Appendix 1

PUBLICATION AND LETTER OF ACCEPTANCE/

ABSTRACTS/ CERTIFICATE

FOR ORAL/ POSTER PRESENTATION

IN NATIONAL/INTERNATIONAL

CONFERENCES AND SEMINARS

Appendix 2

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.

$$K_2[Cu_2(p\text{-}OC_6H_4COO)_2(CH_3(CH_2)_{14}COO)_2(p\text{-}HOC_6H_4COOH)_2].2H_2O \downarrow$$

$$2CuO + K_2O + \text{volatiles}$$

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

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

Formula weight of K_20 = 94.2 g mol^{-1}

Based on the above assumptions and equation,

1 mol of **Complex 1** ⟶ 2 mol CuO + 1 mol K_2O

1300.6 g ⟶ (2 x 79.6 g) + 94.2 g = 253.3 g

The expected percentage of residue = 253.3 / 1300.6 x 100 %

= 19.5 %

Appendix 3

CALCULATION OF EFFECTIVE MAGNETIC MOMENT, μ_{eff} OF COMPLEX 1

χ_M = χ_g x MW

= 2.97 x 10^{-6} cm^3g^{-1} x 1300.6 $gmol^{-1}$

= 386.28 x 10^{-5} cm^3mol^{-1}

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

χ_M^{corr} = χ_M - χ^{dia}

C aromatic	= 24 x (6.24 x 10^{-6})	= 149.76 x 10^{-6}
C aliphatic	= 36 x (-6.00 x 10^{-6})	= -216.00 x 10^{-6}
Hydrogen	= 82 x (-2.93 x 10^{-6})	= -240.26 x 10^{-6}
O alcohol	= 10 x (-4.61 x 10^{-6})	= -46.10 x 10^{-6}
O carbonyl	= 6 x (1.73 x 10^{-6})	= 10.38 x 10^{-6}
Cu(II)	= 2 x (-1.28 x 10^{-5})	= -2.56 x 10^{-5}
K	= 2 x (1.50 x 10^{-5})	= 3.00 x10^{-5}
H_2O	= 2 x (-1.30 x 10^{-5})	= -2.60 x 10^{-5}
Total χ^{dia}	**= -36.38 x 10^{-5}**	

So,

χ_M^{corr} = 386.28 - (-36.38) x 10^{-5} cm^3mol^{-1}

= 422.66 x 10^{-5} cm^3mol^{-1}

μ_{eff} = 2.824 $(\chi_M^{corr} T - N\alpha)^{1/2}$

Nα is the temperature-independent paramagnetism, 60 x 10^{-6} c.g.s e.m.u

Hence,

μ_{eff} = 2.824 [2.98 (422.66 – 12)x 10^{-5})]$^{1/2}$ B.M.

= 3.12 B.M.

Appendix 4

CALCULATION OF EXCHANGE INTEGRAL OF COMPLEX 1

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

$$\chi_M = \frac{2\,Ng^2\beta^2}{3kT}\{1 + {}^1/_3 \exp(-2J/kT)\}^{-1} + 2N\alpha$$

where :

χ_m = Molar Magnetic susceptibility (cm^3/mol)

T = Room temperature in Kelvin (298 K)

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

g = lande factor, 2.2

β = Bohr Magneton (4.6686×10^{-5} cm^{-1} G^{-1})

κ = Boltzmann constant, 0.695 cm^{-1} K^{-1}

N = Avogadro's number

$$\chi_M = \frac{2\,Ng^2\beta^2}{3kT}\{1 + {}^1/_3 \exp(-2J/kT)\}^{-1} + 0.12 \times 10^{-3}$$

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 $\chi_M = 4.2266 \times 10^{-3}$

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

Appendix 5

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.

$$[Cu_2(p\text{-}HOC_6H_4COO)_2(CH_3(CH_2)_{14}COO)_2(CH_3(CH_2)_{14}COOH)(H_2O)].CH_3CH_2OH \downarrow$$

$$2CuO + \text{volatiles}$$

Amount of residue	=	14.3 g
Formula weight of CuO	=	79.6 g mol^{-1}
Mol of CuO	=	14.3 g/79.6 g mol^{-1} = 0.18 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,

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

Appendix 6

GRAVIMETRIC CALCULATION OF FORMULA MASS OF COMPLEX 4

The amount of residue for **Complex 4** at temperatures above 550^{o}C to 900^{o}C is 18.0%. The formula mass is calculated based on the assumption that, the residue are K_2O and CuO; the weight of the complex, 100% equivalent to 100g and the reaction is proceeded as below.

$$2\ K[Cu_2(p\text{-}OC_6H_4COO)(CH_3(CH_2)_{14}COO)_3] \longrightarrow 4CuO + K_2O + \text{volatiles}$$

Amount of residue	=	18.0 g
Formula weight of CuO	=	79.6 g/mol
Formula weight of K_20	=	94.2 g/mol
Percentage of CuO	=	(4 x 79.6) / [(4 x 79.6) + 94.2] x 100%
	=	77.2 %
Mass of CuO	=	(77.2/100) x 18.0 g
	=	13.9 g
Mole CuO	=	13.9 g/79.6 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 g mol^{-1}

Appendix 7

The crystal data and structure refinement of the peacock-blue crystal of $[Cu_2(CH_3(CH_2)_8COO)_4]$ are shown in **Table A.1** while selected bond lengths are shown in **Table A.2**.

Table A.1 : Crystallographic and refinement details of $[Cu_2(CH_3(CH_2)_8COO)_4]$ crystal

Empirical formula	$[Cu(C_{20}H_{38}O_4)]$
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 α = 65.3320 (10)º b = 14.3270 (3) Å β = 86.85 (10)º c = 16.4384 (4) Å γ = 82.8710 (10)º
Volume	1105.24 (4) A^3
Z, Calculated density	2, 1.220 Mg/m^3
Absorption coefficient	1.007 mm^{-1}
F(000)	438
Crystal size	0.26 x 0.20 x 0.10 mm
Theta range for data collection	1.36 to 28.4 º
Limiting indices ($\pm h$, $\pm k$, $\pm l$)	-6/6, -19/19, -21/21
Reflections collected / unique	11169 / 5497 [R_{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 > 2σ(I)]	R1 = 0.0352, wR2 = 0.1064
$\Delta°_{max}$ and $\Delta°_{min}$	0.504 and -0.812 e $Å^{-3}$

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 $[Cu_2(CH_3(CH_2)_6COO)_4]$ are shown in **Table A.3** while selected bond lengths are shown in **Table A.4**.

Table A.3 : Crystallographic and refinement details of $[Cu_2(CH_3(CH_2)_6COO)_4]$ crystal

Empirical formula	$[Cu(C_{16}H_{30}O_4)]$
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 α = 97.451 (2)° b = 12.0209 (3) Å β = 90.507 (2)° c = 14.1881 (3) Å γ = 98.376 (2)°
Volume	862.71 (3) A^3
Z, Calculated density	2, 1.347 Mg/m^3
Absorption coefficient	1.278 mm^{-1}
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_{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 > 2σ(I)]	R1 = 0.0360, wR2 = 0.1010
$\Delta°_{max}$ and $\Delta°_{min}$	0.608 and -1.369 e $Å^{-3}$

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)