

Synthesis, DFT and X-Ray Studies of Trans CuCl₂L₂ with L is (E)-(4-chlorophenyl)-N-(3-phenyl-4H-1,2,4-triazol-4-yl)methanimine

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SUPPLEMENTARY INFORMATION

Crystal structure Supplementary information

Table S1. Crystal data of copper(II) complex (6) trans-CuCl₂L₂ (CCDC No. 2217976)

| | |
|---|---|
| Identification code | Cu Complex |
| Empirical formula | C ₃₀ H ₂₂ N ₈ Cl ₄ Cu |
| Formula weight | 699.90 |
| Temperature/K | 150.0 |
| Crystal system | monoclinic |
| Space group | P2 ₁ /c |
| a/Å, b/Å, c/Å | 10.933(2), 13.1221(14), 11.2068(16) |
| α/°, β/°, γ/° | 90.00, 114.68(2), 90.00 |
| Volume/Å ³ | 1460.9(4) |
| Z | 2 |
| ρ _{calc} /mg mm ⁻³ | 1.591 |
| μ/mm ⁻¹ | 1.151 |
| F(000) | 710 |
| Crystal size/mm ³ | 0.2 × 0.1 × 0.05 |
| 2θ range for data collection | 6.2 to 50.7° |
| Index ranges | -11 ≤ h ≤ 13, -15 ≤ k ≤ 15, -13 ≤ l ≤ 13 |
| Reflections collected | 10555 |
| Independent reflections | 2661 [R(int) = 0.0375] |
| Data/restraints/parameters | 2661/0/196 |
| Goodness-of-fit on F ² | 1.041 |
| Final R indexes [I > 2J (I)] | R ₁ = 0.0318, wR ₂ = 0.0735 |
| Final R indexes [all data] | R ₁ = 0.0394, wR ₂ = 0.0779 |
| Largest diff. peak/hole/e Å ⁻³ | 0.465/-0.474 |

DFT Supplementary Information

Table S2. Computed Energies and Cartesian Coordinates for copper(II) complex (6) trans-CuCl₂L₂

Computed Energies [values are in Hartree] (6-31G(d)/LanL2DZ)

| Method | Total Electronic Energy | Sum of Electronic and Zero-point Energies | Sum of Electronic and Thermal Enthalpies | Gibbs Free Energy |
|-----------|----------------------------|---|--|---------------------------|
| CAM-B3LYP | -1849.3559064 | -1848.876464 | -1848.836448 | -1848.959825 |
| | -1849.4185592* | -1848.940462* | -1848.900218* | -1849.024638* |
| | -1849.3892385 [†] | -1848.910599 [†] | -1848.870586 [†] | -1848.993939 [†] |
| | -1849.4516009 [‡] | -1848.974274 [‡] | -1848.934032 [‡] | -1849.058388 [‡] |
| ωB97XD | -1849.8827604 | -1849.403261 | -1849.363333 | -1849.485606 |
| B3LYP | -1850.3767652 | -1849.904940 | -1849.864351 | -1849.988412 |
| MPW1PW91 | -1850.0841113 | -1849.606888 | -1849.566649 | -1849.689788 |
| B3PW91 | -1849.8971297 | -1849.423566 | -1849.383075 | -1849.506738 |
| PBEPBE | -1848.4243762 | -1847.965984 | -1847.924469 | -1848.050141 |

*6-31+G(d)/LanL2DZ, [†]6-31G(d,p)/LanL2DZ, [‡]6-31+G(d,p)/LanL2DZ.

Cartesian Coordinates [CAM-B3LYP/6-31G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|-------------|
| Cu | -0.00000800 | -0.00018000 | 0.54586800 |
| N | -1.91097700 | -0.55415600 | 0.52108700 |
| C | -3.00680500 | 0.15416600 | 0.36678800 |
| C | -3.48000200 | -1.97945800 | 0.31727900 |
| H | -4.04034700 | -2.90028700 | 0.29166700 |
| N | 1.91091900 | 0.55393900 | 0.52101100 |
| C | 3.00680200 | -0.15430700 | 0.36675100 |
| C | 3.47982200 | 1.97935200 | 0.31702800 |
| H | 4.04009000 | 2.90022500 | 0.29131100 |
| N | -2.20112900 | -1.88350500 | 0.50732500 |
| N | -4.03919500 | -0.72935000 | 0.21083100 |
| N | 2.20096100 | 1.88331100 | 0.50710600 |
| N | 4.03911400 | 0.72928000 | 0.21068300 |
| C | -3.10430500 | 1.61471800 | 0.36335400 |
| C | -3.93415900 | 2.28480100 | -0.53921400 |
| C | -2.32675900 | 2.33929400 | 1.27165400 |
| C | -3.98302700 | 3.67136500 | -0.53245600 |
| H | -4.52368500 | 1.72415800 | -1.25486200 |
| C | -2.38226700 | 3.72725700 | 1.26823300 |
| H | -1.69432800 | 1.81514100 | 1.98323500 |
| C | -3.20805900 | 4.39386100 | 0.37007600 |
| H | -4.62088300 | 4.18982700 | -1.24107100 |
| H | -1.77678500 | 4.28559000 | 1.97448800 |
| H | -3.24712700 | 5.47880100 | 0.36997200 |
| C | 3.10443000 | -1.61485200 | 0.36343300 |
| C | 3.93432500 | -2.28493000 | -0.53910100 |

| | | | |
|----|--------------|-------------|-------------|
| C | 2.32697400 | -2.33943000 | 1.27180900 |
| C | 3.98332300 | -3.67148900 | -0.53223600 |
| H | 4.52378400 | -1.72428900 | -1.25480600 |
| C | 2.38261000 | -3.72738800 | 1.26849500 |
| H | 1.69451300 | -1.81528000 | 1.98336600 |
| C | 3.20844300 | -4.39398600 | 0.37037000 |
| H | 4.62121000 | -4.18994700 | -1.24082500 |
| H | 1.77719800 | -4.28572100 | 1.97480900 |
| H | 3.24761100 | -5.47892200 | 0.37035100 |
| N | -5.35824700 | -0.34793300 | 0.12248600 |
| N | 5.35819500 | 0.34796300 | 0.12233700 |
| C | -6.15877200 | -1.16546600 | -0.44307500 |
| C | 6.15863900 | 1.16551000 | -0.44331700 |
| H | -5.81576500 | -2.10640700 | -0.88178000 |
| H | 5.81554400 | 2.10638400 | -0.88209700 |
| C | -7.58747300 | -0.87020500 | -0.54834200 |
| C | -8.41723600 | -1.76519300 | -1.22575700 |
| C | -8.13650000 | 0.28925900 | 0.01114100 |
| C | -9.77694400 | -1.51446700 | -1.35233400 |
| H | -7.99833400 | -2.66749800 | -1.66203200 |
| C | -9.49074700 | 0.54995300 | -0.10979100 |
| H | -7.48864300 | 0.97912100 | 0.54011000 |
| C | -10.29323800 | -0.35773400 | -0.79093200 |
| H | -10.42675100 | -2.20395700 | -1.87749300 |
| H | -9.92692400 | 1.44398200 | 0.31953900 |
| C | 7.58736200 | 0.87035900 | -0.54858900 |
| C | 8.41703500 | 1.76535700 | -1.22610200 |
| C | 8.13649900 | -0.28900800 | 0.01098500 |
| C | 9.77676100 | 1.51473400 | -1.35268600 |
| H | 7.99804800 | 2.66758800 | -1.66244800 |
| C | 9.49076500 | -0.54959900 | -0.10995300 |
| H | 7.48871100 | -0.97887900 | 0.54002900 |
| C | 10.29316500 | 0.35809500 | -0.79119200 |
| H | 10.42649900 | 2.20423200 | -1.87792000 |
| H | 9.92702700 | -1.44355300 | 0.31944700 |
| Cl | -12.03243800 | -0.02559500 | -0.94329100 |
| Cl | 12.03238900 | 0.02608900 | -0.94355800 |
| Cl | -0.00002400 | 0.00000900 | 2.89124700 |
| Cl | -0.00003900 | -0.00022900 | -1.77658400 |

Cartesian Coordinates [CAM-B3LYP/6-31+G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|------------|
| Cu | 0.00000800 | 0.00002200 | 0.71072800 |
| N | -1.92342600 | -0.54819700 | 0.67082500 |
| C | -3.00940000 | 0.16588800 | 0.47431900 |
| C | -3.48855700 | -1.96500800 | 0.38629000 |
| H | -4.05225400 | -2.88315600 | 0.33104700 |
| N | 1.92344300 | 0.54823800 | 0.67074200 |
| C | 3.00941100 | -0.16585800 | 0.47425100 |
| C | 3.48856800 | 1.96503200 | 0.38609100 |
| H | 4.05226400 | 2.88317600 | 0.33078300 |
| N | -2.21792000 | -1.87566400 | 0.63315400 |
| N | -4.03660000 | -0.71152300 | 0.26440700 |
| N | 2.21793600 | 1.87570300 | 0.63298700 |
| N | 4.03660700 | 0.71153900 | 0.26426600 |
| C | -3.10146600 | 1.62762900 | 0.48147700 |

| | | | |
|----|--------------|-------------|-------------|
| C | -3.87480400 | 2.31065000 | -0.46181300 |
| C | -2.37658500 | 2.34029700 | 1.44204700 |
| C | -3.92192300 | 3.69873700 | -0.44271400 |
| H | -4.42031700 | 1.76073100 | -1.22037300 |
| C | -2.43025800 | 3.72969600 | 1.45296500 |
| H | -1.78316000 | 1.80753200 | 2.18008600 |
| C | -3.20068000 | 4.40979600 | 0.51420200 |
| H | -4.51454900 | 4.22686600 | -1.18341300 |
| H | -1.86463300 | 4.27841500 | 2.19935400 |
| H | -3.23697500 | 5.49518800 | 0.52413800 |
| C | 3.10147600 | -1.62760000 | 0.48149100 |
| C | 3.87479200 | -2.31067500 | -0.46177800 |
| C | 2.37661600 | -2.34021200 | 1.44211800 |
| C | 3.92191000 | -3.69876100 | -0.44260100 |
| H | 4.42028800 | -1.76080000 | -1.22038100 |
| C | 2.43028800 | -3.72961100 | 1.45311400 |
| H | 1.78320900 | -1.80740500 | 2.18014000 |
| C | 3.20068800 | -4.40976400 | 0.51437100 |
| H | 4.51451800 | -4.22693300 | -1.18328400 |
| H | 1.86468000 | -4.27828600 | 2.19954600 |
| H | 3.23698100 | -5.49515600 | 0.52436800 |
| N | -5.35620200 | -0.33448300 | 0.13636000 |
| N | 5.35620600 | 0.33449100 | 0.13621000 |
| C | -6.11038700 | -1.12125300 | -0.52886700 |
| C | 6.11037600 | 1.12122200 | -0.52908000 |
| H | -5.71950900 | -2.01852800 | -1.01756400 |
| H | 5.71948800 | 2.01847000 | -1.01781800 |
| C | -7.54011000 | -0.85001400 | -0.68504000 |
| C | -8.30731600 | -1.70205100 | -1.48318100 |
| C | -8.15135400 | 0.24573500 | -0.06262000 |
| C | -9.66537900 | -1.47005500 | -1.66880500 |
| H | -7.84162900 | -2.55482800 | -1.96982500 |
| C | -9.50448600 | 0.48654500 | -0.24160300 |
| H | -7.55579300 | 0.90309200 | 0.56160100 |
| C | -10.24314300 | -0.37643900 | -1.04354500 |
| H | -10.26480400 | -2.12730200 | -2.28810100 |
| H | -9.98693000 | 1.33165500 | 0.23609600 |
| C | 7.54009500 | 0.84997400 | -0.68527000 |
| C | 8.30728300 | 1.70196300 | -1.48348000 |
| C | 8.15135300 | -0.24574000 | -0.06280100 |
| C | 9.66534100 | 1.46995400 | -1.66912300 |
| H | 7.84158500 | 2.55471100 | -1.97016300 |
| C | 9.50448000 | -0.48656100 | -0.24180200 |
| H | 7.55580600 | -0.90305900 | 0.56147300 |
| C | 10.24311900 | 0.37637500 | -1.04381300 |
| H | 10.26475200 | 2.12716400 | -2.28847300 |
| H | 9.98693500 | -1.33164400 | 0.23593500 |
| Cl | -11.97846300 | -0.06913000 | -1.26990900 |
| Cl | 11.97843300 | 0.06905100 | -1.27020100 |
| Cl | 0.00004100 | 0.00008900 | 3.05047700 |
| Cl | -0.00002200 | -0.00004600 | -1.61435200 |

Cartesian Coordinates [CAM-B3LYP/6-31G(d,p)/LanL2DZ]

| | | | |
|----|-------------|-------------|------------|
| Cu | -0.00001100 | -0.00021900 | 0.54186700 |
| N | -1.91031000 | -0.55577800 | 0.51729300 |

| | | | |
|---|--------------|-------------|-------------|
| C | -3.00610200 | 0.15286200 | 0.36357400 |
| C | -3.48009200 | -1.98095000 | 0.31568800 |
| H | -4.04054200 | -2.90143900 | 0.29105900 |
| N | 1.91023800 | 0.55551300 | 0.51721700 |
| C | 3.00609700 | -0.15303600 | 0.36354300 |
| C | 3.47987600 | 1.98082100 | 0.31542900 |
| H | 4.04023500 | 2.90136300 | 0.29068900 |
| N | -2.20079100 | -1.88470000 | 0.50440100 |
| N | -4.03865100 | -0.73034400 | 0.20918000 |
| N | 2.20058900 | 1.88446300 | 0.50417300 |
| N | 4.03855400 | 0.73025800 | 0.20903300 |
| C | -3.10193600 | 1.61346000 | 0.35941700 |
| C | -3.93635400 | 2.28393300 | -0.53841700 |
| C | -2.31718300 | 2.33718000 | 1.26203500 |
| C | -3.98262200 | 3.67034400 | -0.53240400 |
| H | -4.53174100 | 1.72358400 | -1.24906400 |
| C | -2.37031600 | 3.72497200 | 1.25748700 |
| H | -1.68160200 | 1.81218300 | 1.97020000 |
| C | -3.20058900 | 4.39204300 | 0.36422700 |
| H | -4.62399500 | 4.18943100 | -1.23693300 |
| H | -1.75968200 | 4.28292600 | 1.95917600 |
| H | -3.23776000 | 5.47677700 | 0.36345200 |
| C | 3.10208400 | -1.61362500 | 0.35950700 |
| C | 3.93655500 | -2.28408000 | -0.53829000 |
| C | 2.31743400 | -2.33735900 | 1.26220500 |
| C | 3.98297700 | -3.67048500 | -0.53216600 |
| H | 4.53186500 | -1.72372400 | -1.24899600 |
| C | 2.37072000 | -3.72514400 | 1.25776800 |
| H | 1.68181300 | -1.81237600 | 1.97034300 |
| C | 3.20104400 | -4.39219800 | 0.36454300 |
| H | 4.62439100 | -4.18955900 | -1.23666700 |
| H | 1.76016500 | -4.28310900 | 1.95951800 |
| H | 3.23833600 | -5.47692800 | 0.36385600 |
| N | -5.35749500 | -0.34846500 | 0.12099500 |
| N | 5.35743300 | 0.34850000 | 0.12085000 |
| C | -6.15920000 | -1.16770900 | -0.44037300 |
| C | 6.15904200 | 1.16776700 | -0.44062000 |
| H | -5.81827200 | -2.11065000 | -0.87660200 |
| H | 5.81801000 | 2.11063300 | -0.87693000 |
| C | -7.58767000 | -0.87072300 | -0.54400500 |
| C | -8.41973700 | -1.76702300 | -1.21651600 |
| C | -8.13373200 | 0.29153400 | 0.01224300 |
| C | -9.77905200 | -1.51478900 | -1.34144800 |
| H | -8.00295200 | -2.67134500 | -1.65006700 |
| C | -9.48755100 | 0.55366200 | -0.10718300 |
| H | -7.48339700 | 0.98192000 | 0.53723400 |
| C | -10.29241600 | -0.35533300 | -0.78341800 |
| H | -10.43121900 | -2.20475900 | -1.86261500 |
| H | -9.92209400 | 1.44958900 | 0.31935500 |
| C | 7.58754000 | 0.87091500 | -0.54425400 |
| C | 8.41950200 | 1.76723400 | -1.21686900 |
| C | 8.13373100 | -0.29123400 | 0.01209300 |
| C | 9.77884000 | 1.51512500 | -1.34180700 |
| H | 8.00261700 | 2.67147300 | -1.65049800 |
| C | 9.48757400 | -0.55323700 | -0.10733700 |

| | | | |
|----|--------------|-------------|-------------|
| H | 7.48347700 | -0.98163500 | 0.53716500 |
| C | 10.29233300 | 0.35577500 | -0.78367700 |
| H | 10.43092600 | 2.20511100 | -1.86305400 |
| H | 9.92221700 | -1.44907900 | 0.31927800 |
| Cl | -12.03125500 | -0.02121200 | -0.93377000 |
| Cl | 12.03120200 | 0.02181500 | -0.93403400 |
| Cl | -0.00003600 | -0.00000400 | 2.88756200 |
| Cl | -0.00004100 | -0.00026900 | -1.78045700 |

Cartesian Coordinates [CAM-B3LYP/6-31+G(d,p)/LanL2DZ]

| | | | |
|----|-------------|-------------|-------------|
| Cu | -0.00003900 | -0.00067800 | 0.69635900 |
| N | -1.92304800 | -0.54921200 | 0.65729400 |
| C | -3.00940100 | 0.16533000 | 0.46394200 |
| C | -3.48994500 | -1.96579300 | 0.37925900 |
| H | -4.05371100 | -2.88349000 | 0.32620600 |
| N | 1.92285200 | 0.54829600 | 0.65746300 |
| C | 3.00937100 | -0.16594100 | 0.46390100 |
| C | 3.48942800 | 1.96532200 | 0.37986100 |
| H | 4.05298300 | 2.88316400 | 0.32708000 |
| N | -2.21820100 | -1.87617500 | 0.62157800 |
| N | -4.03750500 | -0.71174300 | 0.25834700 |
| N | 2.21770100 | 1.87533800 | 0.62213000 |
| N | 4.03727300 | 0.71143400 | 0.25857500 |
| C | -3.09920800 | 1.62712200 | 0.47006600 |
| C | -3.88171000 | 2.31054300 | -0.46518800 |
| C | -2.36125400 | 2.33915700 | 1.42100700 |
| C | -3.92481700 | 3.69859000 | -0.44752000 |
| H | -4.43771600 | 1.76119600 | -1.21576100 |
| C | -2.41093200 | 3.72847300 | 1.43000400 |
| H | -1.76126600 | 1.80576700 | 2.15313900 |
| C | -3.19042600 | 4.40906700 | 0.49943400 |
| H | -4.52444200 | 4.22702600 | -1.18157500 |
| H | -1.83541200 | 4.27659000 | 2.16850800 |
| H | -3.22360700 | 5.49407400 | 0.50801200 |
| C | 3.09953100 | -1.62771400 | 0.46954400 |
| C | 3.88220700 | -2.31062800 | -0.46593600 |
| C | 2.36176100 | -2.34025300 | 1.42025000 |
| C | 3.92566500 | -3.69867000 | -0.44873200 |
| H | 4.43807800 | -1.76089100 | -1.21632300 |
| C | 2.41178900 | -3.72956000 | 1.42878200 |
| H | 1.76164000 | -1.80726200 | 2.15256100 |
| C | 3.19145300 | -4.40964800 | 0.49798400 |
| H | 4.52542500 | -4.22671000 | -1.18296300 |
| H | 1.83640600 | -4.27806800 | 2.16710200 |
| H | 3.22490700 | -5.49465000 | 0.50620000 |
| N | -5.35709200 | -0.33395000 | 0.13378000 |
| N | 5.35694600 | 0.33398100 | 0.13388700 |
| C | -6.11545100 | -1.12407300 | -0.52274100 |
| C | 6.11511700 | 1.12447400 | -0.52240400 |
| H | -5.72941900 | -2.02507600 | -1.00805700 |
| H | 5.72887100 | 2.02553100 | -1.00745100 |
| C | -7.54541400 | -0.85052200 | -0.67260700 |
| C | -8.31841600 | -1.70474900 | -1.46251200 |
| C | -8.15077200 | 0.24940400 | -0.05205200 |
| C | -9.67670100 | -1.47058100 | -1.64217100 |

| | | | |
|----|--------------|-------------|-------------|
| H | -7.85728700 | -2.56060000 | -1.94710200 |
| C | -9.50404000 | 0.49232900 | -0.22523200 |
| H | -7.55020000 | 0.90755700 | 0.56593400 |
| C | -10.24847500 | -0.37273400 | -1.01924100 |
| H | -10.28103400 | -2.12884700 | -2.25483800 |
| H | -9.98241500 | 1.34023500 | 0.25067700 |
| C | 7.54514200 | 0.85130100 | -0.67236000 |
| C | 8.31793900 | 1.70593800 | -1.46202400 |
| C | 8.15076400 | -0.24866100 | -0.05212600 |
| C | 9.67627700 | 1.47214100 | -1.64176000 |
| H | 7.85660500 | 2.56182000 | -1.94636400 |
| C | 9.50408800 | -0.49121800 | -0.22538600 |
| H | 7.55035100 | -0.90713400 | 0.56567400 |
| C | 10.24831400 | 0.37425000 | -1.01915000 |
| H | 10.28045100 | 2.13072600 | -2.25424100 |
| H | 9.98266600 | -1.33914800 | 0.25027600 |
| Cl | -11.98415700 | -0.06260200 | -1.23809000 |
| Cl | 11.98406800 | 0.06458900 | -1.23810000 |
| Cl | -0.00011000 | -0.00082100 | 3.03670200 |
| Cl | -0.00006700 | -0.00023100 | -1.62826800 |

Cartesian Coordinates [ω B97XD/6-31G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|-------------|
| Cu | 0.00001200 | 0.00007200 | 0.79924600 |
| N | -1.89601900 | -0.61918100 | 0.77201000 |
| C | -2.97566500 | 0.09495200 | 0.54055600 |
| C | -3.47640300 | -2.03101500 | 0.57400900 |
| H | -4.05281200 | -2.94283400 | 0.57286500 |
| N | 1.89605200 | 0.61929400 | 0.77191000 |
| C | 2.97568000 | -0.09487300 | 0.54047800 |
| C | 3.47645200 | 2.03108900 | 0.57374800 |
| H | 4.05287700 | 2.94289800 | 0.57251700 |
| N | -2.20151700 | -1.94315200 | 0.81226300 |
| N | -4.01166500 | -0.78033500 | 0.38573400 |
| N | 2.20157500 | 1.94326300 | 0.81206700 |
| N | 4.01169200 | 0.78038400 | 0.38557700 |
| C | -3.03840000 | 1.55379300 | 0.44478100 |
| C | -3.79890900 | 2.18120700 | -0.54623100 |
| C | -2.27914200 | 2.31595800 | 1.33964200 |
| C | -3.79530900 | 3.56682000 | -0.64238400 |
| H | -4.37120900 | 1.58784100 | -1.25076500 |
| C | -2.27773100 | 3.70196900 | 1.22983200 |
| H | -1.70302200 | 1.82488400 | 2.12138700 |
| C | -3.03321600 | 4.32764100 | 0.24196400 |
| H | -4.37704700 | 4.05326400 | -1.41917500 |
| H | -1.68188100 | 4.29025000 | 1.92001200 |
| H | -3.02658200 | 5.41025000 | 0.15678000 |
| C | 3.03839000 | -1.55372300 | 0.44481900 |
| C | 3.79887100 | -2.18122800 | -0.54615800 |
| C | 2.27913800 | -2.31580400 | 1.33975600 |
| C | 3.79525000 | -3.56684800 | -0.64219900 |
| H | 4.37116700 | -1.58792600 | -1.25074800 |
| C | 2.27770600 | -3.70182500 | 1.23005800 |
| H | 1.70303900 | -1.82466000 | 2.12147200 |
| C | 3.03316300 | -4.32758700 | 0.24222600 |
| H | 4.37696700 | -4.05336300 | -1.41896100 |

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|----|--------------|-------------|-------------|
| H | 1.68186100 | -4.29004100 | 1.92029700 |
| H | 3.02651300 | -5.41020200 | 0.15713000 |
| N | -5.31976500 | -0.38424700 | 0.21794700 |
| N | 5.31978300 | 0.38426300 | 0.21779900 |
| C | -6.07390600 | -1.18257200 | -0.43669500 |
| C | 6.07392800 | 1.18254300 | -0.43689400 |
| H | -5.69537200 | -2.10952400 | -0.87903600 |
| H | 5.69540600 | 2.10948500 | -0.87926500 |
| C | -7.48830500 | -0.86875000 | -0.64528200 |
| C | -8.26838800 | -1.72490800 | -1.42694600 |
| C | -8.06829100 | 0.27817700 | -0.08712000 |
| C | -9.61072400 | -1.44794100 | -1.65862400 |
| H | -7.82587200 | -2.61587800 | -1.86446600 |
| C | -9.40572200 | 0.56489500 | -0.31108000 |
| H | -7.46004900 | 0.93884000 | 0.52160600 |
| C | -10.15796300 | -0.30422400 | -1.09514500 |
| H | -10.22128800 | -2.10561400 | -2.26610000 |
| H | -9.86478500 | 1.44876600 | 0.11633500 |
| C | 7.48831100 | 0.86866800 | -0.64551200 |
| C | 8.26840100 | 1.72478100 | -1.42721800 |
| C | 8.06827400 | -0.27826500 | -0.08733800 |
| C | 9.61072200 | 1.44776400 | -1.65892400 |
| H | 7.82590500 | 2.61575800 | -1.86474400 |
| C | 9.40568800 | -0.56503500 | -0.31132900 |
| H | 7.46002500 | -0.93889400 | 0.52141800 |
| C | 10.15793800 | 0.30404100 | -1.09543400 |
| H | 10.22129500 | 2.10540400 | -2.26642600 |
| H | 9.86473200 | -1.44891200 | 0.11609300 |
| Cl | -11.87268200 | 0.06132200 | -1.38171600 |
| Cl | 11.87263600 | -0.06157100 | -1.38204200 |
| Cl | 0.00005400 | 0.00014000 | 3.14259900 |
| Cl | -0.00002100 | -0.00001400 | -1.52658400 |

Cartesian Coordinates [B3LYP/6-31G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|-------------|
| Cu | -0.00006100 | -0.00013400 | 0.53383400 |
| N | -1.93637800 | -0.53966300 | 0.50576800 |
| C | -3.04031500 | 0.17366500 | 0.35807300 |
| C | -3.50783000 | -1.97247600 | 0.25675100 |
| H | -4.06558800 | -2.89443300 | 0.20849100 |
| N | 1.93617300 | 0.53959300 | 0.50530700 |
| C | 3.04017500 | -0.17364600 | 0.35774500 |
| C | 3.50753300 | 1.97251400 | 0.25634000 |
| H | 4.06522600 | 2.89451300 | 0.20811700 |
| N | -2.22432300 | -1.87702800 | 0.46133900 |
| N | -4.07522400 | -0.71724300 | 0.17288600 |
| N | 2.22400900 | 1.87698300 | 0.46081600 |
| N | 4.07503200 | 0.71733000 | 0.17255600 |
| C | -3.14747800 | 1.63389300 | 0.38446400 |
| C | -3.98963800 | 2.32222900 | -0.50427900 |
| C | -2.36982900 | 2.35207300 | 1.30932700 |
| C | -4.05070400 | 3.71319700 | -0.46677100 |
| H | -4.57536200 | 1.77344300 | -1.23307300 |
| C | -2.43862500 | 3.74412800 | 1.33617300 |
| H | -1.73092700 | 1.81917500 | 2.00915100 |
| C | -3.27670200 | 4.42647500 | 0.45220100 |

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|----|--------------|-------------|-------------|
| H | -4.69586000 | 4.24105500 | -1.16347000 |
| H | -1.83590600 | 4.29253300 | 2.05416700 |
| H | -3.32564400 | 5.51181500 | 0.47599800 |
| C | 3.14758600 | -1.63384800 | 0.38426900 |
| C | 3.98976400 | -2.32205200 | -0.50455800 |
| C | 2.37018800 | -2.35212900 | 1.30925300 |
| C | 4.05114000 | -3.71300300 | -0.46697300 |
| H | 4.57525600 | -1.77317600 | -1.23347800 |
| C | 2.43929500 | -3.74416600 | 1.33618500 |
| H | 1.73124600 | -1.81930200 | 2.00909300 |
| C | 3.27741600 | -4.42638500 | 0.45215200 |
| H | 4.69630800 | -4.24077000 | -1.16373000 |
| H | 1.83678400 | -4.29266600 | 2.05427900 |
| H | 3.32659600 | -5.51171400 | 0.47601800 |
| N | -5.39901800 | -0.33779100 | 0.09557400 |
| N | 5.39884700 | 0.33795400 | 0.09533500 |
| C | -6.20633200 | -1.15434500 | -0.48308100 |
| C | 6.20612100 | 1.15442100 | -0.48349200 |
| H | -5.86215000 | -2.08545400 | -0.94429900 |
| H | 5.86189200 | 2.08538100 | -0.94497300 |
| C | -7.63689300 | -0.86865300 | -0.57111000 |
| C | -8.46720200 | -1.75870500 | -1.27070800 |
| C | -8.20230800 | 0.27474400 | 0.02370200 |
| C | -9.83508000 | -1.51965700 | -1.38537200 |
| H | -8.04117400 | -2.64577200 | -1.73281400 |
| C | -9.56475700 | 0.52422400 | -0.08464000 |
| H | -7.56175800 | 0.95929300 | 0.56965200 |
| C | -10.36280300 | -0.37870600 | -0.78897600 |
| H | -10.47901700 | -2.20391400 | -1.92593500 |
| H | -10.00828300 | 1.40231600 | 0.37117200 |
| C | 7.63672200 | 0.86878900 | -0.57136500 |
| C | 8.46701400 | 1.75857800 | -1.27129700 |
| C | 8.20215400 | -0.27433000 | 0.02396600 |
| C | 9.83491100 | 1.51954000 | -1.38580100 |
| H | 8.04097400 | 2.64543700 | -1.73379300 |
| C | 9.56462300 | -0.52378600 | -0.08420000 |
| H | 7.56160700 | -0.95867300 | 0.57017000 |
| C | 10.36266500 | 0.37887300 | -0.78888900 |
| H | 10.47883600 | 2.20359800 | -1.92663000 |
| H | 10.00817700 | -1.40165000 | 0.37202600 |
| Cl | -12.12052400 | -0.06005300 | -0.92525800 |
| Cl | 12.12039900 | 0.06024600 | -0.92495400 |
| Cl | 0.00048500 | 0.00029200 | 2.90795200 |
| Cl | -0.00025000 | -0.00088600 | -1.81767700 |

Cartesian Coordinates [MPW1PW91/6-31G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|------------|
| Cu | -0.00000400 | -0.00006900 | 0.59471300 |
| N | -1.91701400 | -0.55883600 | 0.56380800 |
| C | -3.01148500 | 0.15470900 | 0.39677700 |
| C | -3.48217900 | -1.97878800 | 0.31649500 |
| H | -4.04172400 | -2.89891300 | 0.27657100 |
| N | 1.91698700 | 0.55876300 | 0.56372500 |
| C | 3.01148200 | -0.15475100 | 0.39671900 |
| C | 3.48209300 | 1.97875800 | 0.31627300 |
| H | 4.04160100 | 2.89890200 | 0.27626800 |

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|----|--------------|-------------|-------------|
| N | -2.20467700 | -1.88344700 | 0.53308600 |
| N | -4.04113700 | -0.72910900 | 0.21286500 |
| N | 2.20459800 | 1.88338400 | 0.53289400 |
| N | 4.04109500 | 0.72909400 | 0.21272100 |
| C | -3.10599300 | 1.61014500 | 0.40542000 |
| C | -3.94079700 | 2.29520900 | -0.48514300 |
| C | -2.31673200 | 2.32421200 | 1.31623000 |
| C | -3.98329600 | 3.68323600 | -0.46227000 |
| H | -4.53470400 | 1.74597300 | -1.20562000 |
| C | -2.36559700 | 3.71319600 | 1.32719500 |
| H | -1.68435400 | 1.78923100 | 2.02089600 |
| C | -3.19702100 | 4.39398300 | 0.44208700 |
| H | -4.62342900 | 4.21168300 | -1.16098600 |
| H | -1.75214900 | 4.26073600 | 2.03456900 |
| H | -3.23113700 | 5.47871800 | 0.45341700 |
| C | 3.10605600 | -1.61018300 | 0.40546400 |
| C | 3.94088200 | -2.29526700 | -0.48506300 |
| C | 2.31685600 | -2.32422700 | 1.31634500 |
| C | 3.98346400 | -3.68329000 | -0.46208500 |
| H | 4.53474700 | -1.74605300 | -1.20559100 |
| C | 2.36580200 | -3.71320800 | 1.32741500 |
| H | 1.68446600 | -1.78923000 | 2.02098800 |
| C | 3.19724900 | -4.39401400 | 0.44234200 |
| H | 4.62361500 | -4.21175300 | -1.16077200 |
| H | 1.75240300 | -4.26072900 | 2.03484500 |
| H | 3.23143100 | -5.47874600 | 0.45375700 |
| N | -5.35125500 | -0.34921600 | 0.11058400 |
| N | 5.35122500 | 0.34924200 | 0.11043400 |
| C | -6.14447000 | -1.15992200 | -0.48509800 |
| C | 6.14439700 | 1.15993500 | -0.48532200 |
| H | -5.79199000 | -2.08845100 | -0.94283300 |
| H | 5.79187400 | 2.08842300 | -0.94310900 |
| C | -7.56729800 | -0.86770700 | -0.59994300 |
| C | -8.38484000 | -1.74317800 | -1.32313600 |
| C | -8.13420600 | 0.27007100 | -0.00701000 |
| C | -9.74428300 | -1.49436000 | -1.46338500 |
| H | -7.95557300 | -2.62740500 | -1.78496400 |
| C | -9.48835100 | 0.52899000 | -0.14052700 |
| H | -7.50006300 | 0.94335000 | 0.55848400 |
| C | -10.27554000 | -0.35881600 | -0.86838800 |
| H | -10.38176600 | -2.16719100 | -2.02349700 |
| H | -9.93623100 | 1.40413300 | 0.31420300 |
| C | 7.56723200 | 0.86776100 | -0.60018200 |
| C | 8.38472900 | 1.74321500 | -1.32344500 |
| C | 8.13419100 | -0.26996200 | -0.00719200 |
| C | 9.74417800 | 1.49443400 | -1.46370800 |
| H | 7.95542300 | 2.62740100 | -1.78531700 |
| C | 9.48834100 | -0.52884600 | -0.14072500 |
| H | 7.50008200 | -0.94322800 | 0.55835500 |
| C | 10.27548500 | 0.35894200 | -0.86865600 |
| H | 10.38162600 | 2.16725200 | -2.02387400 |
| H | 9.93625900 | -1.40394800 | 0.31404700 |
| Cl | -12.01071000 | -0.02986500 | -1.03643100 |
| Cl | 12.01066100 | 0.03003600 | -1.03671900 |
| Cl | 0.00001400 | 0.00003500 | 2.94469100 |

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|----|-------------|-------------|-------------|
| Cl | -0.00003300 | -0.00014500 | -1.73226100 |
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Cartesian Coordinates [B3PW91/6-31G(d)/LanL2DZ]

| | | | |
|----|--------------|-------------|-------------|
| Cu | -0.00000900 | -0.00013800 | 0.55493300 |
| N | -1.92297400 | -0.54885200 | 0.52538800 |
| C | -3.02127000 | 0.16733200 | 0.36960200 |
| C | -3.49372500 | -1.97094400 | 0.28473500 |
| H | -4.05440800 | -2.89223500 | 0.24664200 |
| N | 1.92292200 | 0.54869500 | 0.52530700 |
| C | 3.02126100 | -0.16743000 | 0.36955500 |
| C | 3.49357500 | 1.97087100 | 0.28450400 |
| H | 4.05419700 | 2.89219600 | 0.24632100 |
| N | -2.21192600 | -1.87662200 | 0.49220700 |
| N | -4.05497300 | -0.71866600 | 0.19008500 |
| N | 2.21178600 | 1.87648100 | 0.49200700 |
| N | 4.05490100 | 0.71862300 | 0.18994500 |
| C | -3.11913300 | 1.62408200 | 0.38496600 |
| C | -3.96014600 | 2.31201200 | -0.50128400 |
| C | -2.32984600 | 2.33880000 | 1.29879300 |
| C | -4.00948600 | 3.70166100 | -0.47065800 |
| H | -4.55340300 | 1.76364000 | -1.22520400 |
| C | -2.38605600 | 3.72935000 | 1.31791600 |
| H | -1.69146600 | 1.80230200 | 1.99886700 |
| C | -3.22405400 | 4.41238300 | 0.43749300 |
| H | -4.65470000 | 4.23138200 | -1.16640300 |
| H | -1.77283100 | 4.27668400 | 2.02824900 |
| H | -3.26365000 | 5.49856200 | 0.45526100 |
| C | 3.11923400 | -1.62417100 | 0.38503100 |
| C | 3.96029100 | -2.31210000 | -0.50117800 |
| C | 2.33002800 | -2.33888600 | 1.29893200 |
| C | 4.00975900 | -3.70174200 | -0.47043700 |
| H | 4.55349000 | -1.76373600 | -1.22515100 |
| C | 2.38636400 | -3.72942900 | 1.31816800 |
| H | 1.69161800 | -1.80238900 | 1.99897800 |
| C | 3.22440800 | -4.41246000 | 0.43778700 |
| H | 4.65500900 | -4.23146300 | -1.16615000 |
| H | 1.77320300 | -4.27675900 | 2.02855900 |
| H | 3.26410400 | -5.49863400 | 0.45564500 |
| N | -5.36943600 | -0.33898800 | 0.10477800 |
| N | 5.36938700 | 0.33902300 | 0.10463500 |
| C | -6.17009600 | -1.15015000 | -0.48720500 |
| C | 6.16998000 | 1.15019000 | -0.48743300 |
| H | -5.81998300 | -2.07576200 | -0.95656900 |
| H | 5.81979500 | 2.07574300 | -0.95685900 |
| C | -7.59677900 | -0.86383600 | -0.58141300 |
| C | -8.42054400 | -1.73966300 | -1.30212900 |
| C | -8.16476400 | 0.26712200 | 0.02898800 |
| C | -9.78505500 | -1.49785100 | -1.42299400 |
| H | -7.99175700 | -2.61898800 | -1.77740100 |
| C | -9.52398700 | 0.51930700 | -0.08515100 |
| H | -7.52733600 | 0.94081500 | 0.59312600 |
| C | -10.31636800 | -0.36870300 | -0.81109400 |
| H | -10.42603000 | -2.17166200 | -1.98099400 |
| H | -9.97121600 | 1.38937900 | 0.38352700 |
| C | 7.59667900 | 0.86395900 | -0.58165400 |

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|----|--------------|-------------|-------------|
| C | 8.42037200 | 1.73978400 | -1.30245400 |
| C | 8.16474900 | -0.26691900 | 0.02881600 |
| C | 9.78489600 | 1.49804800 | -1.42333200 |
| H | 7.99152000 | 2.61904700 | -1.77778200 |
| C | 9.52398400 | -0.51902900 | -0.08533600 |
| H | 7.52737500 | -0.94061100 | 0.59301700 |
| C | 10.31629300 | 0.36897700 | -0.81136200 |
| H | 10.42581500 | 2.17185900 | -1.98139500 |
| H | 9.97127800 | -1.38903800 | 0.38339500 |
| Cl | -12.06083200 | -0.04838200 | -0.95439900 |
| Cl | 12.06077400 | 0.04875400 | -0.95468600 |
| Cl | 0.00000300 | -0.00001400 | 2.91513400 |
| Cl | -0.00003700 | -0.00021800 | -1.78147500 |

Cartesian Coordinates [PBEPBE/6-31G(d)/LanL2DZ]

| | | | |
|----|-------------|-------------|-------------|
| Cu | -0.00002400 | -0.00035700 | 0.60170200 |
| N | -1.91290100 | -0.56358000 | 0.56873700 |
| C | -3.01608700 | 0.16735500 | 0.39751400 |
| C | -3.50102400 | -1.98750700 | 0.30149800 |
| H | -4.07217100 | -2.91124300 | 0.25715400 |
| N | 1.91276900 | 0.56314900 | 0.56864600 |
| C | 3.01606800 | -0.16763300 | 0.39749100 |
| C | 3.50066300 | 1.98729700 | 0.30120600 |
| H | 4.07166300 | 2.91111800 | 0.25673700 |
| N | -2.20929400 | -1.90134700 | 0.53241700 |
| N | -4.05999300 | -0.72333800 | 0.20024100 |
| N | 2.20895100 | 1.90095900 | 0.53215700 |
| N | 4.05982800 | 0.72320300 | 0.20009100 |
| C | -3.10354700 | 1.62618500 | 0.40893200 |
| C | -3.97808000 | 2.32423200 | -0.45212100 |
| C | -2.26630300 | 2.34407600 | 1.29305800 |
| C | -4.01129000 | 3.72255700 | -0.42682200 |
| H | -4.60977500 | 1.77393100 | -1.15349300 |
| C | -2.30747000 | 3.74266800 | 1.30479800 |
| H | -1.60740000 | 1.80084500 | 1.98257400 |
| C | -3.17722300 | 4.43471200 | 0.44885400 |
| H | -4.68340500 | 4.25872700 | -1.10440300 |
| H | -1.65677500 | 4.29074100 | 1.99317800 |
| H | -3.20428500 | 5.52926500 | 0.46100600 |
| C | 3.10377600 | -1.62644800 | 0.40905900 |
| C | 3.97841200 | -2.32442600 | -0.45194600 |
| C | 2.26668900 | -2.34440100 | 1.29328300 |
| C | 4.01187500 | -3.72274300 | -0.42650700 |
| H | 4.60999200 | -1.77408200 | -1.15338800 |
| C | 2.30811000 | -3.74298500 | 1.30516300 |
| H | 1.60771300 | -1.80122200 | 1.98277000 |
| C | 3.17796200 | -4.43495900 | 0.44926400 |
| H | 4.68407100 | -4.25886000 | -1.10405100 |
| H | 1.65753600 | -4.29110400 | 1.99362100 |
| H | 3.20522300 | -5.52950600 | 0.46152700 |
| N | -5.37772400 | -0.33225500 | 0.09736300 |
| N | 5.37761800 | 0.33231600 | 0.09722800 |
| C | -6.18258300 | -1.15698500 | -0.50200400 |
| C | 6.18232900 | 1.15709800 | -0.50226500 |
| H | -5.82803600 | -2.09466200 | -0.96517400 |

| | | | |
|----|--------------|-------------|-------------|
| H | 5.82762000 | 2.09465800 | -0.96554600 |
| C | -7.60833200 | -0.86552200 | -0.61072500 |
| C | -8.43824100 | -1.75618100 | -1.32573400 |
| C | -8.18022500 | 0.28697500 | -0.02184600 |
| C | -9.80814800 | -1.50964400 | -1.46050600 |
| H | -8.00552800 | -2.65204300 | -1.78465800 |
| C | -9.54477700 | 0.54477700 | -0.15021300 |
| H | -7.53696500 | 0.97254000 | 0.53710000 |
| C | -10.34116000 | -0.35946200 | -0.86895700 |
| H | -10.45398900 | -2.19520200 | -2.01387600 |
| H | -9.99520100 | 1.43164400 | 0.30194200 |
| C | 7.60812400 | 0.86585500 | -0.61097900 |
| C | 8.43787000 | 1.75655700 | -1.32612200 |
| C | 8.18022100 | -0.28647000 | -0.02195900 |
| C | 9.80781600 | 1.51023000 | -1.46088800 |
| H | 8.00500000 | 2.65228700 | -1.78515400 |
| C | 9.54481300 | -0.54406100 | -0.15031900 |
| H | 7.53708600 | -0.97206800 | 0.53709000 |
| C | 10.34103100 | 0.36021500 | -0.86919800 |
| H | 10.45353200 | 2.19582200 | -2.01436200 |
| H | 9.99539300 | -1.43079300 | 0.30194400 |
| Cl | -12.09438500 | -0.03282300 | -1.02928000 |
| Cl | 12.09430700 | 0.03384800 | -1.02951200 |
| Cl | -0.00004700 | -0.00011200 | 2.99146400 |
| Cl | -0.00005000 | -0.00046200 | -1.76067800 |

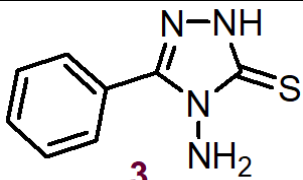
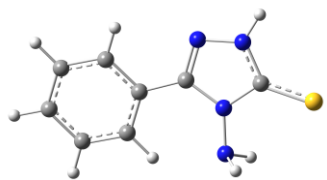
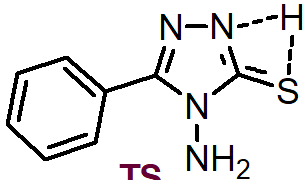
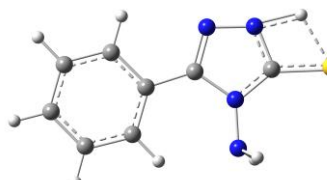
Table S3. Calculations of selected bond lengths for the copper(II) complex (6) using higher basis set.

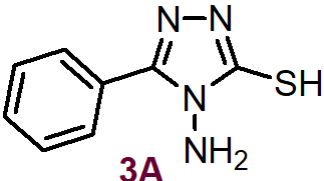
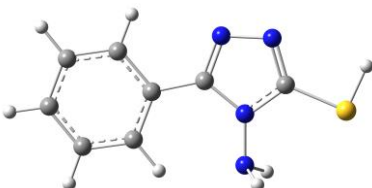
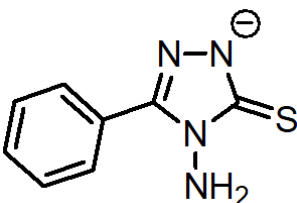
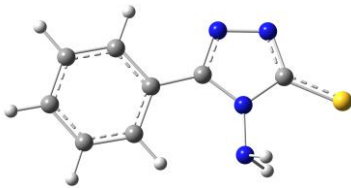
| No. | Atoms * | Experimental | CAM-B3LYP | | |
|-----|----------|--------------|-------------------|--------------------|---------------------|
| | | | 6-31+G(d)/LanL2DZ | 6-31G(d,p)/LanL2DZ | 6-31+G(d,p)/LanL2DZ |
| 1 | Cu1-Cl65 | 2.2552 | 2.32508 | 2.32232 | 2.32463 |
| 2 | Cu1-N6 | 1.9603 | 2.00044 | 1.98960 | 2.00010 |
| 3 | N6-N12 | 1.3780 | 1.36026 | 1.36036 | 1.35986 |
| 4 | N6-C7 | 1.3010 | 1.31448 | 1.31399 | 1.31458 |
| 5 | N12-C8 | 1.2890 | 1.29748 | 1.29672 | 1.29772 |
| 6 | N13-C8 | 1.3610 | 1.37347 | 1.37381 | 1.37371 |
| 7 | N13-C7 | 1.3600 | 1.36713 | 1.36750 | 1.36694 |
| 8 | C7-C25 | 1.4540 | 1.46466 | 1.46375 | 1.46456 |
| 9 | N13-N37 | 1.3840 | 1.37837 | 1.37585 | 1.37824 |
| 10 | N37-C39 | 1.2670 | 1.27684 | 1.27633 | 1.27688 |
| 11 | C39-C52 | 1.4490 | 1.46358 | 1.46269 | 1.46359 |
| 12 | Cl63-C59 | 1.7300 | 1.77680 | 1.77702 | 1.77670 |

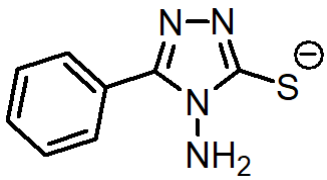
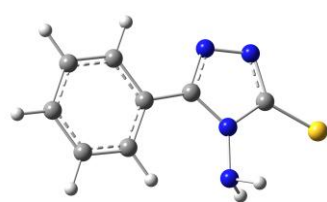
* The numbers described here for the atoms are according to the numbers mentioned for the optimized geometry of the complex in Figure 3a, generated during the visualization using GaussView software.

Table S4. Reaction Energies and Bond Dissociation Energies for Tautomers (3) and (3A)

Computed Energies [values are in Hartree], Optimized structures and Cartesian Coordinates (B3LYP/6-31+G(d,p))

| Species | Total Electronic Energy | Sum of Electronic and Zero-point Energies | Sum of Electronic and Thermal Enthalpies | Gibbs Free Energy |
|---|--|--|---|-------------------|
|  3 | -926.8696219 | -926.709329 | -926.697429 | -926.747848 |
|  | N -0.53911900 C -0.07971800 N -1.15000600 C -2.34348800 N -1.90019300 C 1.36084000 C 2.25406500 C 3.62855000 C 4.13866100 C 3.25906000 C 1.87747700 S -3.89733400 N -1.08653100 H 1.85753500 H 4.30370900 H 5.21162400 H 3.64470200 H 1.20065600 H -1.67970700 H -1.53488700 H -2.48802100 | -1.67307200 -0.44554900 0.44291800 -0.27002000 -1.54764800 -0.14034300 -1.22256400 -1.00510500 0.29258900 1.36836700 1.16102900 0.34054700 1.83646100 -2.22729300 -1.84957400 0.46060400 2.37925500 1.99951700 2.21282900 2.10009200 -2.36522800 | -0.10800200 -0.03222700 0.02629100 -0.01385500 -0.09486000 -0.00988100 0.11902900 0.12674900 0.00657500 -0.12052400 -0.12841000 0.02639900 0.12506300 0.21254400 0.22868700 0.01363600 -0.21456100 -0.22047200 -0.61603800 1.00366600 -0.15402800 | |
|  TS | -926.7920054 | -926.638715 | -926.627809 | -926.674843 |
|  | N -0.61605000 N -1.97269400 C -2.26739600 N -1.10199500 S -3.97964200 H -3.34694000 C -0.07696900 | -1.56951400 -1.38077400 -0.09126000 0.60480100 0.11059400 -1.49841400 -0.36459200 | -0.00005300 -0.00006500 -0.00002400 -0.00001400 0.00003400 -0.00000300 -0.00002900 | |

| | | | | | |
|---|--------------|-------------|-------------|-------------|--|
| | N | -0.96677200 | 2.00024900 | 0.00005700 | |
| | H | -1.43102100 | 2.37007300 | -0.82725100 | |
| | H | -1.43093600 | 2.36998300 | 0.82745400 | |
| | C | 1.37746200 | -0.13672500 | -0.00001500 | |
| | C | 1.97096300 | 1.13782500 | -0.00006600 | |
| | C | 2.20951200 | -1.27509600 | 0.00005000 | |
| | C | 3.36244500 | 1.26405600 | -0.00004700 | |
| | H | 1.34761400 | 2.02144600 | -0.00012200 | |
| | C | 3.59416400 | -1.13809200 | 0.00006900 | |
| | H | 1.75444300 | -2.25895600 | 0.00008500 | |
| | C | 4.17966900 | 0.13314100 | 0.00002100 | |
| | H | 3.80498600 | 2.25599200 | -0.00008800 | |
| | H | 4.21895400 | -2.02644500 | 0.00012100 | |
| | H | 5.26065100 | 0.23792800 | 0.00003700 | |
|  | -926.8412128 | -926.685153 | -926.672885 | -926.723954 | |
|  | N | 0.54236300 | -1.67686700 | -0.00051400 | |
| | C | 0.05993700 | -0.44936400 | -0.00006700 | |
| | N | 1.12965100 | 0.43930000 | 0.00004000 | |
| | C | 2.25186100 | -0.35666500 | -0.00024300 | |
| | N | 1.92211000 | -1.62303900 | -0.00065100 | |
| | C | -1.37946400 | -0.14215100 | -0.00012300 | |
| | C | -2.27090900 | -1.23407900 | 0.00066200 | |
| | C | -3.64670800 | -1.02317700 | 0.00080500 | |
| | C | -4.16375900 | 0.27735100 | -0.00001600 | |
| | C | -3.28728200 | 1.36329600 | -0.00080200 | |
| | C | -1.90459000 | 1.16191000 | -0.00093900 | |
| | S | 3.87567100 | 0.33421200 | -0.00008100 | |
| | N | 1.09073100 | 1.83907100 | 0.00136300 | |
| | H | -1.86520800 | -2.23939200 | 0.00132700 | |
| | H | -4.31841900 | -1.87673900 | 0.00163400 | |
| | H | -5.23771600 | 0.43955600 | 0.00013200 | |
| | H | -3.67634200 | 2.37753500 | -0.00149600 | |
| | H | -1.23485100 | 2.01122600 | -0.00155600 | |
| | H | 4.46084400 | -0.87908500 | 0.00101400 | |
| | H | 1.55668400 | 2.19298100 | 0.83404100 | |
| | H | 1.55578300 | 2.19455400 | -0.83114100 | |
|  | -926.3263849 | -926.180145 | -926.168341 | -926.218261 | |
|  | N | -0.57355200 | -1.70096500 | -0.02446400 | |
| | C | -0.09893800 | -0.46459400 | -0.00563300 | |
| | N | -1.17545100 | 0.40220700 | 0.01139500 | |
| | C | -2.33152400 | -0.37839800 | -0.00318400 | |
| | N | -1.94333400 | -1.66342500 | -0.02647600 | |
| | C | 1.32984900 | -0.14895100 | -0.00310000 | |
| | C | 2.25068900 | -1.22155600 | 0.03440200 | |
| | C | 3.62239400 | -0.98867300 | 0.03425200 | |
| | C | 4.12585000 | 0.31969000 | -0.00289100 | |
| | C | 3.22516800 | 1.38683200 | -0.04116300 | |
| | C | 1.84540400 | 1.16340700 | -0.04132900 | |

| | | | | |
|--|---|--------------|-------------|-------------|
| | S | -3.90555900 | 0.31676000 | -0.00439200 |
| | N | -1.16178200 | 1.80786500 | 0.04038800 |
| | H | 1.85657500 | -2.23164200 | 0.06250900 |
| | H | 4.30693800 | -1.83359100 | 0.06407800 |
| | H | 5.19805700 | 0.49948900 | -0.00219700 |
| | H | 3.59566900 | 2.40929600 | -0.07209300 |
| | H | 1.15353900 | 1.99585600 | -0.07364500 |
| | H | -1.84904500 | 2.09072000 | -0.66401100 |
| | H | -1.60729700 | 2.07540400 | 0.92160700 |
|  | | -926.3263844 | -926.180134 | -926.168338 |
| | | | | -926.218210 |
|  | N | -0.57326800 | -1.70113300 | -0.02464100 |
| | C | -0.09886500 | -0.46475900 | -0.00604900 |
| | N | -1.17535100 | 0.40201000 | 0.01078900 |
| | C | -2.33126200 | -0.37871800 | -0.00377600 |
| | N | -1.94340700 | -1.66340400 | -0.02686200 |
| | C | 1.32994300 | -0.14894300 | -0.00323800 |
| | C | 2.25064200 | -1.22150800 | 0.03449400 |
| | C | 3.62236100 | -0.98854800 | 0.03485700 |
| | C | 4.12565800 | 0.31986000 | -0.00228800 |
| | C | 3.22499000 | 1.38703400 | -0.04142100 |
| | C | 1.84517800 | 1.16348100 | -0.04203500 |
| | S | -3.90550300 | 0.31704300 | -0.00389400 |
| | N | -1.16187700 | 1.80753000 | 0.04071200 |
| | H | 1.85639000 | -2.23152600 | 0.06324700 |
| | H | 4.30713500 | -1.83325500 | 0.06521500 |
| | H | 5.19789600 | 0.49954700 | -0.00132400 |
| | H | 3.59541300 | 2.40947400 | -0.07376700 |
| | H | 1.15327000 | 1.99582400 | -0.07585600 |
| | H | -1.85140500 | 2.09018600 | -0.66170400 |
| | H | -1.60522000 | 2.07464000 | 0.92325500 |

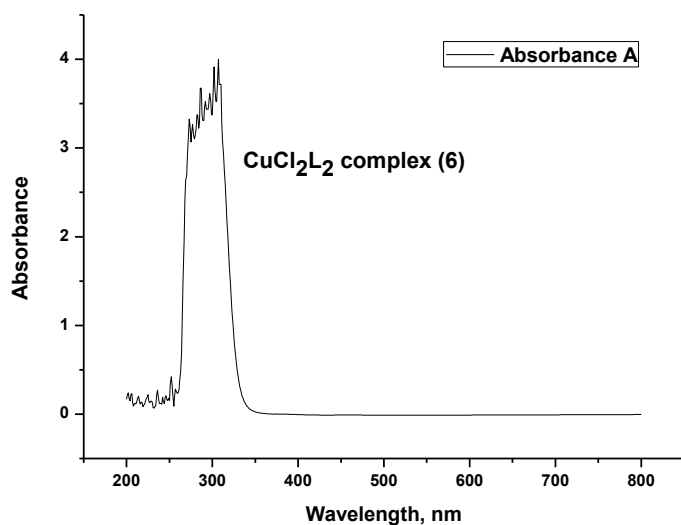


Figure S1. UV-visible spectrum of the copper(II) complex (6).

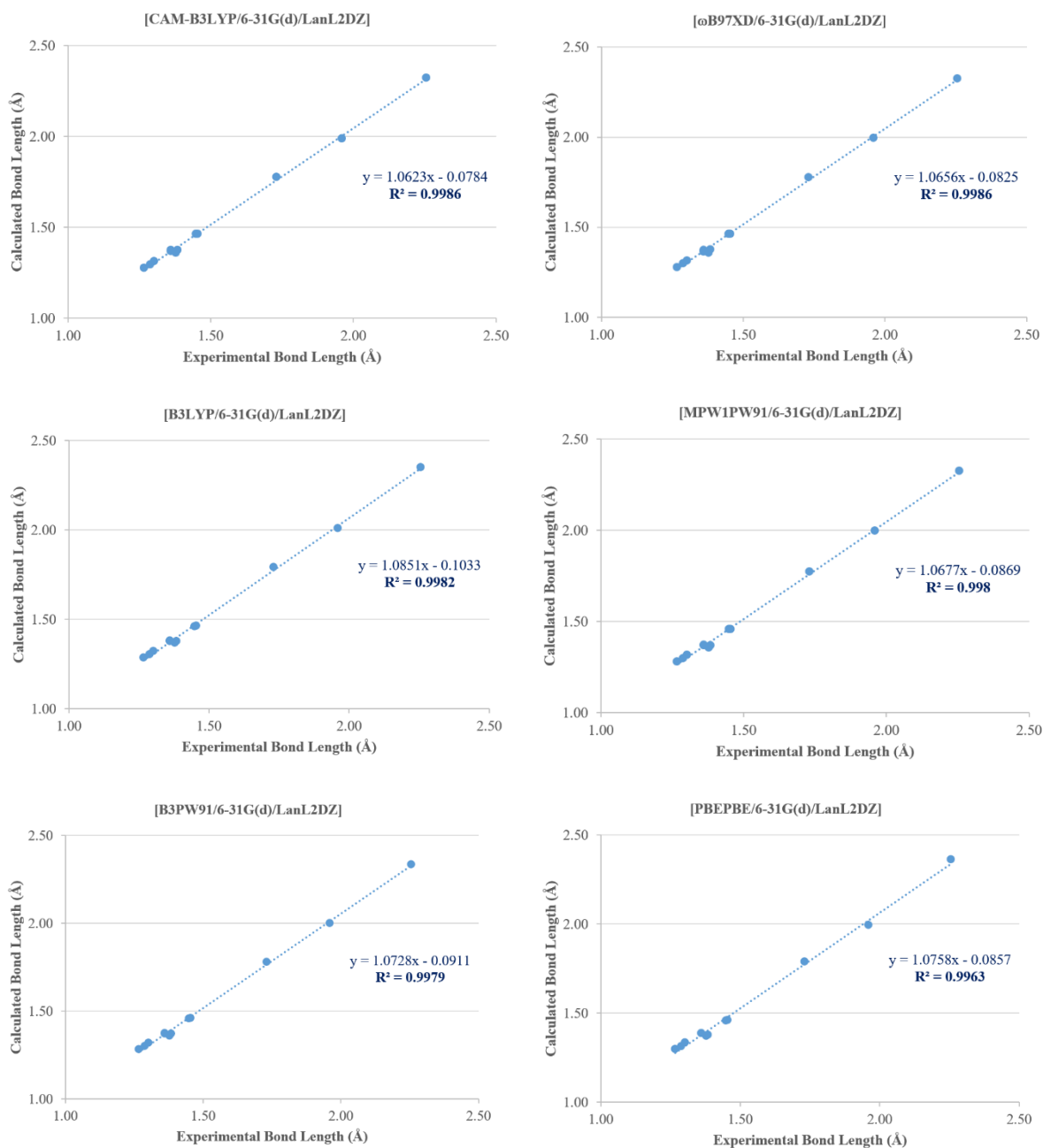


Figure S2. The correlation between experimental and computed values for the selected bond lengths present in the copper(II) complex (6) using pure and hybrid functionals with 6-31G(d)/LanL2DZ mixed basis set.

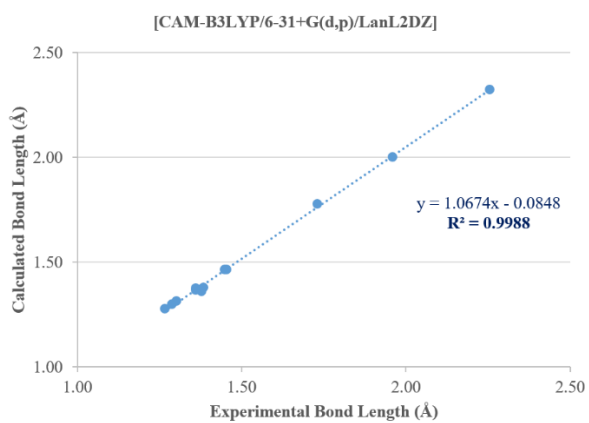
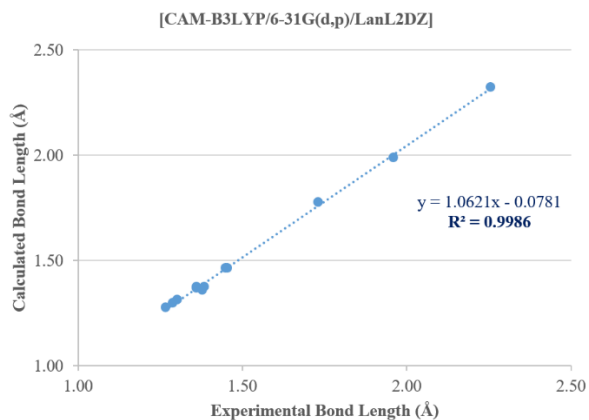
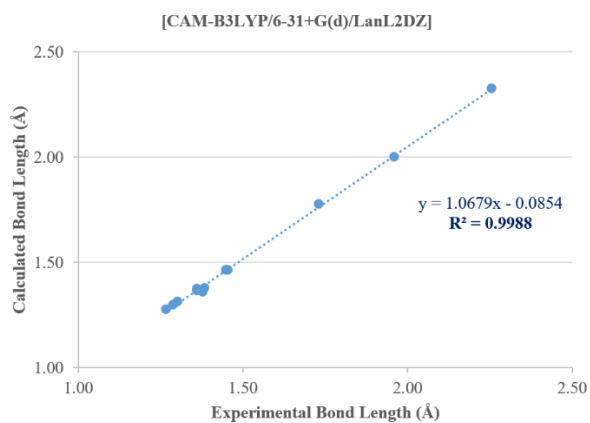


Figure S3. A comparative correlation to evaluate the performance of various basis sets using CAM-B3LYP method for experimental and calculated bond lengths, for the selected bond lengths present in the copper(II) complex (6).