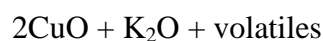
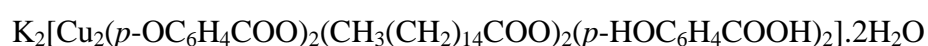


**PUBLICATION AND LETTER OF ACCEPTANCE/  
ABSTRACTS/ CERTIFICATE  
FOR ORAL/ POSTER PRESENTATION  
IN NATIONAL/INTERNATIONAL  
CONFERENCES AND SEMINARS**

**GRAVIMETRIC CALCULATION OF THE EXPECTED RESIDUE OF COMPLEX 1**

The expected residue of **Complex 1** is calculated based on the assumption that, the residue of the complex are copper oxide and potassium oxide, and the weight of the complex, 100 % equivalent to 100 g. The reaction is proceeded as below.



$$\text{Formula weight of Complex 1} = 1300.6 \text{ g mol}^{-1}$$

$$\text{Formula weight of CuO} = 79.6 \text{ g mol}^{-1}$$

$$\text{Formula weight of K}_2\text{O} = 94.2 \text{ g mol}^{-1}$$

Based on the above assumptions and equation,



$$1300.6 \text{ g} \longrightarrow (2 \times 79.6 \text{ g}) + 94.2 \text{ g} = 253.3 \text{ g}$$

$$\text{The expected percentage of residue} = 253.3 / 1300.6 \times 100 \%$$

$$= 19.5 \%$$

### CALCULATION OF EFFECTIVE MAGNETIC MOMENT, $\mu_{\text{eff}}$ OF COMPLEX 1

$$\begin{aligned} M &= g \times MW \\ &= 2.97 \times 10^{-6} \text{ cm}^3 \text{g}^{-1} \times 1300.6 \text{ gmol}^{-1} \\ &= 386.28 \times 10^{-5} \text{ cm}^3 \text{mol}^{-1} \end{aligned}$$

The molar susceptibility obtained has to be corrected for the inherent diamagnetic contribution from the ligands and metal ions using the table of Pascal's constants

$$M^{\text{corr}} = M - \text{dia}$$

C aromatic	= 24 x (6.24 x 10 <sup>-6</sup> )	= 149.76 x 10 <sup>-6</sup>
C aliphatic	= 36 x (-6.00 x 10 <sup>-6</sup> )	= -216.00 x 10 <sup>-6</sup>
Hydrogen	= 82 x (-2.93 x 10 <sup>-6</sup> )	= -240.26 x 10 <sup>-6</sup>
O alcohol	= 10 x (-4.61 x 10 <sup>-6</sup> )	= -46.10 x 10 <sup>-6</sup>
O carbonyl	= 6 x (1.73 x 10 <sup>-6</sup> )	= 10.38 x 10 <sup>-6</sup>
Cu(II)	= 2 x (-1.28 x 10 <sup>-5</sup> )	= -2.56 x 10 <sup>-5</sup>
K	= 2 x (1.50 x 10 <sup>-5</sup> )	= 3.00 x 10 <sup>-5</sup>
H <sub>2</sub> O	= 2 x (-1.30 x 10 <sup>-5</sup> )	= -2.60 x 10 <sup>-5</sup>
<b>Total dia</b>	<b>= -36.38 x 10<sup>-5</sup></b>	

So,

$$\begin{aligned} M^{\text{corr}} &= 386.28 - (-36.38) \times 10^{-5} \text{ cm}^3 \text{mol}^{-1} \\ &= 422.66 \times 10^{-5} \text{ cm}^3 \text{mol}^{-1} \end{aligned}$$

$$\mu_{\text{eff}} = 2.824 (M^{\text{corr}} T - N)^{1/2}$$

N is the temperature-independent paramagnetism,  $60 \times 10^{-6}$  c.g.s e.m.u

Hence,

$$\begin{aligned} \mu_{\text{eff}} &= 2.824 [2.98 (422.66 - 12) \times 10^{-5}]^{1/2} \text{ B.M.} \\ &= 3.12 \text{ B.M.} \end{aligned}$$

**CALCULATION OF EXCHANGE INTEGRAL OF COMPLEX 1**

**Bleany and Bowers equation for two copper(II) centres:**

$$M = \frac{2Ng^2}{3kT} \{1 + \frac{1}{3} \exp(-2J/kT)\}^{-1} + 2N$$

where :

$\chi_m$  = Molar Magnetic susceptibility ( $\text{cm}^3/\text{mol}$ )

T = Room temperature in Kelvin (298 K)

N = Temperature independent paramagnetism,  $60 \times 10^{-6}$  c.g.s e.m.u

g = lande factor, 2.2

$\mu_B$  = Bohr Magneton ( $4.6686 \times 10^{-5} \text{ cm}^{-1} \text{ G}^{-1}$ )

k = Boltzmann constant,  $0.695 \text{ cm}^{-1} \text{ K}^{-1}$

N = Avogadro's number

$$M = \frac{2Ng^2}{3kT} \{1 + \frac{1}{3} \exp(-2J/kT)\}^{-1} + 0.12 \times 10^{-3}$$

After rearranging the above equation and by putting the necessary values for all constants,

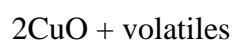
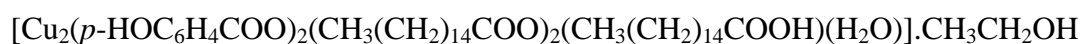
$$-2J = \{\ln[\{1.2186 \times 10^{-2}/(\chi_m - 0.12 \times 10^{-3})\} - 3]\}207.11$$

Putting in the  $\chi_m = 4.2266 \times 10^{-3}$

$$-2J = -60 \text{ cm}^{-1}$$

## GRAVIMETRIC CALCULATION OF FORMULA MASS OF COMPLEX 2

The formula mass of **Complex 2** is calculated based on the assumption that, the residue of the complex is copper oxide, the weight of the complex, 100 % equivalent to 100 g and the reaction is proceeded as below.



$$\text{Amount of residue} = 14.3 \text{ g}$$

$$\text{Formula weight of CuO} = 79.6 \text{ g mol}^{-1}$$

$$\text{Mol of CuO} = 14.3 \text{ g} / 79.6 \text{ g mol}^{-1} = 0.18 \text{ mol}$$

From the above equation, 2 mol of CuO equivalent to 1 mol of **Complex 2**. Thus, 0.18 mole of CuO equivalent to 0.09 mole of **Complex 2**.

As such,

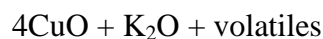
$$\text{Formula weight of the complex} = 100 \text{ g} / 0.09 \text{ mol}$$

$$= 1111.1 \text{ g mol}^{-1}$$

**GRAVIMETRIC CALCULATION OF FORMULA MASS OF COMPLEX 4**

The amount of residue for **Complex 4** at temperatures above 550°C to 900°C is 18.0%.

The formula mass is calculated based on the assumption that, the residue are K<sub>2</sub>O and CuO; the weight of the complex, 100% equivalent to 100g and the reaction is proceeded as below.



Amount of residue	=	18.0 g
Formula weight of CuO	=	79.6 g/mol
Formula weight of K <sub>2</sub> O	=	94.2 g/mol
Percentage of CuO	=	$(4 \times 79.6) / [(4 \times 79.6) + 94.2] \times 100\%$
	=	77.2 %
Mass of CuO	=	$(77.2/100) \times 18.0 \text{ g}$
	=	13.9 g
Mole CuO	=	$13.9 \text{ g} / 79.6 \text{ g mol}^{-1}$
	=	0.17 mol

From the above equation, 4 mol of CuO equivalent to 2 mol of **Complex 4**. Thus, 0.17 mol of CuO equivalent to 0.09 mol of **Complex 4**.

Hence,

Formula weight of the complex	=	$100/0.09$
	=	$1111.1 \text{ g mol}^{-1}$

## Appendix 7

The crystal data and structure refinement of the peacock-blue crystal of  $[\text{Cu}_2(\text{CH}_3(\text{CH}_2)_8\text{COO})_4]$  are shown in **Table A.1** while selected bond lengths are shown in

### Table A.2.

**Table A.1** : Crystallographic and refinement details of  $[\text{Cu}_2(\text{CH}_3(\text{CH}_2)_8\text{COO})_4]$  crystal

Empirical formula	$[\text{Cu}(\text{C}_{20}\text{H}_{38}\text{O}_4)]$
Formula weight	406.04
Temperature	100 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimension	a = 5.20450 (10) Å $\alpha = 65.3320 (10)^\circ$ b = 14.3270 (3) Å      = 86.85 (10)° c = 16.4384 (4) Å      = 82.8710 (10)°
Volume	1105.24 (4) Å <sup>3</sup>
Z, Calculated density	2, 1.220 Mg/m <sup>3</sup>
Absorption coefficient	1.007 mm <sup>-1</sup>
F(000)	438
Crystal size	0.26 x 0.20 x 0.10 mm
Theta range for data collection	1.36 to 28.4 °
Limiting indices ( $\pm h, \pm k, \pm l$ )	-6/6, -19/19, -21/21
Reflections collected / unique	11169 / 5497 [ $R_{\text{int}} = 0.0190$ ]
Absorption correction	Multi-scan
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	5497 / 0 / 236
Goodness-of-fit on $F^2$	1.153
Final R indices [ $I > 2\sigma(I)$ ]	R1 = 0.0352, wR2 = 0.1064
$\Delta\rho_{\text{max}}$ and $\Delta\rho_{\text{min}}$	0.504 and -0.812 e Å <sup>-3</sup>

**Table A.2** : Selected bond lengths [Å] of crystal

Cu1 – O12	1.9358(16)
Cu1 – O14	1.9430(16)
Cu1 – O2	1.9702(16)
Cu1 – O	2.0140(14)

## Appendix 8

The crystal data and structure refinement of the peacock-blue crystal of  $[\text{Cu}_2(\text{CH}_3(\text{CH}_2)_6\text{COO})_4]$  are shown in **Table A.3** while selected bond lengths are shown in

### Table A.4.

**Table A.3 :** Crystallographic and refinement details of  $[\text{Cu}_2(\text{CH}_3(\text{CH}_2)_6\text{COO})_4]$  crystal

Empirical formula	$[\text{Cu}(\text{C}_{16}\text{H}_{30}\text{O}_4)]$
Formula weight	349.94
Temperature	296 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimension	a = 5.14710 (10) Å $\alpha = 97.451 (2)^\circ$ b = 12.0209 (3) Å      = 90.507 (2)° c = 14.1881 (3) Å      = 98.376 (2)°
Volume	862.71 (3) Å <sup>3</sup>
Z, Calculated density	2, 1.347 Mg/m <sup>3</sup>
Absorption coefficient	1.278 mm <sup>-1</sup>
F(000)	374
Crystal size	0.20 x 0.08 x 0.05 mm
Theta range for data collection	1.44 to 27.49 °
Limiting indices ( $\pm h, \pm k, \pm l$ )	-6/6, -15/15, -18/18
Reflections collected / unique	7732 / 3948 [ $R_{\text{int}} = 0.0280$ ]
Absorption correction	Multi-scan
Refinement method	Full-matrix least-squares on $F^2$
Data / restraints / parameters	3948 / 0 / 192
Goodness-of-fit on $F^2$	1.142
Final R indices [ $I > 2\sigma(I)$ ]	$R1 = 0.0360, wR2 = 0.1010$
$\Delta_{\text{max}}$ and $\Delta_{\text{min}}$	0.608 and -1.369 e Å <sup>-3</sup>

**Table A.4** Selected bond lengths [Å] of crystal

Cu1 – O1	1.9445(17)
Cu1 – O3	1.9460(17)
Cu1 – O2	1.963(2)
Cu1 – O4	2.009(2)