Structure and magnetic properties of a 1D alternating Cu(II) monomer—paddlewheel chain

Vanessa Machado[1], Mark Turnbull[2], Louise N. Dawe[1]*

[1] Department of Chemistry and Biochemistry, Wilfrid Laurier University, 75 University Ave. W., ON, Canada, N2L 3C5
[2] Carlson School of Chemistry and Biochemistry, Clark University, 950 Main St., Worcester, MA, USA, 01610
* Correspondence: ldawe@wlu.ca; Tel. 1-519-884-0710 ext. 4963

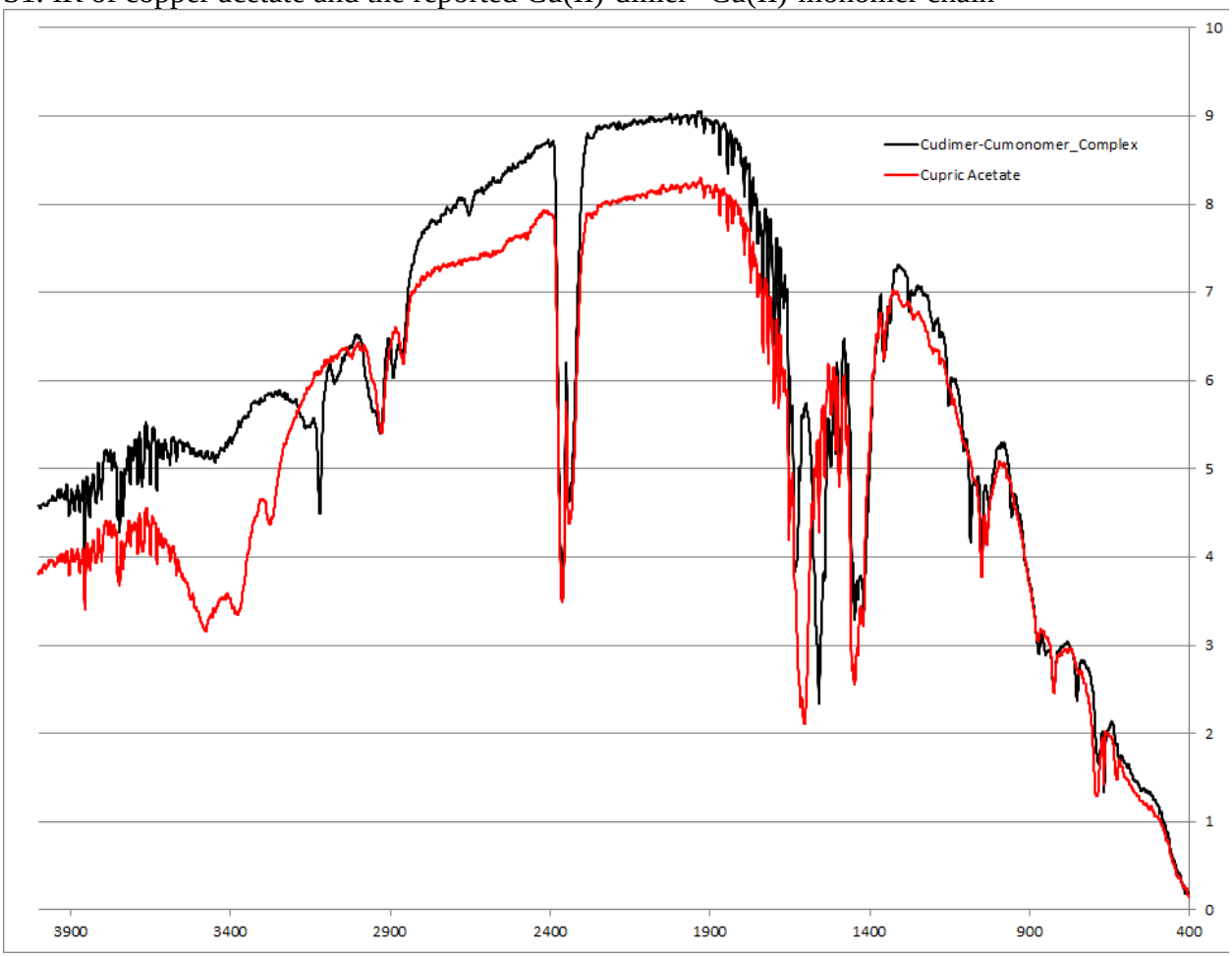
Supplementary Material

S1. IR of copper acetate and the reported Cu(II)-dimer···Cu(II)-monomer chain

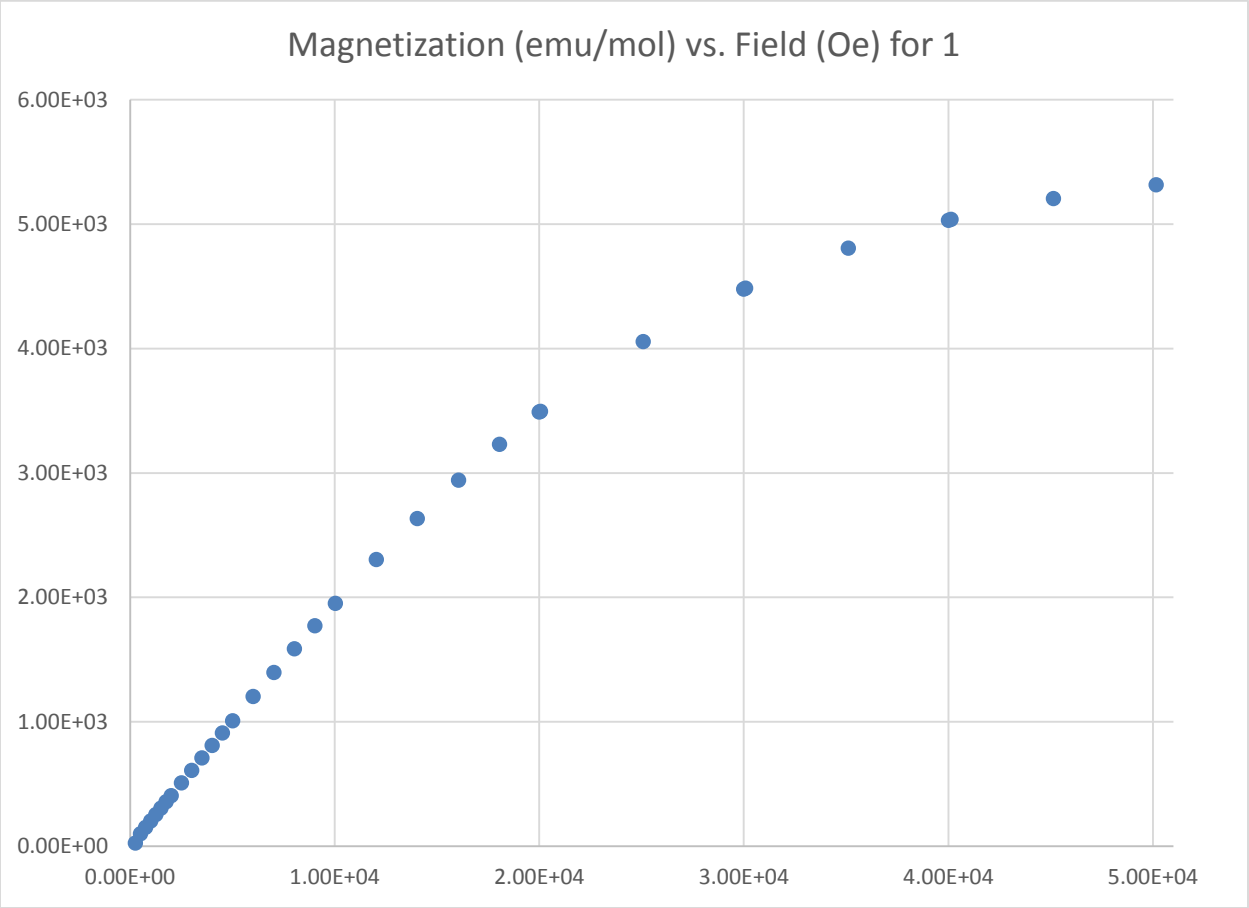
S2. Magnetization as a function of field for Cu(II)-dimer···Cu(II)-monomer chain

S3. checkcif for Cu(II)-dimer···Cu(II)-monomer chain

S1. IR of copper acetate and the reported Cu(II)-dimer···Cu(II)-monomer chain



S2. Magnetization as a function of field for Cu(II)-dimer···Cu(II)-monomer chain



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) n16061_0m

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: n16061_0m

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Bond precision:  C-C = 0.0030 A          Wavelength=1.54184

Cell:           a=11.0485(17)    b=11.7850(17)      c=10.9549(16)
                alpha=90         beta=115.411(4)    gamma=90
Temperature:    110 K

                Calculated                Reported
Volume          1288.4(3)                 1288.4(3)
Space group     P 21/c                    P 1 21/c 1
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C18 H26 Cu3 N4 O12        C18 H26 Cu3 N4 O12
Sum formula     C18 H26 Cu3 N4 O12        C18 H26 Cu3 N4 O12
Mr              681.08                    681.05
Dx,g cm-3       1.756                     1.756
Z               2                         2
Mu (mm-1)       3.475                     3.475
F000            690.0                     690.0
F000'           680.14
h,k,lmax        13,14,13                  13,13,13
Nref            2273                      2247
Tmin,Tmax       0.755,0.829               0.641,0.753
Tmin'           0.424

Correction method= # Reported T Limits: Tmin=0.641 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.989          Theta(max)= 66.616

R(reflections)= 0.0240( 2073)     wR2(reflections)= 0.0637( 2247)

S = 1.108                 Npar= 175
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The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 26 Report

Author Response: Some of these may have been obstructed by the beamstop. This represents a small number of the total reflections, and there are no apparent model problems resulting from these missing reflections.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note

Author Response: H2 was introduced in its difference map position, and refined positionally with a distance restraint using default tolerances.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info

Author Response: This is confirmed.

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report

Author Response: H2 was introduced in its difference map position, and refined positionally with a distance restraint using default tolerances.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2 -- O6 .. 5.6 s.u.

Author Response: This is not unexpected when a heavier metal centre is coordinatively bonded to a lighter ligand donor atom.

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.12 Ratio

Author Response: Better overcomplete than undercomplete! (This is likely due to the inclusion of bonds generated by the inclusion of symmetry related atoms in the polymeric structure.)

PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) ..... 2.36 Note

Author Response: Magnetic properties are detailed in the full paper, and agree with this bond valence assignment.

PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1 Note

Author Response: H2 was introduced in its difference map position, and refined positionally with a distance restraint using default tolerances.

PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still 84 %

Author Response: Crystals diffracted strongly, which is reflected in the excellent refinement values.

PLAT933_ALERT_2_G Number of OMIT records in Embedded RES ..... 3 Note

Author Response: These were three low angle reflections with error/esd greater than |10|, and were likely partially obstructed by the beamstop.

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density 2 Note

Author Response: This is expected for high quality data and model, since all other electron density has been accounted.

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 08/07/2016; check.def file version of 05/07/2016

Datablock n16061_0m - ellipsoid plot