SUPPLEMENTARY MATERIAL TO

**(E)-4-(((2-amino-5-chlorophenyl)imino)methyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis**

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**Figure S1.** The B3LYP optimized geometry of the TSEnol-Keto of the *meta* isomer.

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**Figure S2.** Optimized geometry and the isosurface Fukui map of the **L-**.

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**Figure S3.** The 1H- and 13C-NMR spectra of the **HL** Schiff base.

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**Figure S4.** The QTAIM molecular graphs of the **HL** Schiff base and [Cu(**L**)Cl] complex.

**Table S1.** The elemental analysis of the investigated compounds.

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical formula | Experimental (%) | | | | Calculated (%) | | | | Species |
| Metal | N | H | C | Metal | N | H | C |
| C14H14ClN3O2 | - | 15.01 | 4.76 | 57.34 | - | 14.40 | 4.84 | 57.64 | **HL** |
| C14H13Cl2CuN3O2 | 17.02 | 10.46 | 3.48 | 43.52 | 16.31 | 10.78 | 3.36 | 43.15 | [Cu(**L**)Cl] |

**Table S2.** Relative electronic energies (E+ZPE) for the investigated species of the **HL** Schiff base (in term of kJ.mol-1).

|  |  |  |  |
| --- | --- | --- | --- |
| ΔG  (Methanol solution) | E+ZPE | | **Species** |
| Gas phase | Methanol solution |
| 0 | 0 | 0 | Enol tautomer of the *meta* isomer |
| 24.59 | 29.15 | 27.38 | Keto tautomer of the *meta* isomer |
| 20.94 | 26.34 | 24.23 | Enol tautomer of the *para* isomer |
| 28.63 | 33.67 | 30.89 | Keto tautomer of the *para* isomer |
| 123.91 | 159.11 | 164.90 | TSEnol-Keto |

**Table S3.** Important experimental and the DFT-computed IR vibrational frequencies (cm-1) of the **HL** Schiff base (Enol tautomer of the *meta* isomer) and [Cu(**L**)Cl] complex.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Experimental frequencies | | Calculated frequencies | | | | Vibrational assignment |
| **HL** | [Cu(**L**)Cl] | **HL** | | [Cu(**L**)Cl] | |
| Frequency | Intensity  (km.mol-1) | Frequency | Intensity  (km.mol-1) |
| - | 547 (m) | - | - | 532 | 41 | υasym(Cu-N, Cu-O) |
| - | 640 (w) | - | - | 618 | 5 | υsym(Cu-N, Cu-O) |
| 765 (m) | 767 (m) | 759 | 16 | 744 | 9 | Breathing of the aromatic rings |
| 846 (w) | 851 (w) | 834 | 24 | 836 | 14 | δop(aromatic hydrogens) |
| 809 (m) | - | 802 | 79 | - | - | δop(H12) |
| 912 (w) | 915 (w) | 886 | 51 | 892 | 23 | υ(C13-Cl1) |
| 1032 (vs) | 1027 (s) | 1039 | 73 | 1037 | 95 | υ(C1-O1) |
| 1208 (m) | 1188 (m) | 1173 | 126 | 1160 | 94 | υ(C9-N2) |
| 1298 (m) | 1262 (m) | 1284 | 105 | 1249 | 228 | υ(C9-N2)+ υ(Ar-C) |
| 1380 (vs) | 1416 (vs) | 1370 | 112 | 1421 | 137 | υ(C1-O1) |
| 1471 (m) |  | 1456 | 68 | 1482 | 186 | υ(C9-N2) |
| 1521 (m) | 1507 (m) | 1535 | 16 | 1496 | 127 | υasym(C=C) of the benzene ring |
| 1557 | 32 | 1540 | 24 | υsym(C=C) of the benzene ring |
|  |  | 1570 | 98 | 1563 | 108 | υ(C=N, C=C) of the right pyridine rings + υ(C4-N2) |
| 1617 (vs) | 1605 (vs) | 1584 | 125 | 1567 | 58 | υ(C=N, C=C) of the pyridine rings |
| 1592 | 221 | 1581 | 279 | υ(C4=N2) |
| 2746 (m) | 2741 (s) | 2852 | 40 | 2852 | 65 | υsym(C-H) of -CH2- groups |
| 2840 (s) | 2838 (s) | 2876 | 30 | 2876 | 36 | υasym(C-H) of -CH2- groups |
| 2919 (s) | 2918 (s) | 2914 | 20 | 2930 | 14 | υsym(C-H) of the methyl groups |
| 3110 (vs, br) | 3096 (vs, br) | 2954 | 36 | 3032 | 15 | υ(C4-H1) |
| 3015 | 11 | 3034 | 14 | υasym(C-H) of the methyl groups |
| 3087-3056 | 3 | 3289-3073 | 4 | υasym(C-H) of the aromatic hydrogens |
|  | 3126 | 471 | - | - | υ(O1-H12) |
| 3463 (m, br) | 3362 (s) | 3443 | 28 | 3353 | 45 | υsym(H-N-H) of the -NH2 amine group |
| 3444 (s) | 3547 | 39 | 3417 | 48 | υasym(H-N-H) of the -NH2 amine group |
| 3260 | 59 | 3703 | 55 | υ(O2-H5) |

**Table S4.** Important topological parameters of the investigated species (energies in term of kJ.mol-1).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Bond | ρ(r) | ∇2ρ | Vb | Gb | Hb | -Gb/Vb |
| **HL** Schiff base | |  |  |  |  |  |
| C1-O1 | 0.299251 | -0.38595 | -2027.82 | 887.36 | -1140.45 | 0.44 |
| O1-H12 | 0.331725 | -2.29726 | -1873.5 | 183.54 | -1689.97 | 0.10 |
| N2…H12 | 0.049647 | 0.1126 | -120.763 | 97.30 | -23.48 | 0.81 |
| C4-N2 | 0.365541 | -0.84807 | -2401.46 | 922.68 | -1478.80 | 0.38 |
| C9-N2 | 0.292365 | -0.82668 | -1365.14 | 411.53 | -953.62 | 0.30 |
| C10-N3 | 0.305063 | -0.89704 | -1471.92 | 441.84 | -1030.08 | 0.30 |
| C7-O2 | 0.254508 | -0.48479 | -1429.14 | 555.62 | -873.54 | 0.39 |
| O2-H5 | 0.366696 | -2.55259 | -2048.69 | 187.41 | -1861.28 | 0.09 |
| O2…H2 | 0.015167 | 0.075335 | -31.9744 | 40.69 | 8.72 | 1.27 |
| C13-Cl1 | 0.189252 | -0.26191 | -504.796 | 166.52 | -338.26 | 0.33 |
| [Cu(**L**)Cl] complex | |  |  |  |  |  |
| C1-O1 | 0.344981 | -0.17071 | -2851.17 | 1369.62 | -1481.55 | 0.48 |
| C4-N2 | 0.348704 | -0.70745 | -2619.77 | 1077.93 | -1541.85 | 0.41 |
| C9-N2 | 0.294602 | -0.93463 | -1471.63 | 429.38 | -1042.28 | 0.29 |
| C10-N3 | 0.276305 | -0.83136 | -1209.91 | 332.37 | -877.52 | 0.27 |
| C7-O2 | 0.258655 | -0.54536 | -1562.55 | 602.46 | -960.07 | 0.39 |
| O2-H5 | 0.350059 | -1.811 | -1535.56 | 173.99 | -1361.55 | 0.11 |
| C13-Cl1 | 0.187947 | -0.24896 | -487.747 | 162.25 | -325.51 | 0.33 |
| Cu-O1 | 0.075907 | 0.521302 | -315.888 | 328.86 | 12.98 | 1.04 |
| Cu-N2 | 0.166307 | 0.872714 | -1020.69 | 796.48 | -224.21 | 0.78 |
| Cu-N3 | 0.07758 | 0.441895 | -304.898 | 297.34 | -7.58 | 0.98 |
| Cu-Cl2 | 0.063669 | 0.272222 | -201.315 | 189.91 | -11.41 | 0.94 |
| O2…H2 | 0.015259 | 0.071397 | -31.9744 | 39.39 | 7.43 | 1.23 |