**Supplementary Data for**

Synthesis and Antibacterial Testing of Cu(II)-3-Picolylamine Complexes

Ninna Arifatun Nurul Azizah, Monica Hening Citra Dewi, Sentot Budi Rahardjo\*, Soerya Dewi Marliyana

Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Sebelas Maret, Jl. Ir. Sutami 36A Kentingan, Surakarta, Indonesia

\* Corresponding author: sentotbr@staff.uns.ac.id

1. Calculation of Cu Content

The Cu content in each sample can be determined by the following calculation:

$$Cu concentration \left(ppm\right)=\frac{weight of Cu (mg)}{volume (L)}$$

Weight of Cu (mg) = Cu concentration (ppm) × solution volume (L)

$$\%Cu=\frac{weight of Cu}{sampel weight (mg)}×100\%$$

**Table S1**. Data from Calculation of Copper Content with SSA in the Cu(II)-(Lamine) Complex

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample weight (mg) | Volume (mL) | Concentration (ppm) | Mass of Cu (mg) | %Cu | %Cu average | STD |
| 1.6 | 100 | 0.5745 | 0.143625 | 8.98 | 8.92 | 0.05 |
| 0.5695 | 0.142375 | 8.90 |
| 0.5685 | 0.142125 | 8.88 |

**Table S2**. Calculation of Cu Content for Various Complex Formulas in Theory

|  | Compound | Molar mass of the compound | Molar mass of Cu | % Cu |
| --- | --- | --- | --- | --- |
| 1:6 | [Cu(L)6].SO4 | 808.451 | 63.55 | 7.861 |
|  | [Cu(L)6].SO4.H2O | 826.451 | 63.55 | 7.689 |
|  | [Cu(L)6].SO4.2H2O | 844.451 | 63.55 | 7.525 |
|  | [Cu(L) 6].SO4.3H2O | 862.451 | 63.55 | 7.369 |
|  | [Cu(L) 6].SO4.4H2O | 880.451 | 63.55 | 7.218 |
|  | [Cu(L) 6].SO4.5H2O | 898.451 | 63.55 | 7.073 |
|  | [Cu(L) 6].SO4.6H2O | 916.451 | 63.55 | 6.934 |
| 1:5 | [Cu(L)5].SO4 | 700.311 | 63.55 | 9.075 |
|  | [Cu(L)5].SO4.H2O | 718.311 | 63.55 | 8.847 |
|  | [Cu(L)5].SO4.2H2O | 736.311 | 63.55 | 8.631 |
|  | [Cu(L) 5].SO4.3H2O | 754.311 | 63.55 | 8.425 |
|  | [Cu(L) 5].SO4.4H2O | 772.311 | 63.55 | 8.229 |
|  | [Cu(L) 5].SO4.5H2O | 790.311 | 63.55 | 8.041 |
|  | [Cu(L) 5].SO4.6H2O | 808.311 | 63.55 | 7.862 |
| 1:4 | [Cu(L)4].SO4 | 592.171 | 63.55 | 10.732 |
|  | [Cu(L)4].SO4.H2O | 610.171 | 63.55 | 10.415 |
|  | [Cu(L)4].SO4.2H2O | 628.171 | 63.55 | 10.117 |
|  | [Cu(L)4].SO4.3H2O | 646.171 | 63.55 | 9.835 |
|  | [Cu(L)4].SO4.4H2O | 664.171 | 63.55 | 9.568 |
|  | [Cu(L)4].SO4.5H2O | 682.171 | 63.55 | 9.316 |
|  | **[Cu(L)4].SO4.6H2O** | **700.171** | 63.55 | **9.076** |
| 1:3 | [Cu(L)3].SO4 | 484.031 | 63.55 | 13.129 |
|  | [Cu(L)3].SO4.H2O | 502.031 | 63.55 | 12.658 |
|  | [Cu(L)3].SO4.2H2O | 520.031 | 63.55 | 12.220 |
|  | [Cu(L)3].SO4.3H2O | 538.031 | 63.55 | 11.812 |
|  | [Cu(L)3].SO4.4H2O | 556.031 | 63.55 | 11.429 |
|  | [Cu(L)3].SO4.5H2O | 574.031 | 63.55 | 11.071 |
|  | [Cu(L)3].SO4.6H2O | 592.031 | 63.55 | 10.734 |
| 1:2 | [Cu(L)2].SO4 | 375.891 | 63.55 | 16.906 |
|  | [Cu(L)2].SO4.H2O | 393.891 | 63.55 | 16.134 |
|  | [Cu(L)2].SO4.2H2O | 411.891 | 63.55 | 15.429 |
|  | [Cu(L)2].SO4.3H2O | 429.891 | 63.55 | 14.783 |
|  | [Cu(L)2].SO4.4H2O | 447.891 | 63.55 | 14.189 |
|  | [Cu(L)2].SO4.5H2O | 465.891 | 63.55 | 13.641 |
|  | [Cu(L)2].SO4.6H2O | 483.891 | 63.55 | 13.133 |
| 1:1 | [Cu(L)].SO4 | 267.751 | 63.55 | 23.735 |
|  | [Cu(L)].SO4.H2O | 285.751 | 63.55 | 22.239 |
|  | [Cu(L)]. SO4.2H2O | 303.751 | 63.55 | 20.922 |
|  | [Cu(L)].SO4.3H2O | 321.751 | 63.55 | 19.751 |
|  | [Cu(L)].SO4.4H2O | 339.751 | 63.55 | 18.705 |
|  | [Cu(L)].SO4.5H2O | 357.751 | 63.55 | 17.764 |
|  | [Cu(L)].SO4.6H2O | 375.751 | 63.55 | 16.913 |

1. TGA Analysis Calculations

**Table S3**. Calculation of Molecule Release in Cu(II)-(L) Complex (n= 4, 5 or 6)

|  |  |  |
| --- | --- | --- |
| T (°C) | Weight Loss (%) | Estimated H2O in formulaCu(L)4.SO4.4H2O (Molecular mass = 664.171 g/mol) |
| Experiment | Theory |
| 55-130 | 13.45 | 13.45% × 664.17 = 89.33~ 5 H2O | 72 (10.84%) |
| T (°C) | Weight loss (%) | Estimated H2O in formulaCu(L)4.SO4.5H2O (Molecular mass = 682.171 g/mol) |
| Experiment | Theory |
| 55-130 | 13.45 | 13.45% × 682.17 = 91.75~ 5 H2O | 90 (13.19%) |
| T (°C) | Weight loss (%) | Estimated H2O in formulaCu(L)4.SO4.6H2O (Molecular mass = 700.171 g/mol) |
| Experiment | Theory |
| 55-130 | 13.45 | 13.45% × 700.17 = 94.17~ 5 H2O | 108 (15.42%) |

1. Conductivity Measurement

The molar electrical conductivity of the standard and sample solutions is obtained as follows:

Ʌ\*m = $\frac{10^{-3} cm^{3} .L^{-1}}{C}$ K\*

Where, K\* is the corrected specific conductivity (μS. cm-1) (K – Ksolvent), K is the specific conductivity of the solution (μS. cm-1), Ʌ\*m is the corrected molar electrical conductivity (S.cm2.mol-1), C is the molar concentration of the electrolyte (mol.L-1).

**Table S4**. Conductivity of standard solutions and Cu(II)-(3-picolylamine) complex samples with methanol solvent (1.10-3 M)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Solution | K | k\* | Ʌ\*m(S.cm2.mol-1) | Ʌ\*m average(S.cm2.mol-1) | Number of ions |
| DMSO | 0 | 0 | 0 | - | - |
| NaCl | 6 | 6 | 6 | 6 | 2 |
| 6 | 6 | 6 |
| 6 | 6 | 6 |
| CuSO4.5H2O | 5 | 5 | 5 | 5 | 2 |
| 5 | 5 | 5 |
| 5 | 5 | 5 |
| CoSO4.7H2O | 7 | 7 | 7 | 7 | 2 |
| 7 | 7 | 7 |
| 7 | 7 | 7 |
| FeSO4.7H2O | 6 | 6 | 6 | 6 | 2 |
| 6 | 6 | 6 |
| 6 | 6 | 6 |
| NiCl2.6H2O | 65 | 65 | 65 | 65 | 3 |
| 65 | 65 | 65 |
| 65 | 65 | 65 |
| CuCl2.2H2O | 28 | 28 | 28 | 29 | 3 |
| 29 | 29 | 29 |
| 29 | 29 | 29 |
| CoCl2.6H2O | 52 | 52 | 52 | 52 | 3 |
| 52 | 52 | 52 |
| 52 | 52 | 52 |
| Cu(NO3)2.3H2O | 86 | 86 | 86 | 86 | 3 |
| 86 | 86 | 86 |
| 86 | 86 | 86 |
| Cu(II)-3-*picolylamine* | 9 | 9 | 9 | 9 | 2 |
| 9 | 9 | 9 |
| 9 | 9 | 9 |

1. Moment Magnetic Measurement

The results of measuring the magnetic susceptibility of the complex [Cu(3-picolylamine)4(H2O)]SO4.5H2O are shown in Table 5.

**Table S5**. Effective Magnetic Moment Measurement Data (μeff) of Complex

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | Mass (gr) | T (K) | Xg (10-6) (cgs) |
| Cu(II) complex | 0.0639 | 298 | 1.489 |
| 0.0654 | 298 | 1.478 |
| 0.0647 | 298 | 1.482 |

The effective magnetic moment is calculated using the formula:

*μeff* =2.828 [XA.T]1/2

Diamagnetic correction of [Cu(3-picolylamine)4.H2O].SO4.5H2O :

Cu2+ = 1 × (-13.00 × 10-6 cgs) = (-13.00 × 10-6 cgs)

SO42-  = 1 × (-40.00 × 10-6 cgs) = (-40.00 × 10-6 cgs)

H = 8 × 4 × (-2.93 × 10-6 cgs) = (-93.76 × 10-6 cgs)

C aromatic = 5 × 4 × (-6.24 × 10-6 cgs) = (-124.8 × 10-6 cgs)

C alifatic = 1 × 4 × (-6.00 × 10-6 cgs) = (-24.00 × 10-6 cgs)

N aromatic = 1 × 4 × (-4.61 × 10-6 cgs) = (-18.44 × 10-6 cgs)

N alifatic = 1 × 4 × (-5.57 × 10-6 cgs) = (-22.28 × 10-6 cgs)

H2O = 6 × (-13.00 × 10-6 cgs) = (-78.00 × 10-6 cgs)

 ΣXL = - 0.414 × 10-3 cgs

1. Complex [Cu(3*-*picolylamine)4.H2O].SO4.5H2O

Xg = 1.489 × 10-6 cgs

Xm = Xg × BM

 = 1.489 × 10-6 × 700.171

 = 1.043 × 10-3 cgs

XA = XM – XL

 = (1.043 × 10-3)-( -0.414 × 10-3) cgs

 = 1.457 10-3 cgs

*μeff* = 2.828 [XA.T]1/2

 = 2.828 [1.457 10-3 cgs × 298]1/2

 = 1.863 BM

1. Complex [Cu(3-picolylamine)4.H2O].SO4.5H2O

Xg = 1.478 × 10-6 cgs

Xm = Xg × BM

 = 1.478 × 10-6 × 700.171

 = 1.034 × 10-3 cgs

XA = XM – XL

 = (1.034 × 10-3)-( -0.414 × 10-3) cgs

 = 1.448 10-3 cgs

*μeff* = 2.828 [XA.T]1/2

 = 2.828 [1.448 10-3 cgs × 298]1/2

 = 1.857 BM

1. Complex [Cu(3-picolylamine)4.H2O].SO4.5H2O

Xg = 1.485 × 10-6 cgs

Xm = Xg × BM

 = 1.485 × 10-6 × 700.171

 = 1.039 × 10-3 cgs

XA = XM – XL

 = (1.039 × 10-3)-( -0.414 × 10-3) cgs

 = 1.453 10-3 cgs

*μeff* = 2.828 [XA.T]1/2

 = 2.828 [1.457 10-3 cgs × 298]1/2

 = 1.861 BM

1. Molar Absorptivity

The molar absorptivity for CuSO4·5H2O and the complex is calculated using the Lambert-Beer law equation:

A = ɛ.b.C

Where, A is the absorbance, ɛ is the molar absorptivity (L.mol-1.cm-1), b is the ray travel distance (1 cm), and C is the concentration (mol.L-1).

1. CuSO4.5H2O in DMSO

A = 0.2551

W = 0.0111

C = $\frac{W}{Mr × V}$ = $\frac{0.0111 gram}{249.69 \frac{gr}{mol} × 0.01 L}$ = 0.0044 M

ɛ = $\frac{A}{b × C}$ = $\frac{0.2551}{1 × 0.0044 M}$ = 57.97 L.mol-1.cm-1

1. Complex in DMSO

A = 0.1533

W = 0.0032

C = $\frac{W}{Mr × V}$ = $\frac{0.0032 gram}{700.17 \frac{gr}{mol} × 0.01 L}$ = 0.00045 M

ɛ = $\frac{A}{b × C}$ = $\frac{0.1533}{1 × 0.00045 M}$ = 340.66 L.mol-1.cm-1