Subtle structural variation in copper metal-organic frameworks: syntheses, structures, magnetic properties and catalytic behaviour

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Supplementary Information

IR Spectrum of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\cdot 2DMF\}_\infty$ (**1**)
TGA of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2].2DMF\}_\infty$ (**1**)
XRPD of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2].2DMF\}_\infty$ (**1**)

IR Spectrum of $\{[Cu_2(5\text{-nbdc})_3(DMF)_2]\cdot 3\frac{1}{3}DMF\}_\infty$ (**2**)
TGA of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\ 3\frac{1}{3}DMF\}_\infty$ (**2**)
Magnetic data for $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\ 3\frac{1}{3}DMF\}_\infty$ (**2**)
XRPD of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\ 3\frac{1}{3}DMF\}_\infty$ (**2**)

IR Spectrum of $[Cu_6(5\text{-nbdc})_6(DMF)_6(H_2O)_{12}]\cdot 57H_2O$ (**3**)
TGA of $[Cu_6(5\text{-nbdc})_6(DMF)_6(H_2O)_{12}]\ 57H_2O$ (**3**)

IR Spectrum of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)
TGA of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)
Magnetic data for $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)
XRPD of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)

IR Spectrum of $[Cu_2(5\text{-abdc})_2\cdot(DMF)_2]_\infty$ (**5**)
TGA of $[Cu_2(5\text{-abdc})_2\cdot(DMF)_2]_\infty$ (**5**)
XRPD of $[Cu_2(5\text{-abdc})_2\cdot(DMF)_2]$ (**5**)
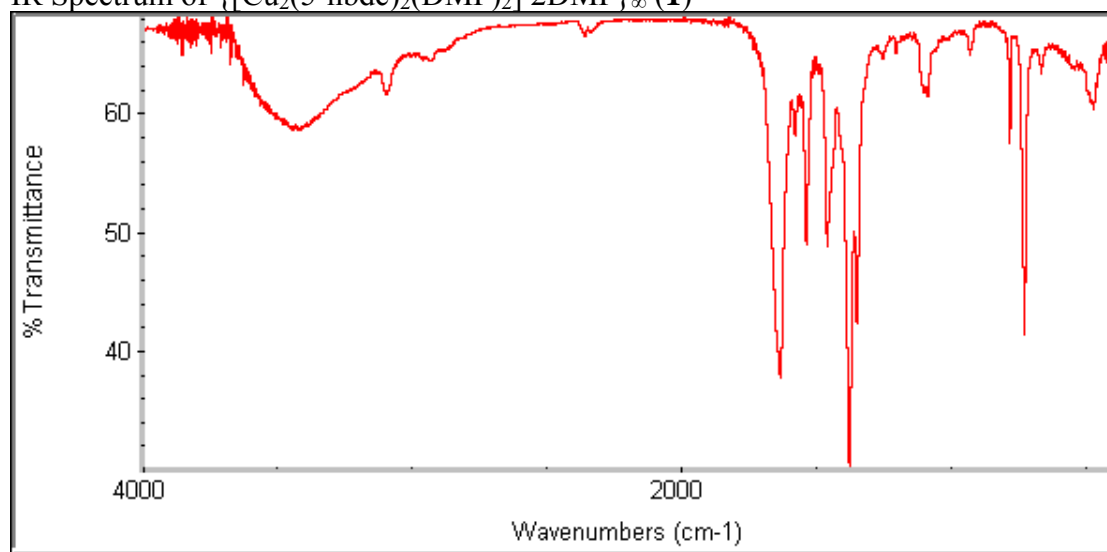
IR Spectrum of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)
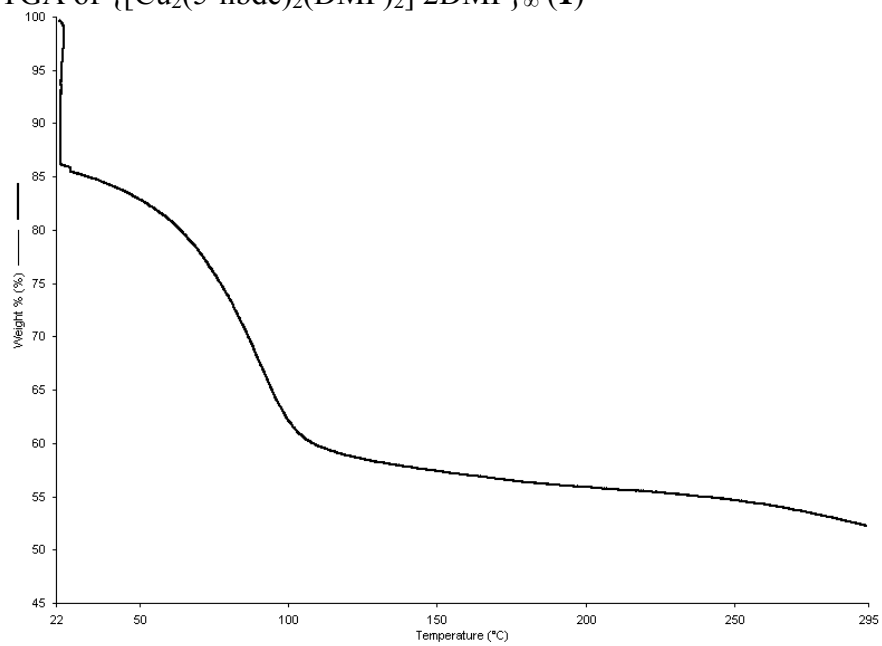TGA of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)
XRPD of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)

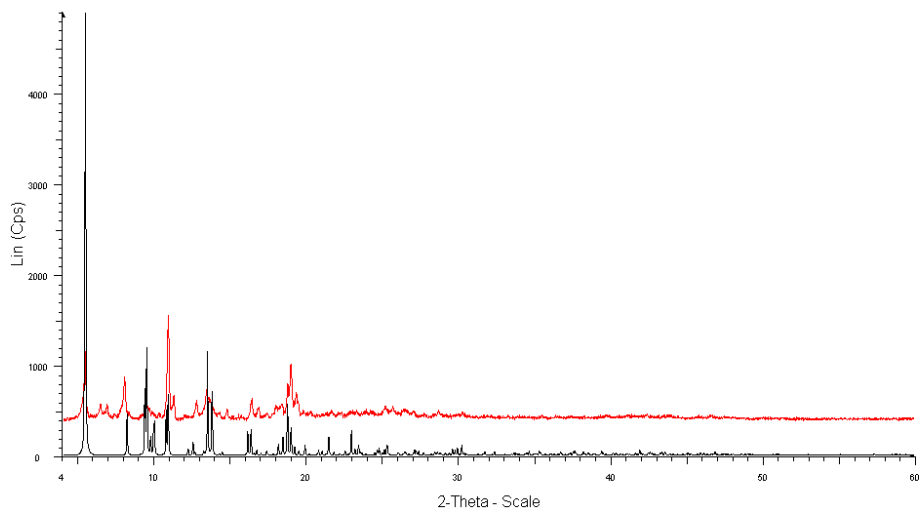IR Spectrum of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\cdot 2DMF\}_\infty$ (**1**)

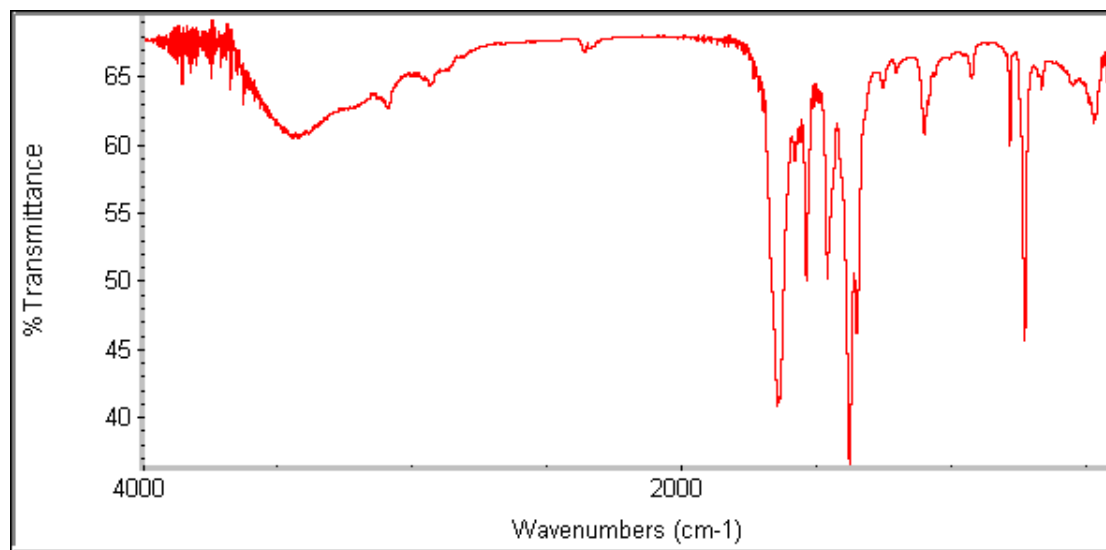TGA of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\cdot 2DMF\}_\infty$ (**1**)

XRPD of {[Cu$_2$(5-nbdc)$_2$(DMF)$_2$]·2DMF}$_\infty$ (**1**)

H06ADB2 & CR2-130
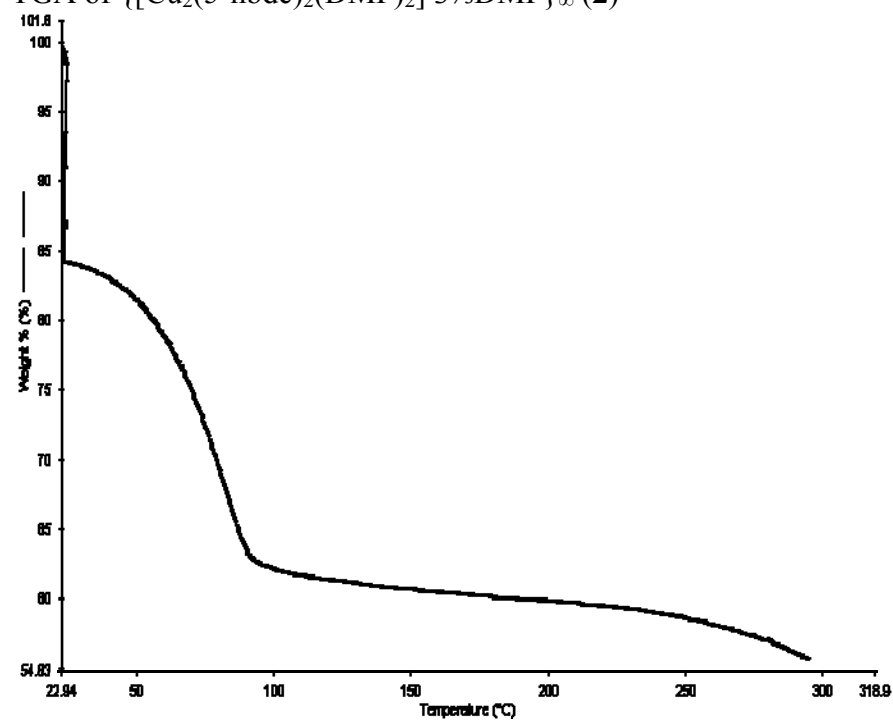
(red experimental, black calculated from X-ray single crystal structure)

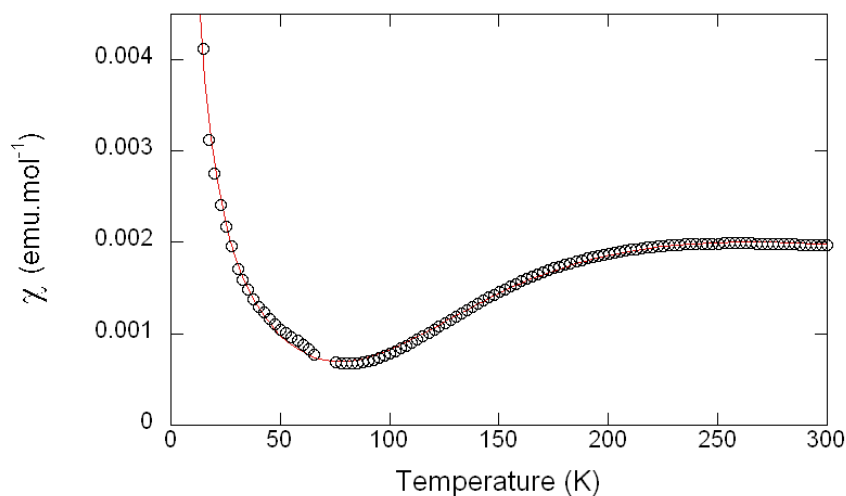IR Spectrum of $\{[Cu_2(5\text{-nbdc})_3(DMF)_2]\cdot 3\frac{1}{3}DMF\}_\infty$ (**2**)

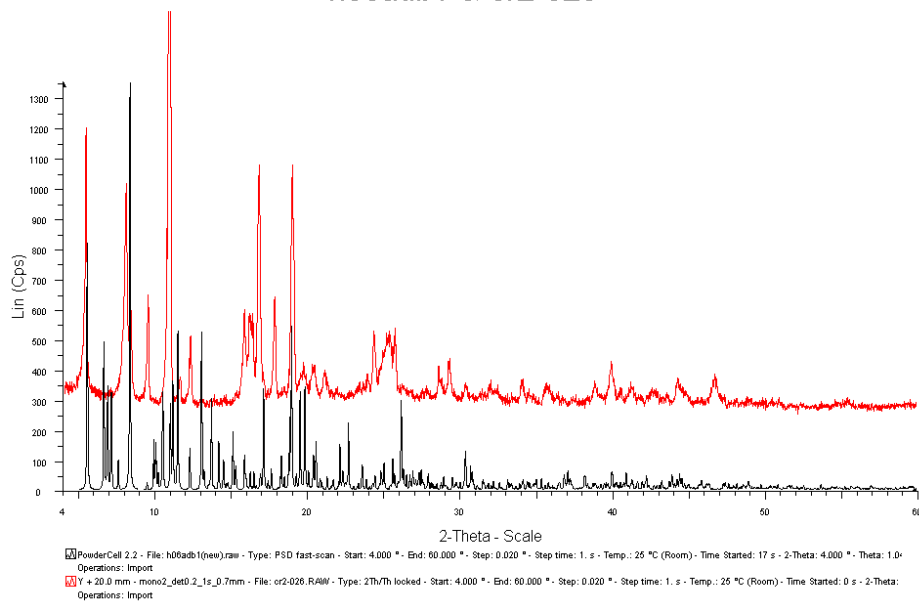

TGA of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\cdot 3\frac{1}{3}DMF\}_\infty$ (**2**)

Magnetic data for $\{[Cu_2(5\text{-nbdc})_2(DMF)_2] \ 3\frac{1}{3}DMF\}_\infty$ (**2**)

(the black circles are the experimental data, the red line shows the fit of the Bleaney-Bowers expression with a Curie contribution)
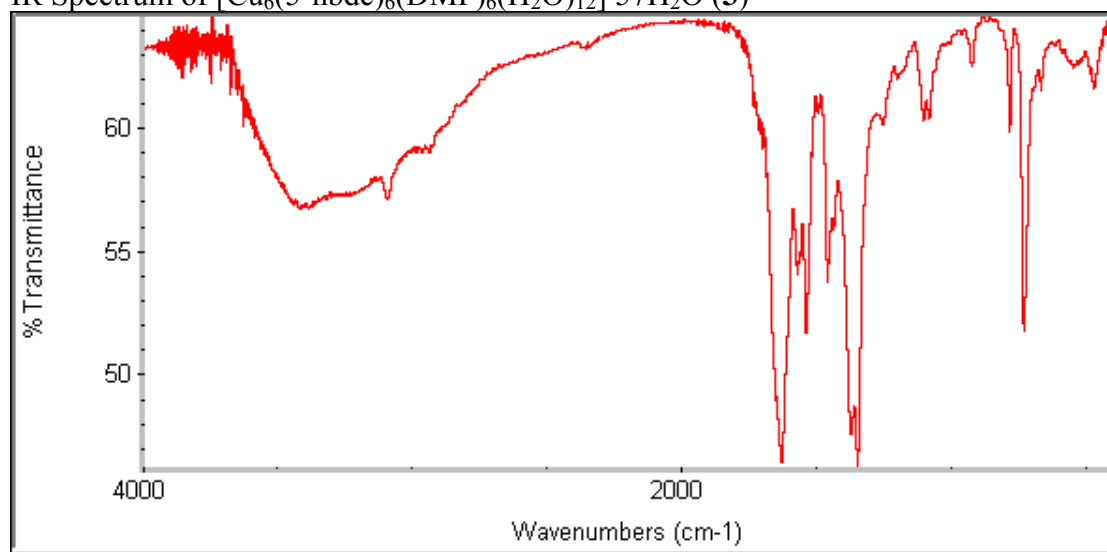
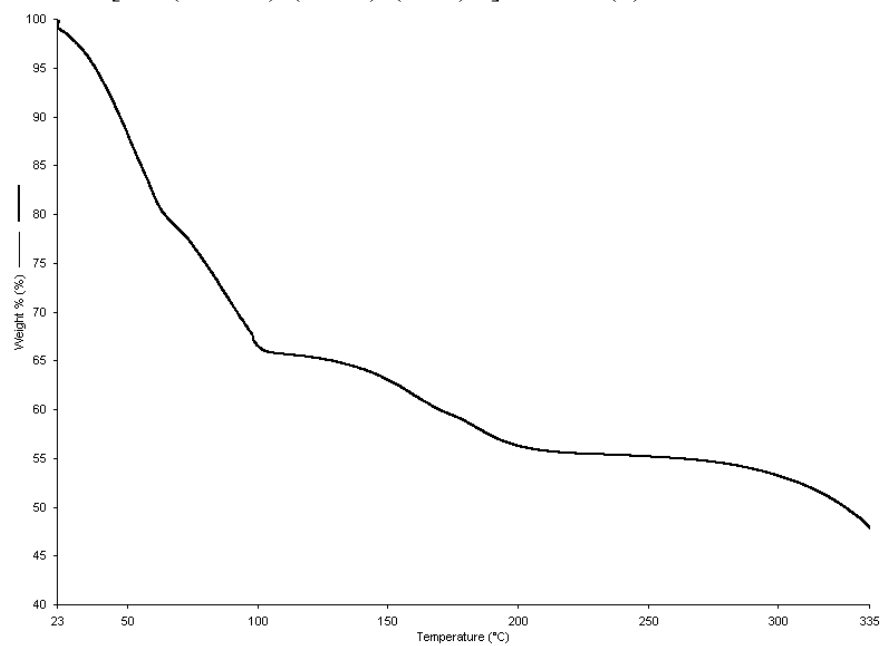XRPD of $\{[Cu_2(5\text{-nbdc})_2(DMF)_2]\cdot 3\frac{1}{3}DMF\}_\infty$ (**2**)

h06adb1 & cr2-026

(red experimental, black calculated from X-ray single crystal structure)

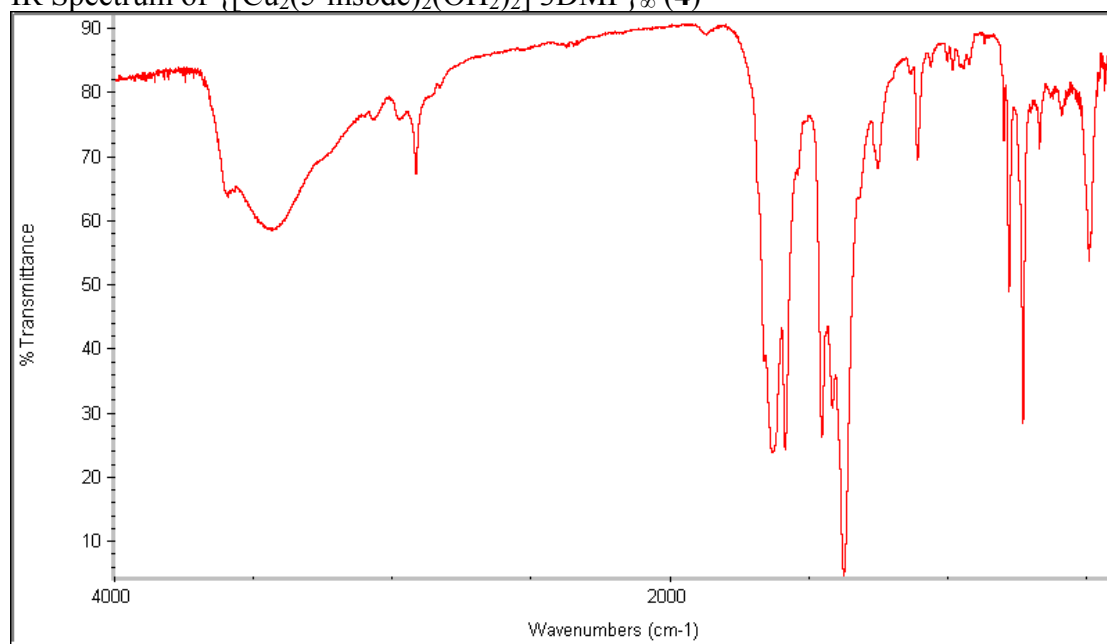IR Spectrum of $[Cu_6(5\text{-nbdc})_6(DMF)_6(H_2O)_{12}]\cdot57H_2O$ (**3**)
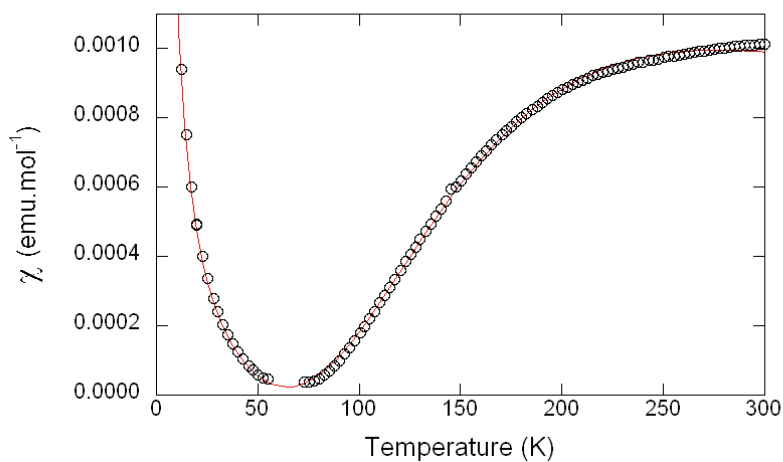

TGA of $[Cu_6(5\text{-nbdc})_6(DMF)_6(H_2O)_{12}]\cdot57H_2O$ (**3**)

IR Spectrum of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)
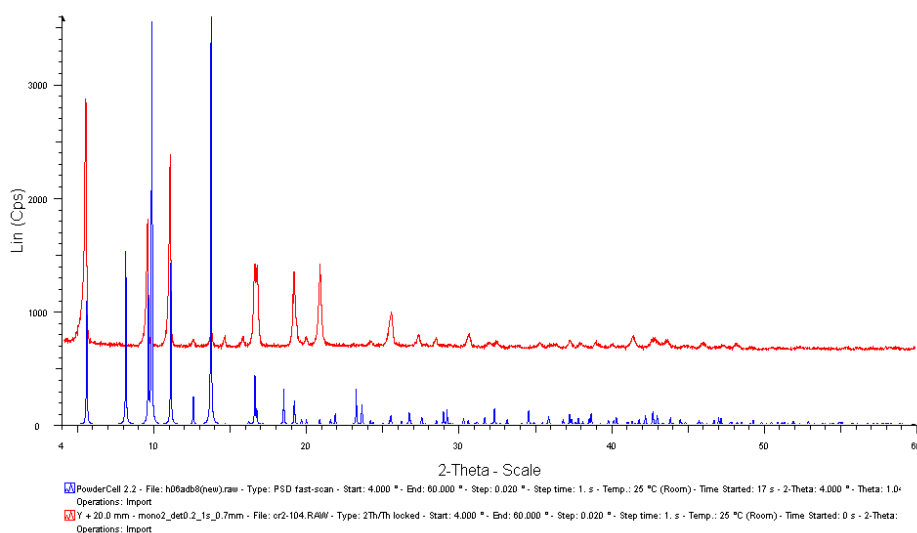

TGA of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)
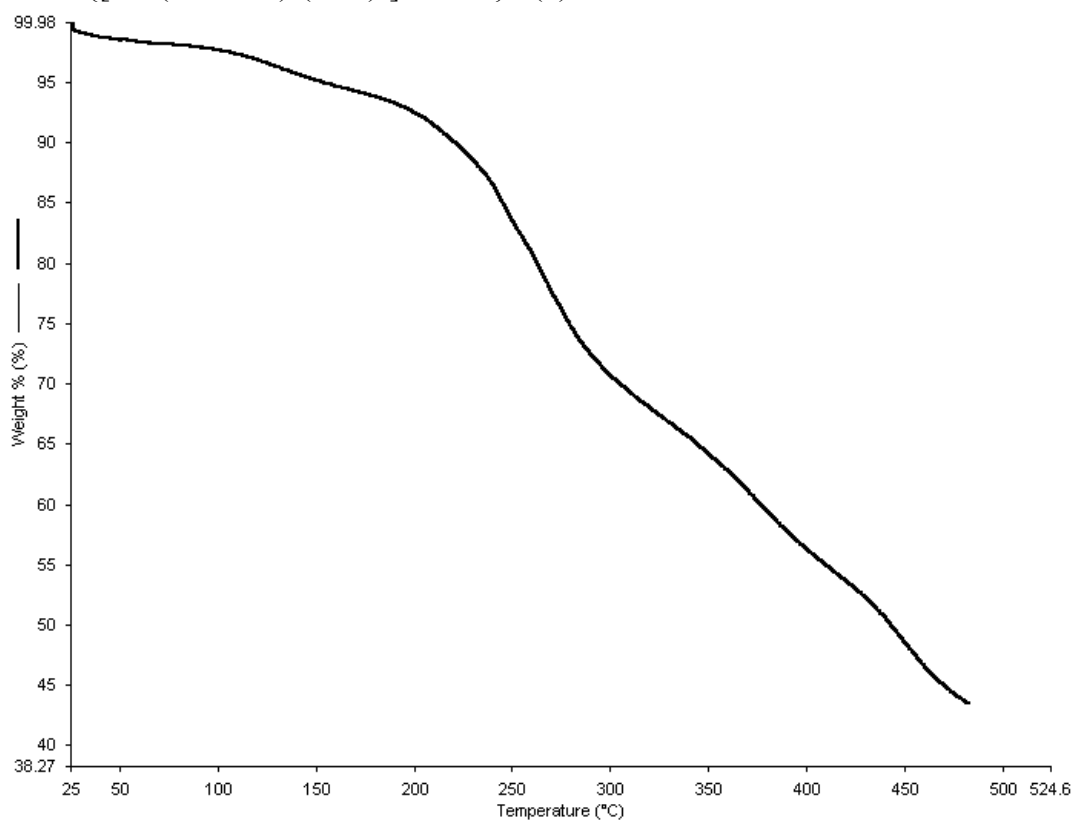
Magnetic data for $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)

(the black circles are the experimental data, the red line shows the fit of the Bleaney-Bowers expression with a Curie contribution)
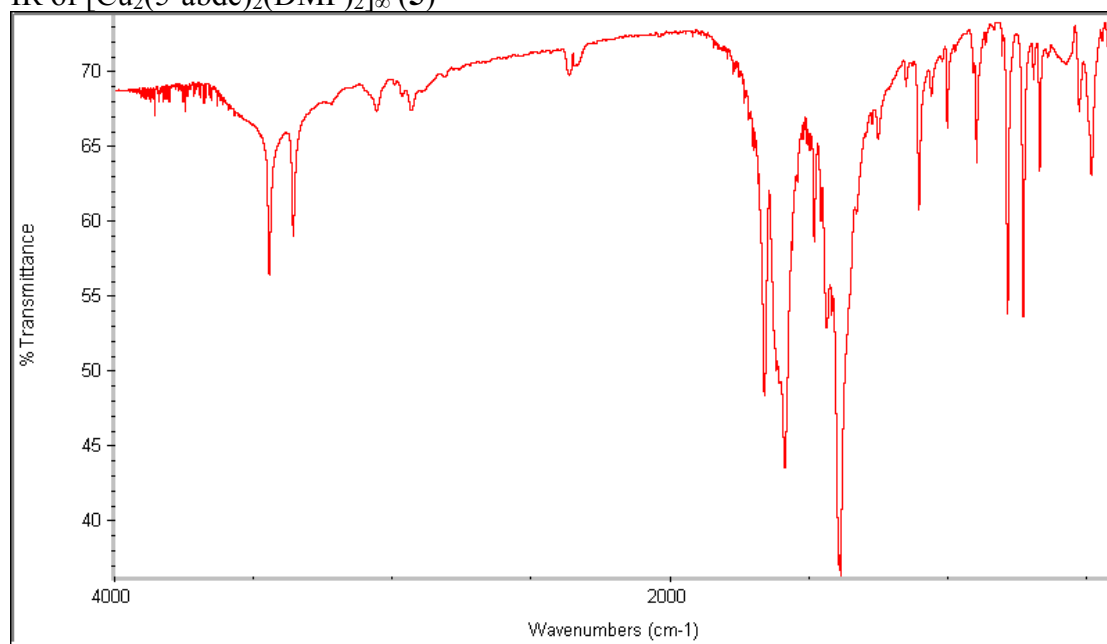
XRPD of $\{[Cu_2(5\text{-msbdc})_2(OH_2)_2]\cdot 3DMF\}_\infty$ (**4**)

h06adb8 & cr2-104
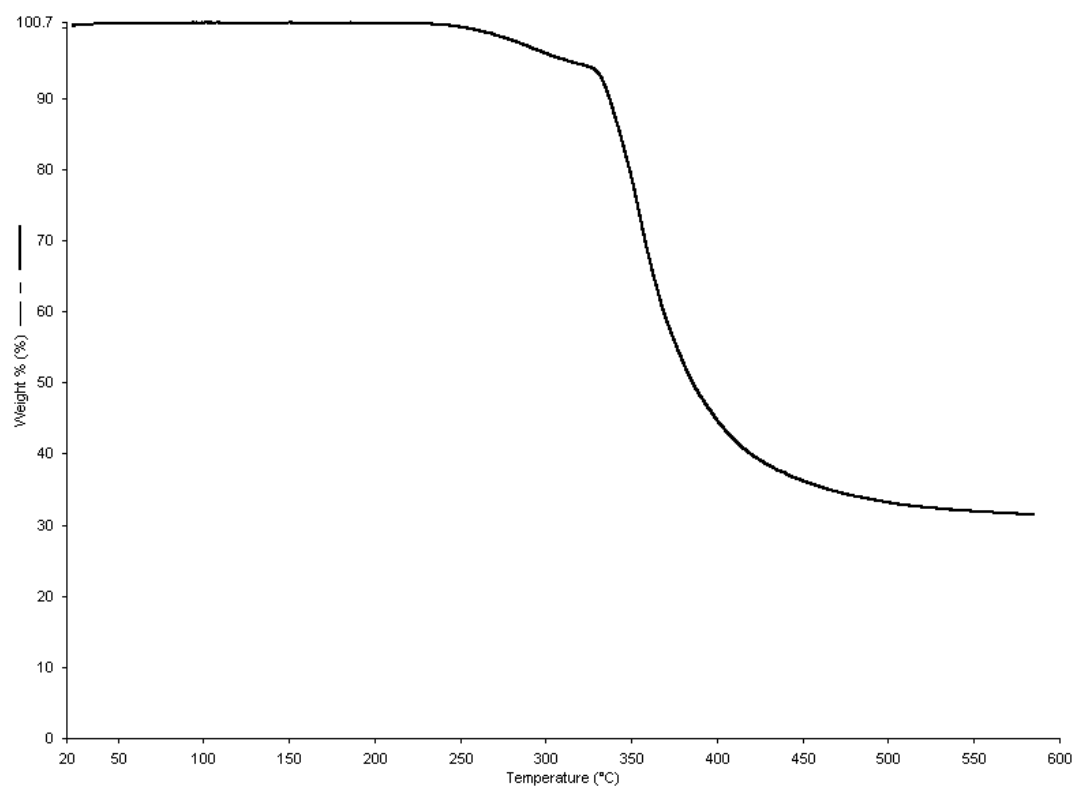

(red experimental, blue calculated from X-ray single crystal structure)
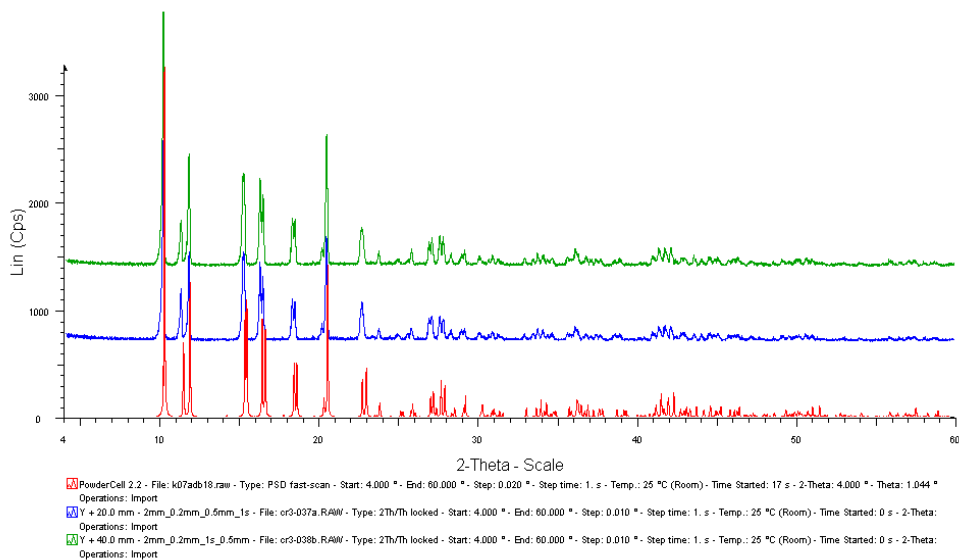
IR of $[Cu_2(5\text{-abdc})_2(DMF)_2]_\infty$ (**5**)

TGA of $[Cu_2(5\text{-abdc})_2(DMF)_2]_\infty$ (**5**)
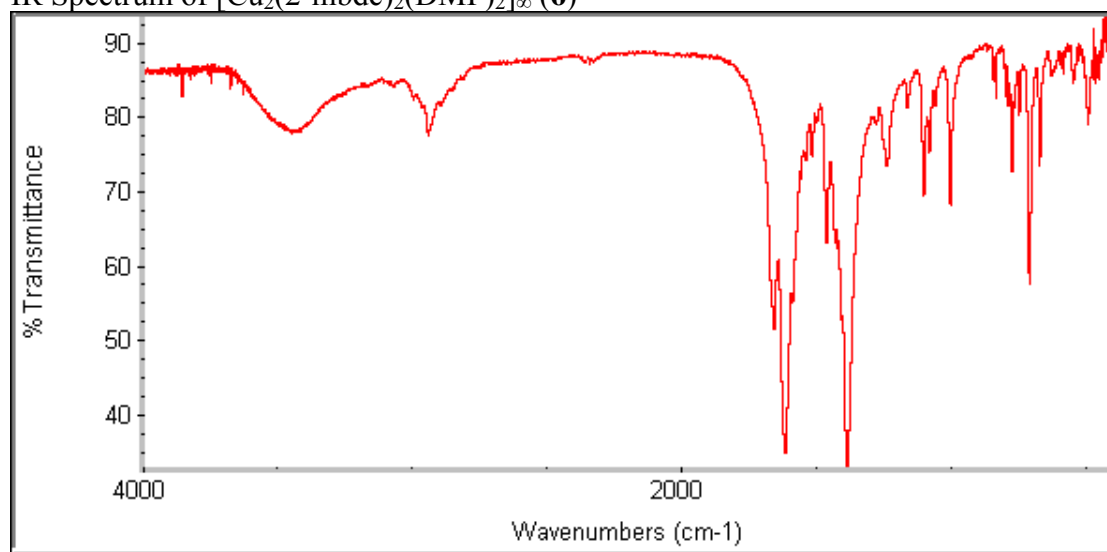
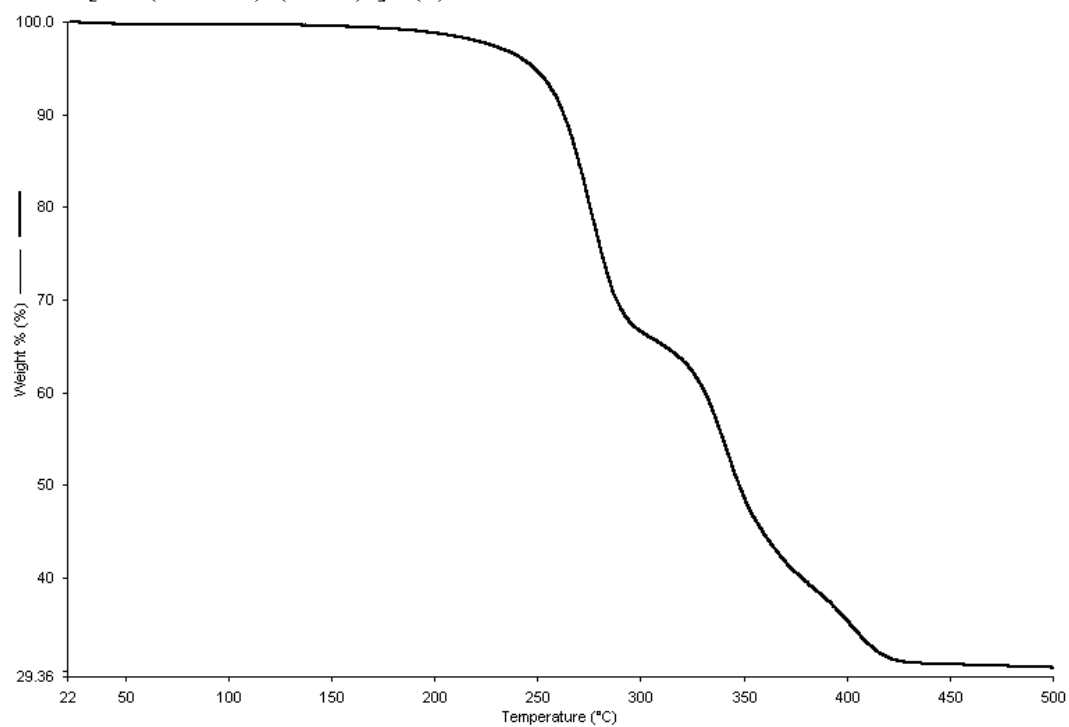XRPD of $[Cu_2(5\text{-}abdc)_2(DMF)_2]$ (**5**)

cr3-037a, cr3-038b & k07adb18(calc)

(green and blue experimental, red calculated from X-ray single crystal structure)

IR Spectrum of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)

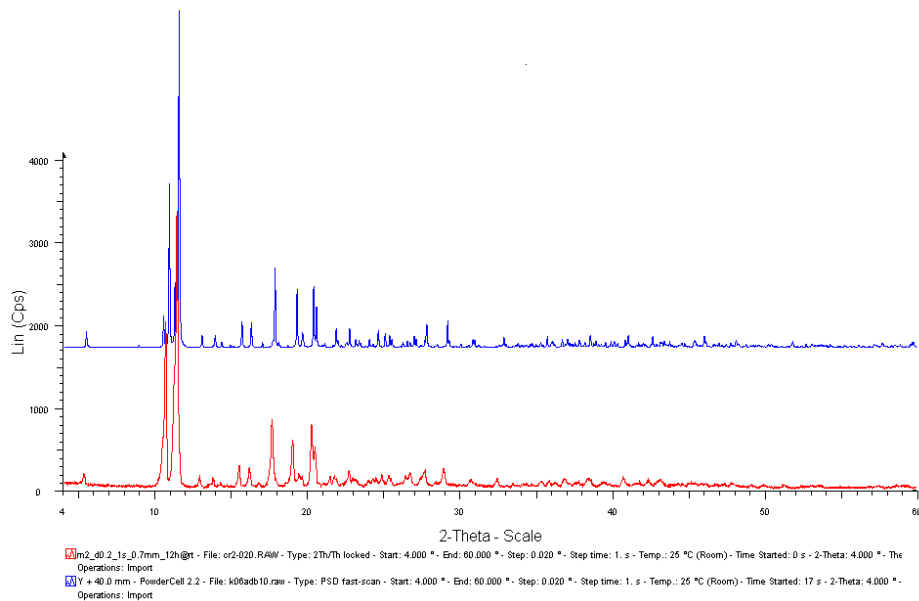TGA of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)

XRPD of $[Cu_2(2\text{-mbdc})_2(DMF)_2]_\infty$ (**6**)

cr2-020 & k06adb10

(red experimental, blue calculated from X-ray single crystal structure)