

Synthesis and characterization of Cu₃N nanoparticles using pyrrole-2-carbaldehydepropyliminato Cu(II) complex and Cu(NO₃)₂ as single-source precursors: the search for an ideal precursor

Rudo K. Sithole¹, Lerato F.E. Machogo¹, Mildred A. Airo¹, Siziwe S. Gqoba¹, Makwena J. Moloto³, Poslet Shumbula⁴, Juanita Van Wyk^{1*} and Nosipho Moloto^{1,2*}

¹Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Wits, 2050, South Africa

²Materials for Energy Research Group, University of the Witwatersrand, Private Bag 3, Wits, 2050, South Africa

³Department of Chemistry, Vaal University of Technology, P/Bag X021, Vanderbijlpark, 1900, South Africa

⁴Nanotechnology Innovation Centre, Advanced Materials Division, Mintek, Private Bag X3015, Randburg, 2125, South Africa

*Corresponding authors: Juanita van Wyk; Nosipho Moloto

Email: Juanita.VanWyk@wits.ac.za; Nosipho.Moloto@wits.ac.za

Tel: +27117176732/74

Fax: +2711 7176749

Supporting information

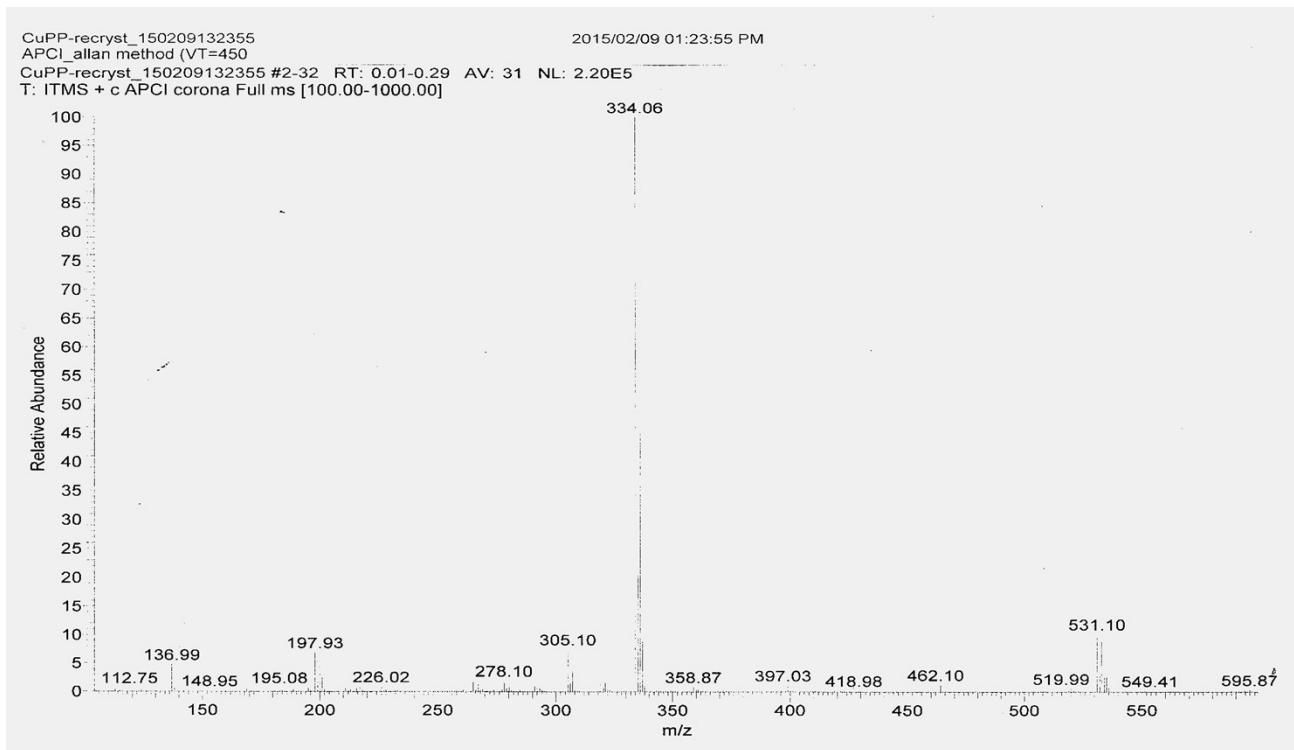


Fig. S1: Mass spectrum of the PPC complex.

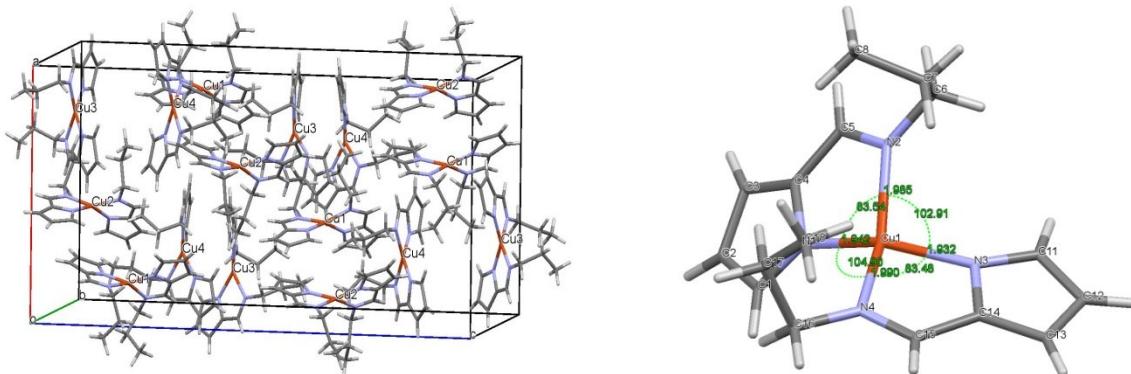


Fig. S2: Crystal structure showing (a) packing of the four different molecules (b) central bond angles and distances on a molecule of the synthesized PPC complex.

Table S1: Crystal data and detailed structure refinement for synthesized and published complex [1]

	Synthesized	Published
Empirical formula	C ₁₆ H ₂₂ N ₄ Cu	C ₁₆ H ₂₂ N ₄ Cu
Formula weight	333.93	333.93
Temperature (K)	293	293
Wavelength (Å)	0.71073	0.71073
Crystal system	orthorhombic	orthorhombic
Space group	P 2 ₁ 2 ₁ 2 ₁	P 2 ₁ 2 ₁ 2 ₁
<i>Unit cell dimensions</i>		
<i>a</i> (Å)	14.6108(5)	14.6053917)
<i>b</i> (Å)	15.9605(7)	15.9508(19)
<i>c</i> (Å)	28.9556(11)	28.957(3)
β (°)	90	90
Volume (Å³)	6752.3(5)	6746.0(13)
Z	16	16
D_{calc} (g/cm³)	1.314	1.315
Absorption coefficient (mm⁻¹)	1.293	1.009
F(0 0 0)	2800	2800
Crystal size (mm)	0.30 × 0.20 × 0.03	0.39 × 0.40 × 0.42
θ Range for data collection (°)	1.406–27.998	1.41–28.32
Index ranges	$-19 \leq h \leq 19$, $-21 \leq k \leq 20$, $-38 \leq l \leq 33$	$-19 \leq h \leq 16$, $-20 \leq k \leq 19$, $-20 \leq l \leq 38$
Reflections collected	54 025	44605
Independent reflections (<i>R</i>_{int})	16 264 (0.057)	16033 (0.0490)
Completeness to θ (%)	100.0 ($\theta = 25.242^\circ$)	97.1 ($\theta = 28.32^\circ$)
Maximum and minimum transmission	-	0.8237 and 0.6884
Goodness-of-fit on <i>F</i>²	0.886	1.031
Final <i>R</i> indices	<i>R</i> ₁ = 0.0322, <i>wR</i> ₂ = 0.0580	<i>R</i> ₁ = 0.0496, <i>wR</i> ₂ = 0.1135
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0541, <i>wR</i> ₂ = 0.0545	<i>R</i> ₁ = 0.0787, <i>wR</i> ₂ = 0.1285

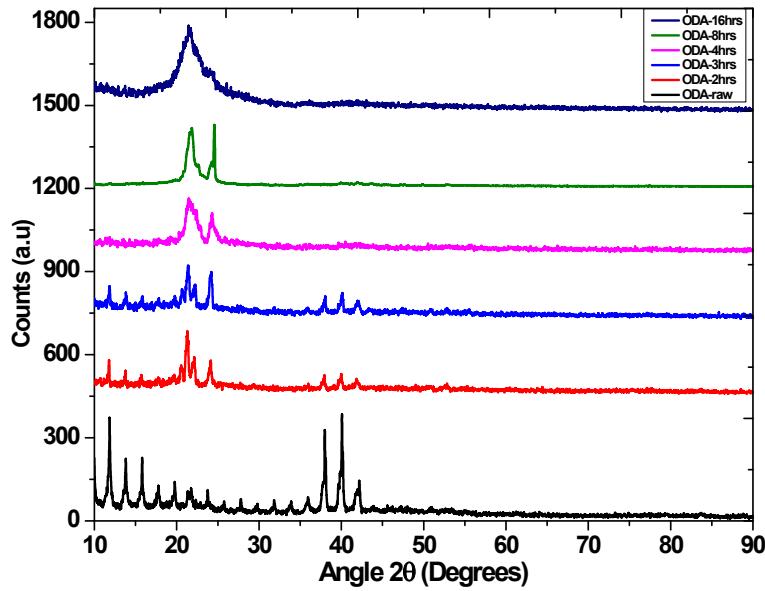


Fig. S3: XRD patterns of products of decomposition of octadecylamine at 260 °C under N₂ (g) flow

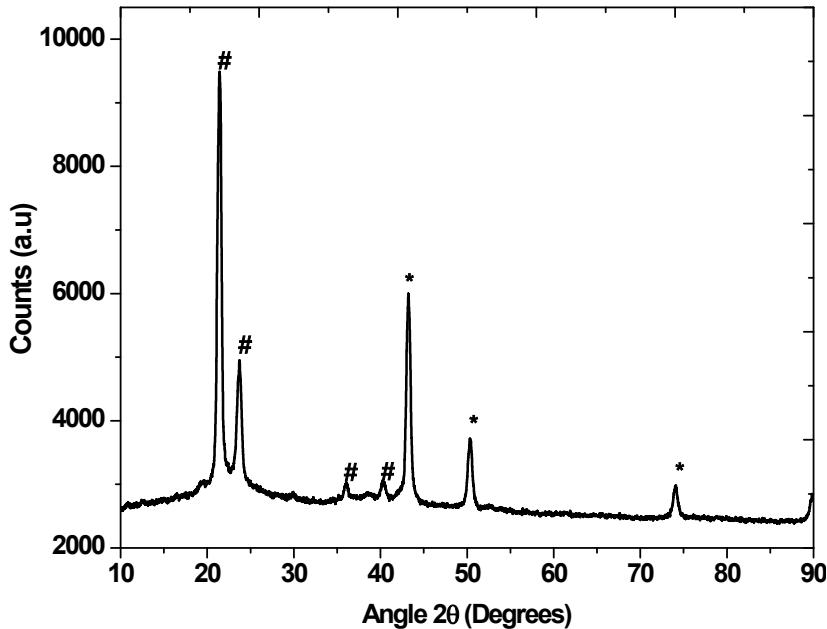


Fig. S4: XRD pattern of a product obtained from the thermolysis of Cu(CO₂CH₃).H₂O in ODA at 260 °C (# ODA and * Cu) JCP2.2CA:01-070-3038.

References

- [1] Cambridge Crystallographic Data Centre CCDC-241810.