Electronic Supplementary Information

Crystalline Cu(II) metal-organic frameworks based on a carboxamide pincer ligand and an $N^{CO}N^{CO}N$-Pd(II) pincer complex

Siphelele S. P. Malaza,[a] Gift Mehlana,*[b] Ocean Cheung[c] , Roger Hunter[d] and Banothile C. E. Makhubela*[a]

*[a]*University of Johannesburg, Centre for Synthesis and Catalysis, Department of Chemical Sciences, Faculty of Science, Kingsway Campus: C2 Lab 328, Auckland Park, 2006, South Africa. E-mail: bmakhubela@uj.ac.za*

*[b]*Department of Chemical Technology, Faculty of Science and Technology, Midlands State University, 9055 Senga Road, Gweru, Zimbabwe. Email : mehlanag@staff.msu.ac.zw*

Nanotechnology and Functional Materials, Department of Materials Sciences and Engineering Angström Laboratory, Uppsala University, Uppsala, Sweden.

Department of Chemistry, University of Cape Town, Rondebosch, 7701, Cape Town, South Africa.

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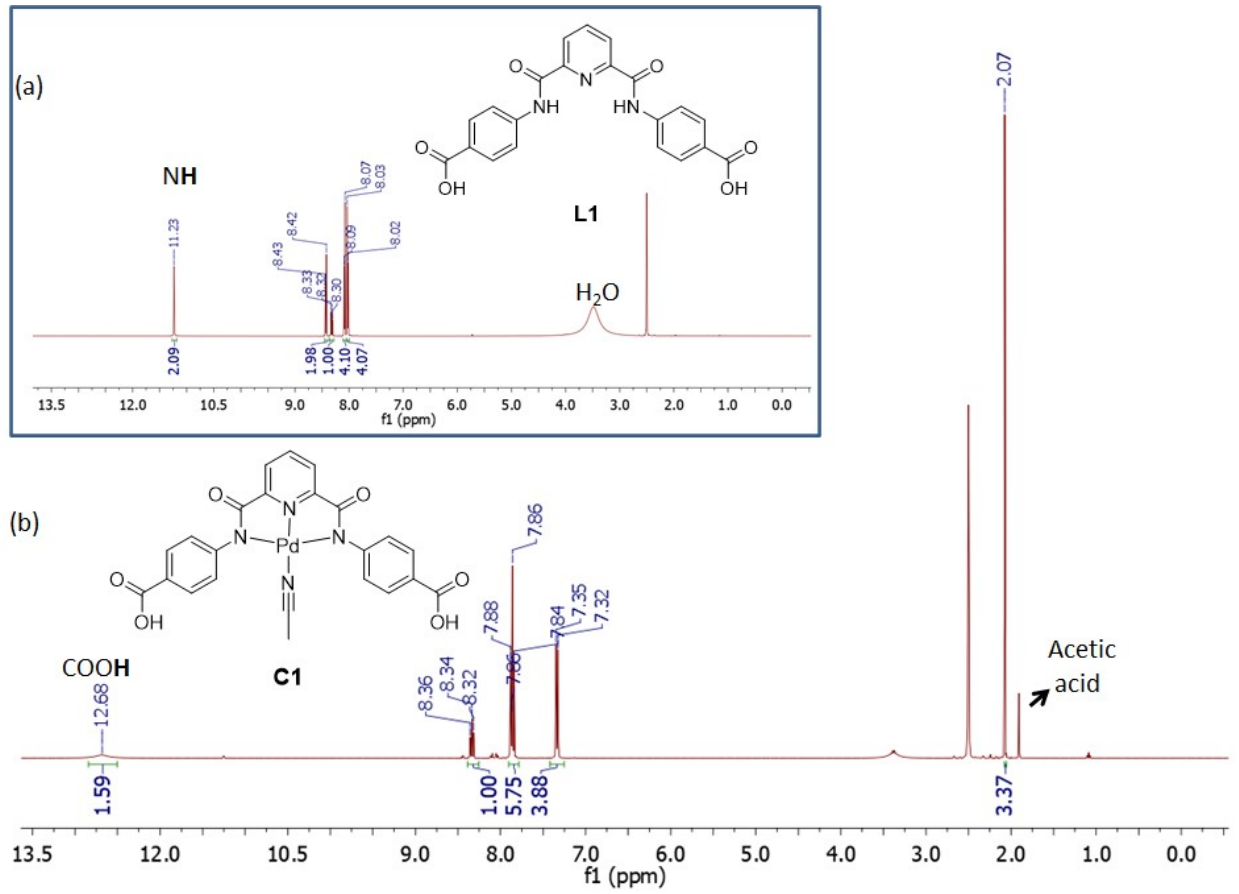

Figure S1: (a) ^{1}H NMR spectrum of **L1** (insert) in DMSO-$_{d6}$ showing the amide protons as a singlet at 11.23 ppm. (b) ^{1}H NMR spectrum in DMSO-$_{d6}$ showing the reaction progress of **C1**. The reaction proceeds with the pincer ligand **L1** forming a tridentate chelate around palladium(II) where the fourth coordination site is occupied by CH_3CN, which is supported by a singlet at 2.07 ppm.

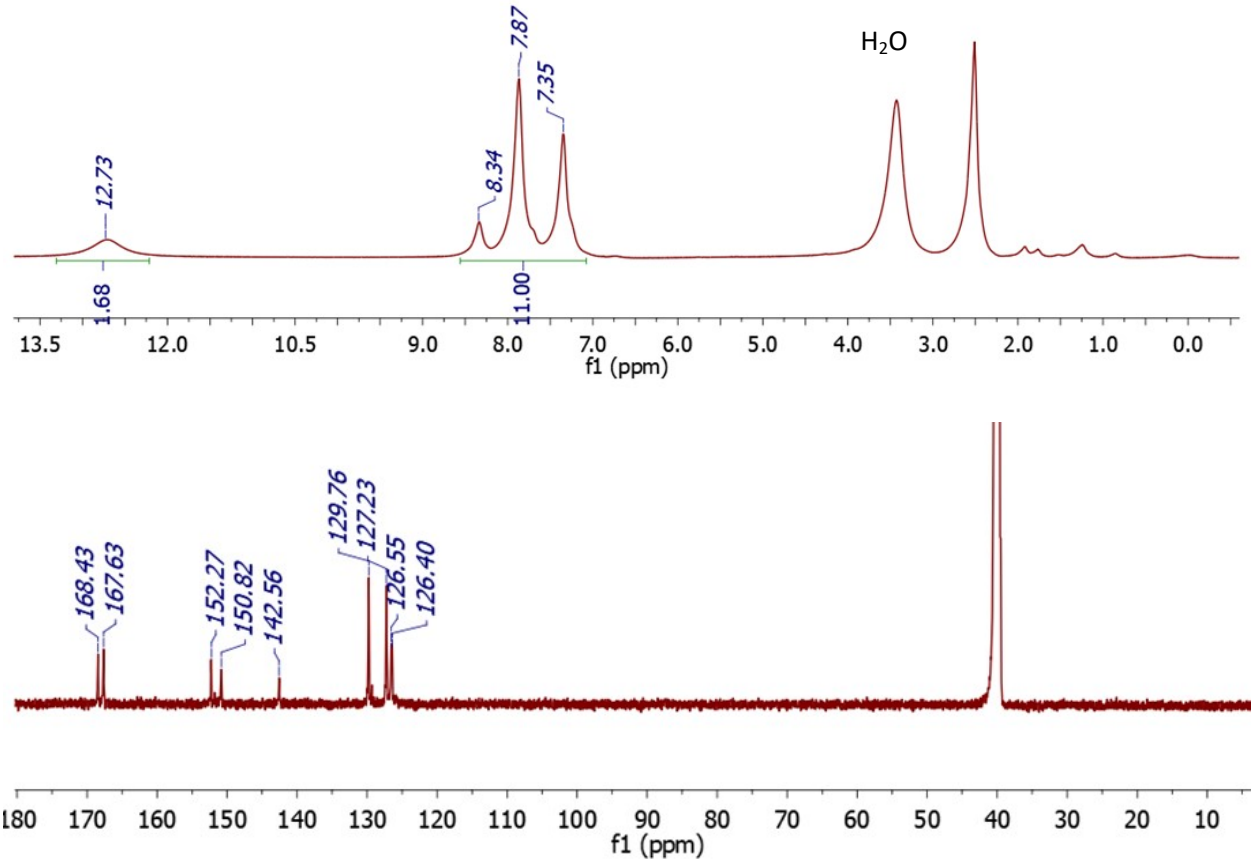

Figure S2: (a) ^{1}H NMR and $^{13}C\{^{1}H\}$ NMR spectra in DMSO-$_{d6}$ corresponding to **C1** after workup. After the workup of the bulk material containing **C1**, the CH_3CN ligand previously observed in **Figure S1 (b)** can be displaced by solvent molecules such as water or DMSO. The $^{13}C\{^{1}H\}$ NMR spectrum further supports this notion as no CH_3CN carbon peaks were observed.

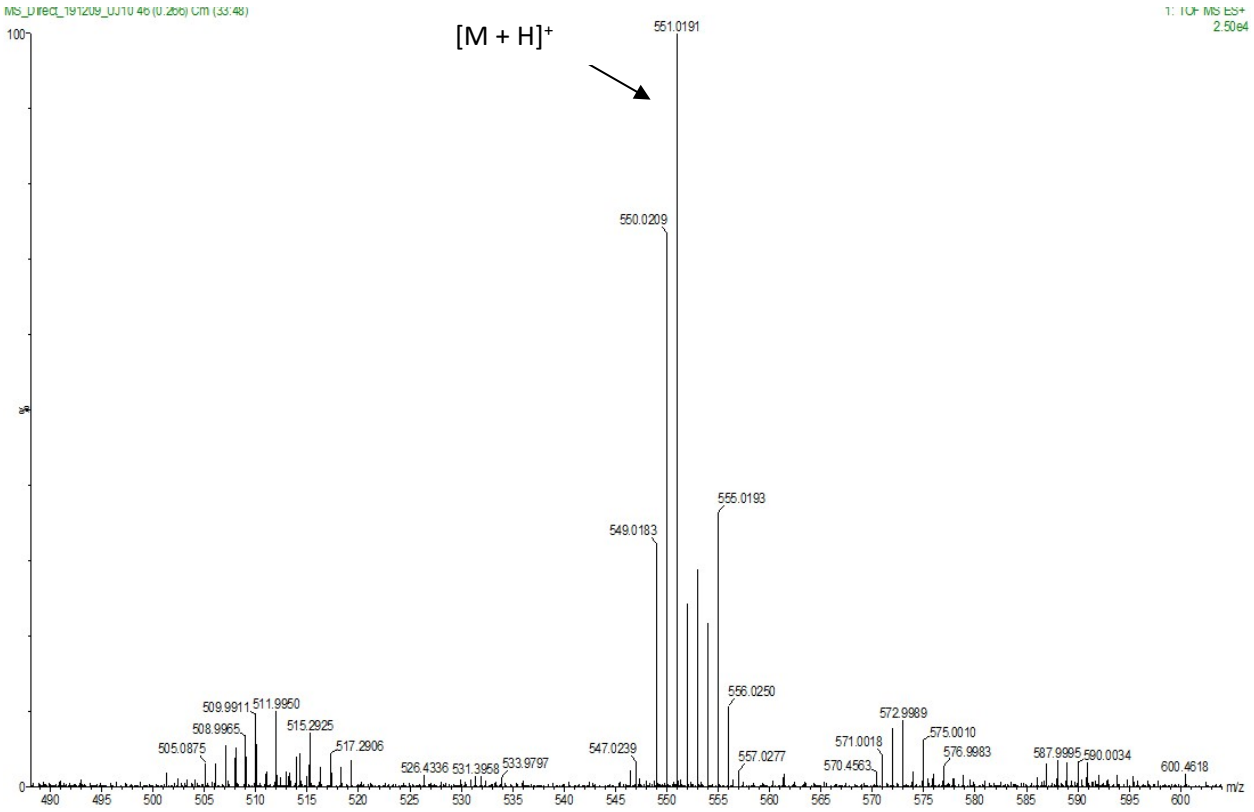

Figure S3: Mass spectrum of **C1** showing a base peak fragment of a monomeric palladium(II) species.

Table S1: <u>The X-ray diffraction data of **Cu-MOF** and **Pd@Cu-MOF**</u>

compound	**Cu-MOF**	**Pd@Cu-MOF**
empirical formula	$C_{57}H_{67}Cu_2N_{11}O_{21}$	$C_{62}H_{64}Cu_2N_{10}O_{21}Pd_2$
formula weight	1369.29	1625.14
crystal system	monoclinic	monoclinic
space group	$P2_1/c$	Cc
a (Å)	21.4117(12)	19.6662(2)
b (Å)	11.5851(6)	20.9151(1)
c (Å)	25.3771(14)	18.3648(2)
α (degrees)	90	90
β (degrees)	103.588(1)	117.440(2)
γ (degrees)	90	90
V (Å^3)	6118.8(6)	6703.96(15)
Z	4	4
D_{cald} (g.cm^{-3})	1.486	1.566
θ_{max} (degress)	28.43	72.125
F(000)	2848.0	3124.0
crystal colour	blue	green
index ranges	h = -28 to 28	h = -24 to 24
	k = -15 to 15	k = -25 to 25
	l = -33 to 33	l = -22 to 22
reflections collected	15 369	11 270
Data completeness	99.7%	85.0%

GOF	1.028	0.999
Final R indexes [all data]	R_1 = 0.0379, wR_2 = 0.1032	R_1 = 0.0542, wR_2 = 0.1439

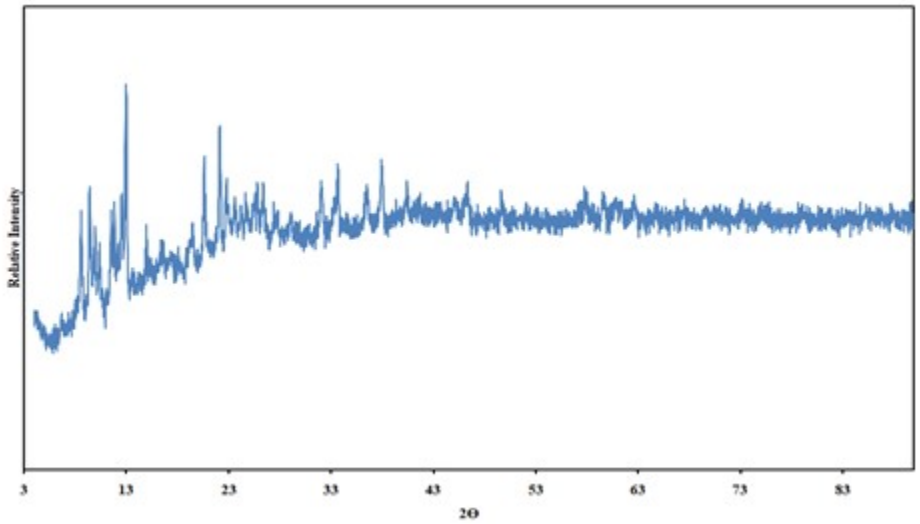

Figure S4: The experimental PXRD pattern of the powder material obtained after attempting a solvothermal method to make **Cu-MOF**.

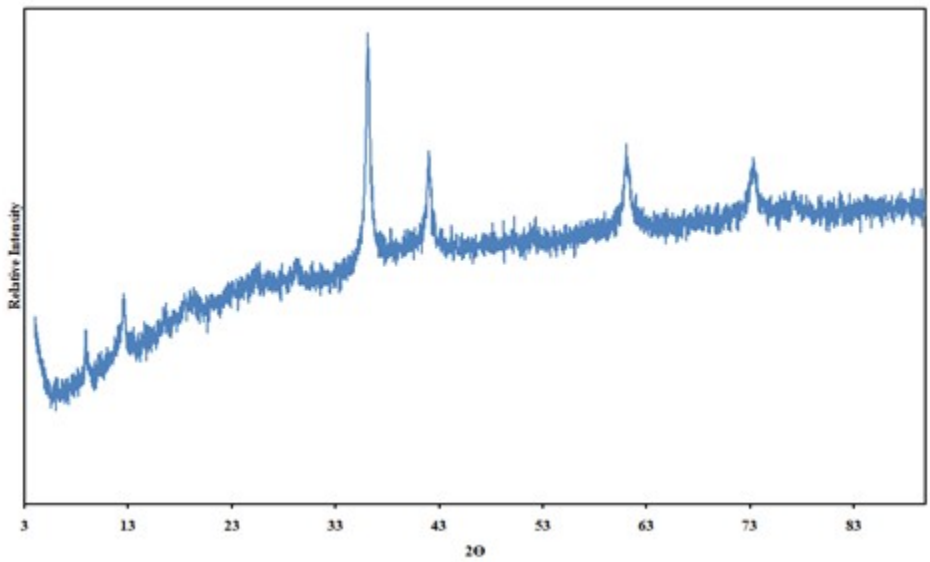

Figure S5: The experimental PXRD pattern of the powder material obtained after attempting a solvothermal method to make **Pd@Cu-MOF**.

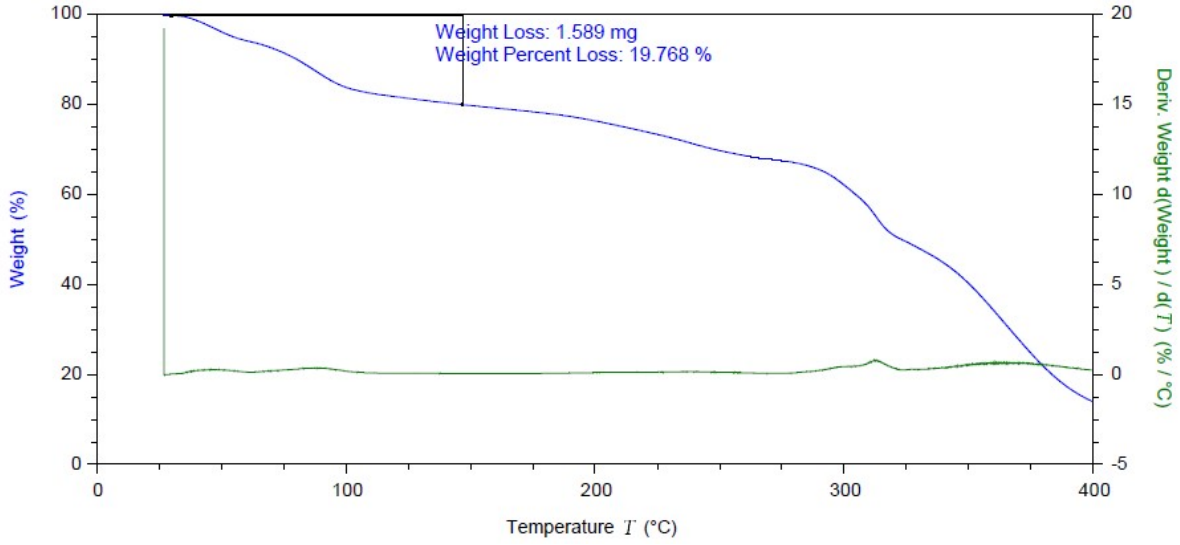

Figure S6: TGA traces of **Cu-MOF**.

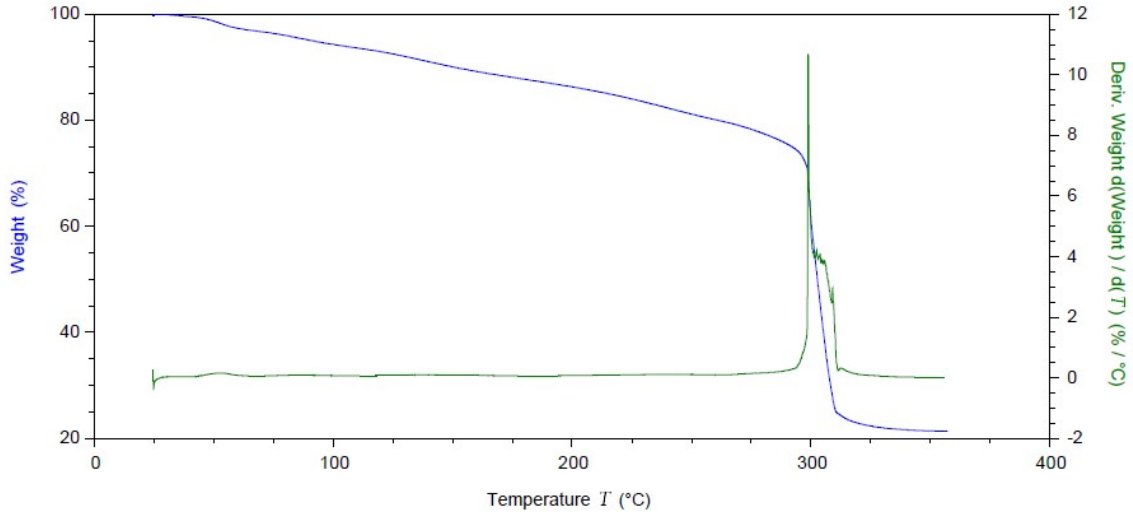

Figure S7: TGA traces of **Pd@Cu-MOF**.

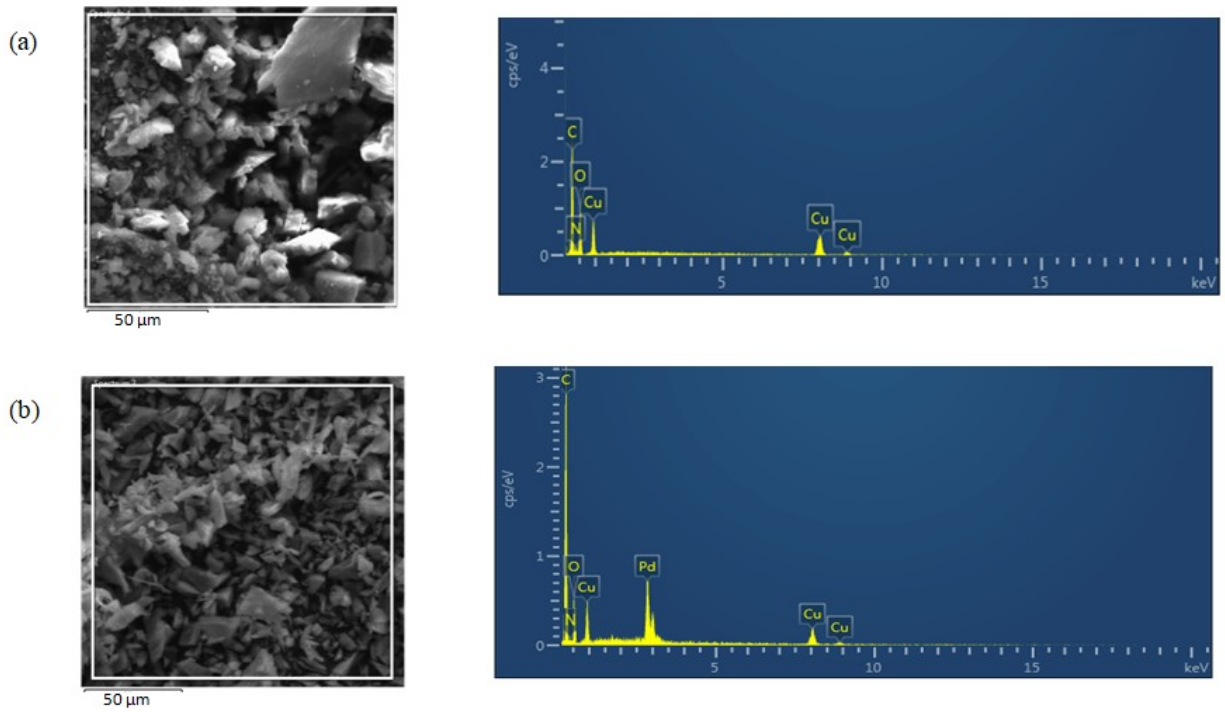

Figure S8: SEM-EDX images of (a) **Cu-MOF** and (b) **Pd@Cu-MOF**.