 0.21231 | 0.00000 | 0.78632 | 0.00137 | 0.78769 |
| H | 30 | 0.25377 | 0.00000 | 0.74484 | 0.00139 | 0.74623 |
| H | 31 | 0.21231 | 0.00000 | 0.78633 | 0.00137 | 0.78769 |
| C | 32 | -0.68908 | 1.99941 | 4.68122 | 0.00845 | 6.68908 |
| H | 33 | 0.23420 | 0.00000 | 0.76403 | 0.00177 | 0.76580 |
| H | 34 | 0.23418 | 0.00000 | 0.76405 | 0.00177 | 0.76582 |
| H | 35 | 0.24758 | 0.00000 | 0.75120 | 0.00122 | 0.75242 |
| * Total * | | -0.00000 | 73.98183 | 117.52606 | 0.49211 | 192.00000 |

**M06/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 157.3 кДж/моль**

**Alpha occupied eigenvalues (highest) = -6.0585786 eV**
**Alpha virtual eigenvalues (lowest) = -2.7356934 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Zn | 1 | 1.07174 | 17.99587 | 10.92718 | 0.00521 | 28.92826 |
| N | 2 | -0.52395 | 1.99928 | 5.49017 | 0.03449 | 7.52395 |
| N | 3 | -0.32612 | 1.99923 | 5.29802 | 0.02887 | 7.32612 |
| N | 4 | -0.52395 | 1.99928 | 5.49017 | 0.03449 | 7.52395 |
| N | 5 | -0.32612 | 1.99923 | 5.29802 | 0.02887 | 7.32612 |
| N | 6 | -0.40734 | 1.99944 | 5.38508 | 0.02282 | 7.40734 |
| N | 7 | -0.40733 | 1.99944 | 5.38508 | 0.02282 | 7.40733 |
| H | 8 | 0.40529 | 0.00000 | 0.59135 | 0.00336 | 0.59471 |
| H | 9 | 0.40529 | 0.00000 | 0.59135 | 0.00336 | 0.59471 |
| C | 10 | 0.21517 | 1.99942 | 3.75133 | 0.03409 | 5.78483 |
| C | 11 | 0.21517 | 1.99942 | 3.75133 | 0.03409 | 5.78483 |
| S | 12 | -0.15410 | 9.99902 | 6.13478 | 0.02030 | 16.15410 |
| S | 13 | -0.15410 | 9.99902 | 6.13478 | 0.02030 | 16.15410 |
| N | 14 | -0.17554 | 1.99929 | 5.15052 | 0.02574 | 7.17554 |
| N | 15 | -0.17554 | 1.99929 | 5.15051 | 0.02574 | 7.17554 |
| C | 16 | 0.22636 | 1.99917 | 3.75322 | 0.02125 | 5.77364 |
| C | 17 | 0.22636 | 1.99917 | 3.75322 | 0.02125 | 5.77364 |
| C | 18 | 0.14651 | 1.99921 | 3.83180 | 0.02249 | 5.85349 |
| C | 19 | 0.14651 | 1.99921 | 3.83180 | 0.02249 | 5.85349 |
| C | 20 | -0.67488 | 1.99939 | 4.66694 | 0.00855 | 6.67488 |
| H | 21 | 0.23513 | 0.00000 | 0.76328 | 0.00159 | 0.76487 |
| H | 22 | 0.22333 | 0.00000 | 0.77489 | 0.00178 | 0.77667 |
| H | 23 | 0.23981 | 0.00000 | 0.75905 | 0.00114 | 0.76019 |
| C | 24 | -0.62345 | 1.99940 | 4.61626 | 0.00779 | 6.62345 |
| H | 25 | 0.20485 | 0.00000 | 0.79380 | 0.00135 | 0.79515 |
| H | 26 | 0.20665 | 0.00000 | 0.79193 | 0.00142 | 0.79335 |
| H | 27 | 0.24643 | 0.00000 | 0.75226 | 0.00131 | 0.75357 |
| C | 28 | -0.62345 | 1.99940 | 4.61626 | 0.00779 | 6.62345 |
| H | 29 | 0.20665 | 0.00000 | 0.79194 | 0.00142 | 0.79335 |
| H | 30 | 0.24643 | 0.00000 | 0.75226 | 0.00131 | 0.75357 |
| H | 31 | 0.20485 | 0.00000 | 0.79380 | 0.00135 | 0.79515 |
| C | 32 | -0.67489 | 1.99939 | 4.66695 | 0.00855 | 6.67489 |
| H | 33 | 0.23513 | 0.00000 | 0.76328 | 0.00159 | 0.76487 |
| H | 34 | 0.22333 | 0.00000 | 0.77488 | 0.00178 | 0.77667 |
| H | 35 | 0.23981 | 0.00000 | 0.75905 | 0.00114 | 0.76019 |
| * Total * | | 0.00000 | 73.98158 | 117.53656 | 0.48186 | 192.00000 |

**OPBE/TZVP level**

**ΔE(multipl.=1) = 0.0 кДж/моль**
**ΔE(multipl.=3) = 124.23 кДж/моль**

**Alpha occupied eigenvalues (highest) = -5.0090889 eV**
**Alpha virtual eigenvalues (lowest) = -3.4390719 eV**

**<S**2> = 0.0000**

**Summary of Natural Population Analysis:**

| Atom | No | Natural Charge | Natural Population: Core | Valence | Rydberg | Total |
|---|---|---|---|---|---|---|
| Zn | 1 | 1.08463 | 17.99595 | 10.91273 | 0.00669 | 28.91537 |
| N | 2 | -0.47478 | 1.99932 | 5.44154 | 0.03392 | 7.47478 |
| N | 3 | -0.31822 | 1.99929 | 5.28956 | 0.02936 | 7.31822 |
| N | 4 | -0.47501 | 1.99932 | 5.44176 | 0.03393 | 7.47501 |
| N | 5 | -0.31857 | 1.99929 | 5.28990 | 0.02938 | 7.31857 |
| N | 6 | -0.36041 | 1.99946 | 5.33959 | 0.02136 | 7.36041 |
| N | 7 | -0.36054 | 1.99946 | 5.33974 | 0.02134 | 7.36054 |
| H | 8 | 0.41160 | 0.00000 | 0.58468 | 0.00372 | 0.58840 |
| H | 9 | 0.41156 | 0.00000 | 0.58472 | 0.00372 | 0.58844 |
| C | 10 | 0.14175 | 1.99944 | 3.82821 | 0.03060 | 5.85825 |
| C | 11 | 0.14186 | 1.99944 | 3.82809 | 0.03061 | 5.85814 |
| S | 12 | -0.12744 | 9.99900 | 6.10918 | 0.01926 | 16.12744 |
| S | 13 | -0.12751 | 9.99900 | 6.10924 | 0.01926 | 16.12751 |
| N | 14 | -0.16515 | 1.99935 | 5.14198 | 0.02382 | 7.16515 |
| N | 15 | -0.16505 | 1.99935 | 5.14190 | 0.02380 | 7.16505 |
| C | 16 | 0.17062 | 1.99920 | 3.81003 | 0.02014 | 5.82938 |
| C | 17 | 0.17062 | 1.99920 | 3.81002 | 0.02015 | 5.82938 |
| C | 18 | 0.11635 | 1.99926 | 3.86262 | 0.02177 | 5.88365 |
| C | 19 | 0.11618 | 1.99926 | 3.86281 | 0.02176 | 5.88382 |
| C | 20 | -0.71116 | 1.99941 | 4.70461 | 0.00714 | 6.71116 |
| H | 21 | 0.24018 | 0.00000 | 0.75803 | 0.00179 | 0.75982 |
| H | 22 | 0.24016 | 0.00000 | 0.75805 | 0.00179 | 0.75984 |
| H | 23 | 0.25625 | 0.00000 | 0.74242 | 0.00133 | 0.74375 |
| C | 24 | -0.66668 | 1.99942 | 4.66056 | 0.00670 | 6.66668 |
| H | 25 | 0.22197 | 0.00000 | 0.77664 | 0.00139 | 0.77803 |
| H | 26 | 0.22197 | 0.00000 | 0.77664 | 0.00139 | 0.77803 |
| H | 27 | 0.26111 | 0.00000 | 0.73735 | 0.00154 | 0.73889 |
| C | 28 | -0.66672 | 1.99942 | 4.66061 | 0.00670 | 6.66672 |
| H | 29 | 0.22196 | 0.00000 | 0.77665 | 0.00139 | 0.77804 |
| H | 30 | 0.26111 | 0.00000 | 0.73735 | 0.00154 | 0.73889 |
| H | 31 | 0.22196 | 0.00000 | 0.77665 | 0.00139 | 0.77804 |
| C | 32 | -0.71122 | 1.99941 | 4.70468 | 0.00714 | 6.71122 |
| H | 33 | 0.24019 | 0.00000 | 0.75802 | 0.00179 | 0.75981 |
| H | 34 | 0.24017 | 0.00000 | 0.75804 | 0.00179 | 0.75983 |
| H | 35 | 0.25626 | 0.00000 | 0.74241 | 0.00133 | 0.74374 |
| * Total * | | -0.00000 | 73.98228 | 117.55701 | 0.46072 | 192.00000 |

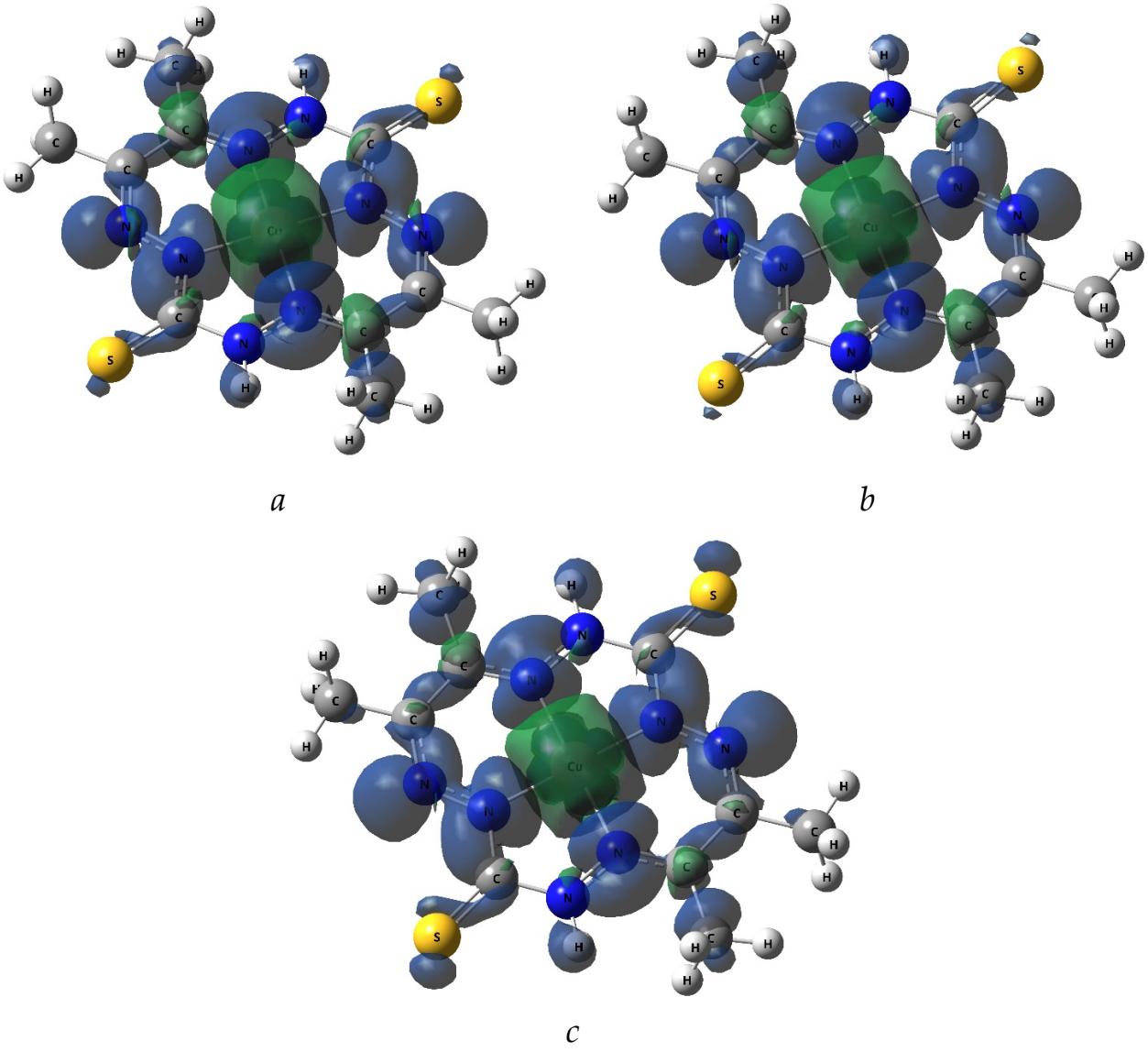


**Figure S1**. Spin density distribution in the Cu**L** complex obtained by DFT B3PW91/ TZVP (*a*), DFT M06/TZVP (*b*) and DFT OPBE/TZVP (*c*) model chemistry.