

1. ABOUT THE DATASET

Title: Copper-chloride linked cage-catenanes

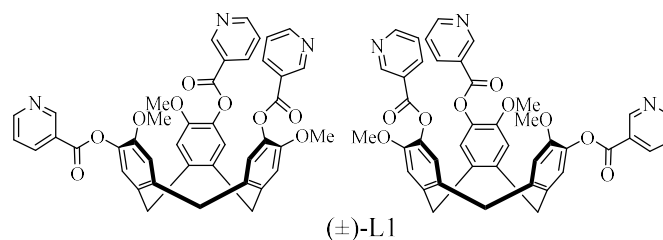
Creators: Matthew Snelgrove, Natalia Sergeeva, Michaele Hardie

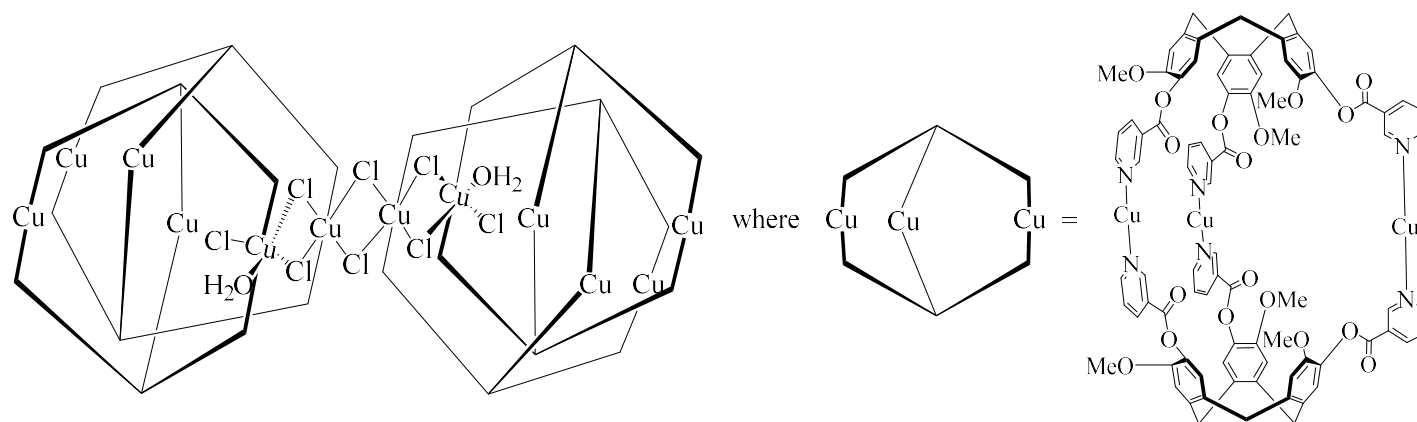
Organisation: University of Leeds

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Publication Year: 2024

Description: Analytical, spectroscopic and X-ray diffraction structural data collected for complexes obtained from a combination of copper nitrate or copper chloride with ligand (\pm)-2,7,12-trimethoxy-3,8,13-*tris*(3-pyridylcarboxy)-10,15-dihydro-5*H*-tribenzo[*a,d,g*]cyclononene designated (\pm)-L1 and pictured below. There are four complexes designated **C1**, **C1a**, **C1b** and **C2** whose compositions are given in the table below along with data available for each. All complexes feature a tetrameric cage motif with two linked cage-catenanes shown schematically for **C1** below. **C1a** and **C1b** were obtained by solvent-exchange from **C1** and have additional dimeric copper chloride links while **C2** is a 2D polymer with three types of copper chloride links. Data for unsuccessful investigation of **C2** as a putative photocatalyst for dye degradation is also supplied.





C1 (not all terminal ligands are shown on Cu centres)

Label	Composition	Single crystal Xray structure	Powder Xray diffraction (XRD)	Elemental analysis CHN, EDX	Infrared	Thermo-gravimetric Analysis (TGA)	UV-visible spectroscopy
C1	$[\text{Cu}_6(\text{L1})_4\text{Cl}_{10.5}(\text{NO}_3)_{1.5}(\text{H}_2\text{O})_4] \cdot 17(\text{DMF})$	x	x	x,x	x	x	
C1a	$[\text{Cu}_6(\text{L1})_4\text{Cl}_{10.5}(\text{NO}_3)_{1.5}(\text{H}_2\text{O})_2] \cdot n(\text{toluene})$	x					
C1b	$[\text{Cu}_{12}(\text{L1})_8\text{Cl}_{20}(\text{NO}_3)_4(\text{H}_2\text{O})_5] \cdot (\text{DMF}) \cdot n(\text{toluene})$	x					
C2	$[\text{Cu}_6(\text{L1})_4\text{Cl}_{12}(\text{H}_2\text{O})_3] \cdot (\text{H}_2\text{O}) \cdot 15(\text{DMF})$	x		x	x		x

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<https://doi.org/10.5518/1585>

Related publication: "Higher Assemblies of Coordination Cage-Catenanes Linked by Copper(II) Chloride Clusters: Networks and Transformations", M. P. Snelgrove, N. N. Sergeeva, M. J. Hardie, *Chemistry- A European Journal* accepted 2024, DOI: 10.1002/chem.202403692

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2. TERMS OF USE

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3. PROJECT AND FUNDING INFORMATION

Title: Metal-organic frameworks and supramolecular assemblies for dyes and other inclusions

Dates: 2019-2023

Funding Organisation: Gunnell and Matthews Scholarship University of Leeds

Funding Organisation: Diamond Light Source

Grant no.: CY26879

4. CONTENTS

Folder	Filename	Contents	File format
Analysis	C1 infrared.pdf C2 infrared.pdf C2_UVvisible.xlsx EDX_L1 and C1.pdf Elemental Analysis_C1 and C2.pdf MS_C1 soln.pdf MS_C2 soln.pdf TGA-sample C1 Data.xlsx	Infrared spectra of C1 Infrared spectrum of C2 UV-visible data for C2 suspension Energy dispersive Xray analysis for L1 and C1 CHN elemental analysis for C1 and C2 Mass spectrometry spectra of reaction mixture for C1 Mass spectrometry spectra of reaction mixture for C1 Thermogravimetric analysis data for C1	pdf pdf MS Excel pdf pdf pdf pdf MS Excel
Structural	C1_powder_XRD.xlsx Complex 1/complex1.cif /complex1.fcf /complex1.hkl /complex1.lst /complex1.res /complex1-mask.txt Complex 1a/complex1a.cif /complex1a.fcf /complex1a.hkl	powder X-Ray diffraction for CH ₂ Cl ₂ washed and dried C1 crystallographic information file for C1 single crystal structure structure factor file for C1 single crystal structure data file for C1 single crystal structure final shelxl refinement output for C1 single crystal structure shelxl results/instruction file for C1 single crystal structure solvent mask/void calculations for C1 single crystal structure crystallographic information file for C1a single crystal structure structure factor file for C1a single crystal structure data file for C1a single crystal structure	MS Excel All other files in this folder are text documents readable as txt files or MS Word, WordPad etc. hkl and res files are formatted for

	/complex1a.lst /complex1a.res /complex1a-mask.txt Complex 1b/complex1b.cif /complex1b.fcf /complex1b.hkl /complex1b.lst /complex1b.res /complex1b-mask.txt Complex 2/complex2.cif /complex2.fcf /complex2.hkl /complex2.lst /complex2.res /complex2-mask.txt	final shelxl refinement output for C1a single crystal structure shelxl results/instruction file for C1a single crystal structure solvent mask/void calculations for C1a single crystal structure crystallographic information file for C1b single crystal structure structure factor file for C1b single crystal structure data file for C1b single crystal structure final shelxl refinement output for C1b single crystal structure shelxl results/instruction file for C1b single crystal structure solvent mask/void calculations for C1b single crystal structure crystallographic information file for C2 single crystal structure structure factor file for C2 single crystal structure data file for C2 single crystal structure final shelxl refinement output for C2 single crystal structure shelxl results/instruction file for C2 single crystal structure solvent mask/void calculations for C2 single crystal structure	SHELX crystallographic programmes
Dye studies	C20.5mgmMB25uM_uncorrected.xlsx C20.5mgmMO25uM_uncorrected.xlsx MB 50uM blank.xlsx MO blank.xlsx	UV-visible for methylene blue photodegradation with C2 UV-visible for methyl orange photodegradation with C2 UV-visible for methylene blue photodegradation without C2 UV-visible for methylene blue photodegradation without C2	All MS excel workbook files

5. METHODS

Detailed information about methods and instrumentation are available within the supplementary information for the related publication, see section 1.