Supplementary Information for

Pyrazine-bridged Cu(II) chains: diaquabis(n-methyl-2-pyridone)copper(II) perchlorate complexes

Emma Kirkman-Davis,[a] Faith E. Witkos,[a] Veli Selmani,[a] Jeffrey C. Monroe,[a] Christopher P. Landee,[b] Mark M. Turnbull,[a,*] Louise N. Dawe,[c] Matthew Polson[d] and Jan L. Wikaira[d]

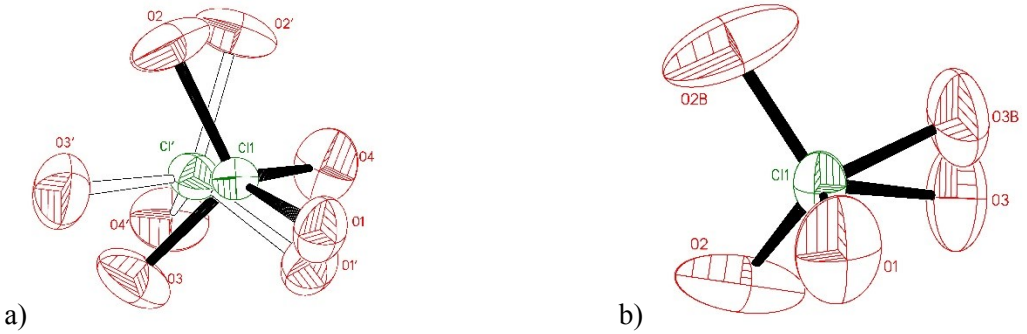
[a]*Carlson School of Chemistry and Biochemistry and the*

[b]*Department of Physics, Clark University, 950 Main Street, Worcester, MA 01610.*

[c]*Department of Chemistry and Biochemistry, Wilfrid Laurier University, 75 University Avenue West, Waterloo, Ontario N2L 3C5.*

[d]*Department of Physical and Chemical Sciences, University of Canterbury, Private Bag 4800, Christchurch, New Zealand.*

Crystallographic Supplementary Information:



a) b)

Figure S1 - a) A thermal ellipsoid plot showing the disordered perchlorate ion of **1**. The occupancy of the Cl1 ion is 0.677 and the occupancy of the Cl' ion is 0.323. b) A thermal ellipsoid plot of the disordered perchlorate ion of **3**. O3 and O3B each have occupancies of 0.5. Attempts to further model the disorder did not improve the refinement.

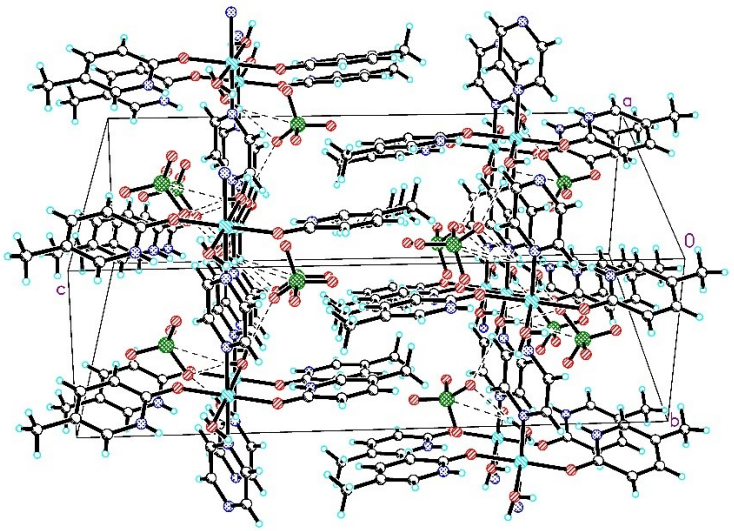


Figure S2 - A packing diagram of **2**(HT) viewed parallel to the *ab*-face diagonal showing interdigitation of the pyridone ligands between chains.

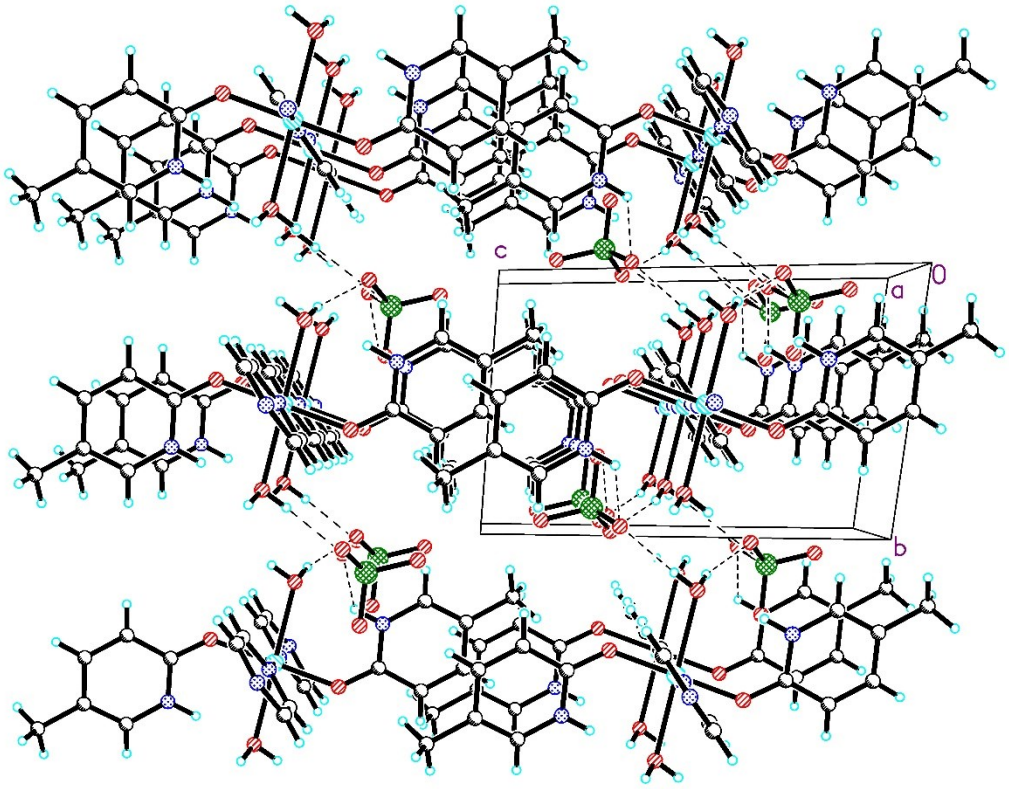


Figure S3 - A packing diagram of **2**(LT) viewed parallel to the *a*-axis (chain axis) showing the isolation of the chains.

Table S1 - Temperature dependent crystallographic data for **2**.

Temp (K)	**SG**	**a (Å)**	**b (Å)**	**c (Å)**	**α (°)**	**β (°)**	**γ (°)**	**V (Å^3)**	**V/molec.**
220	*C*2/*c*	15.016	6.865	22.324		93.368		2297	574
195	*C*2/*c*	14.985	6.859	22.293		93.331		2288	572
170	*P*-1	8.069	15.348	24.304	75.215	84.771	76.940	2833	708
145	*P*-1	6.849	8.059	11.668	79.955	73.917	66.271	565	565
120	*P*-1	6.846	8.051	11.659	79.958	73.894	66.234	564	564

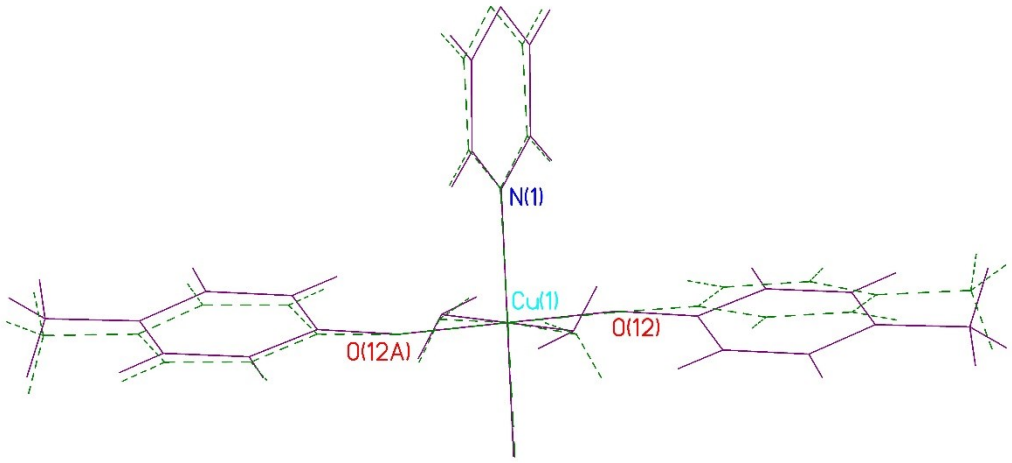


Figure S4 - A wire-frame overlay of the molecular units of **2**(LT) (solid lines) and **2**(HT) (dashed lines).

Table S2 - X-Ray data collection and refinement parameters for the 280 K structures of **1** and **3**.

Compound	**1**	**3**
Formula	$C_{16}H_{22}Cl_2CuN_4O_{12}$	$C_{16}H_{22}Cl_2CuN_4O_{12}$
Mol. Wt.	596.81	596.81
Temp (K)	280(2)	280(2)
Crystal System	Triclinic	Monoclinic
Space Group	$P\bar{1}$	$C2/m$
Unit cell: a(Å) b(Å) c(Å) α (°) β (°) γ (°)	6.8314(6) 8.1609(9) 10.4545(10) 90.984(8) 99.500(7) 93.911(8)	23.0309(19) 6.8184(5) 7.7006(15) 90 90.399(11) 90
Volume (Å)	573.28(10)	1209.2(3)
Z	1	2
Abs. Coef (mm^{-1})	1.256	3.927
Crys. Dim. (mm)	0.49x0.13x0.07	0.13x0.09x0.07
θ/2θ range (°)	3.332-30.708	5.746-76.645
Index ranges	$-7 \leq h \leq 9$	$-28 \leq h \leq 23$

	$-11 \leq k \leq 11$ $-13 \leq l \leq 14$	$-8 \leq k \leq 8$ $-9 \leq l \leq 8$
Total Rlfn	5016	3789
Ind. Rlfn (R_{int})	3882 (0.0606)	1333 (0.0259)
Min-max. trans.	0.437-1.000	0.681-0.887
Data/restr./param.	3882/2/207	1333/1/129
GooF	1.069	1.071
Fin. $R_1(wR_2)I>2\sigma$	0.0792 (0.2060)	0.0398(0.1089)
Fin. $R_1(wR_2)$ all	0.0973 (0.2306)	0.0450(0.1174)
Peak(hole) (e/Å^3)	2.708, near Cu1 (-0.993)	0.368(-0.407)

Magnetism Supplementary Information

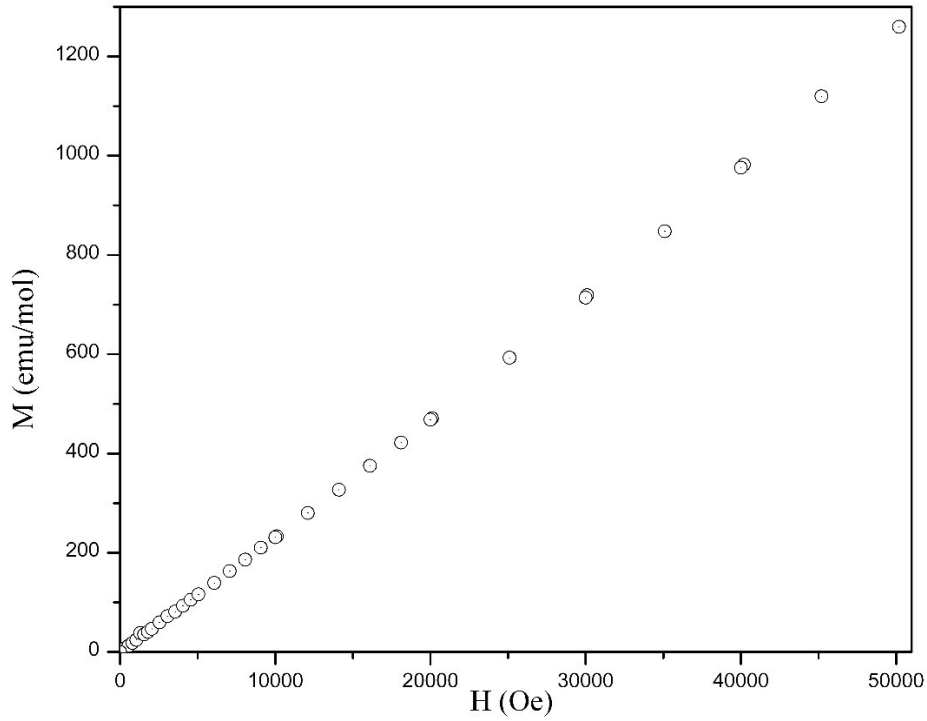


Figure S5 - M(H) for compound **2** at 1.8 K.

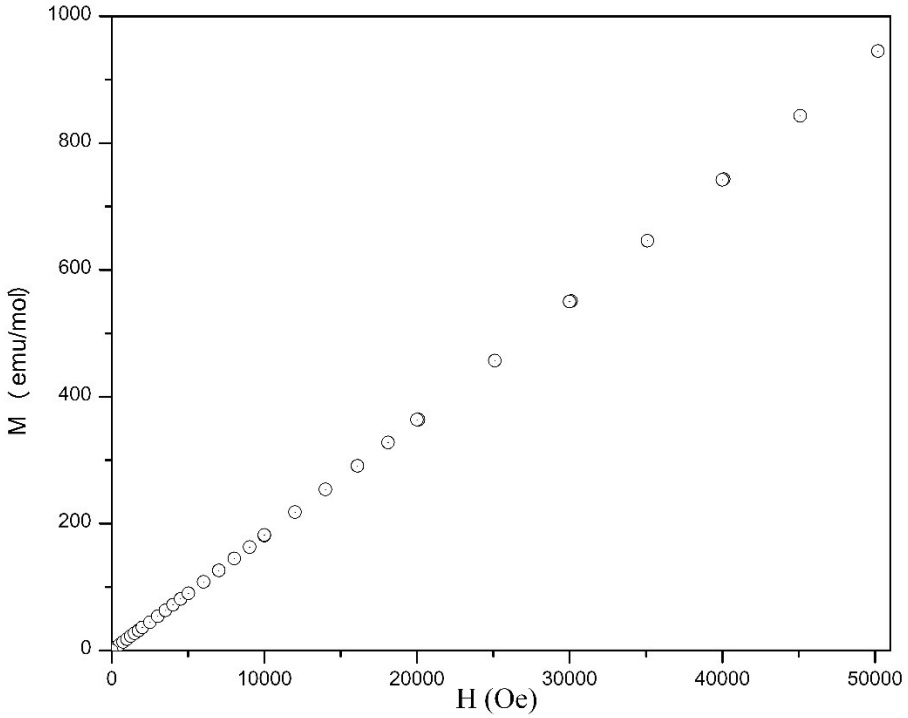


Figure S6 - M(H) for compound **3** at 1.8 K.

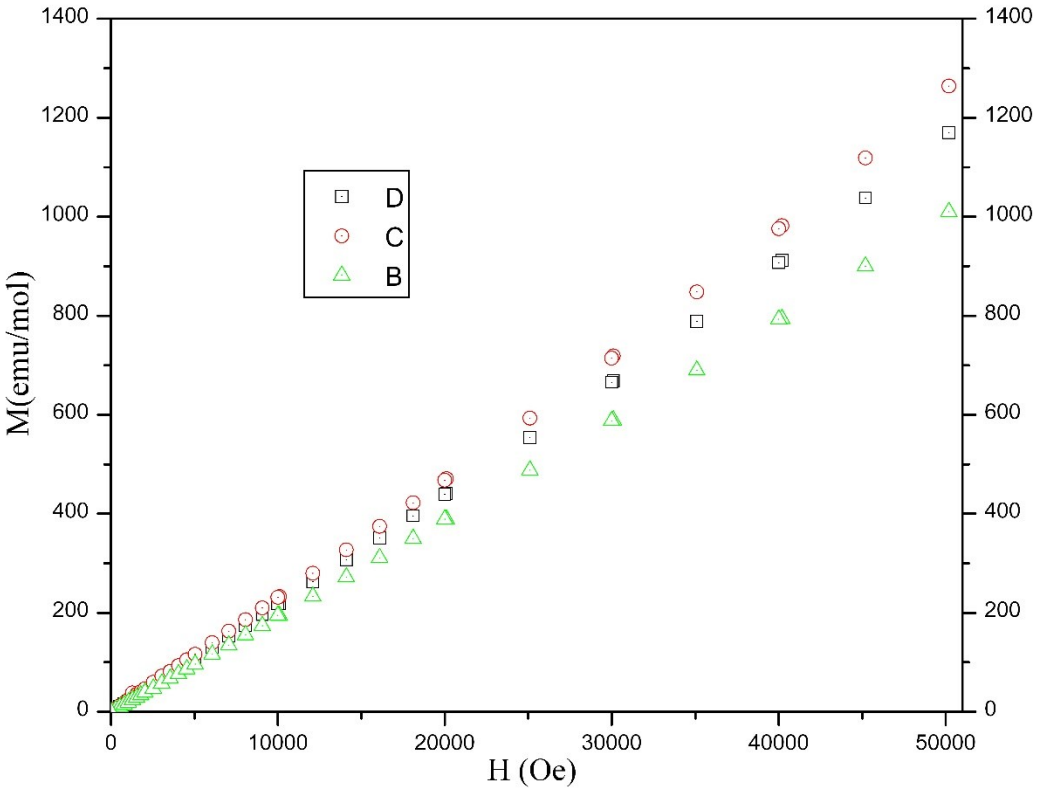


Figure S7 - M(H) for compounds **1-3** at 1.8 K.

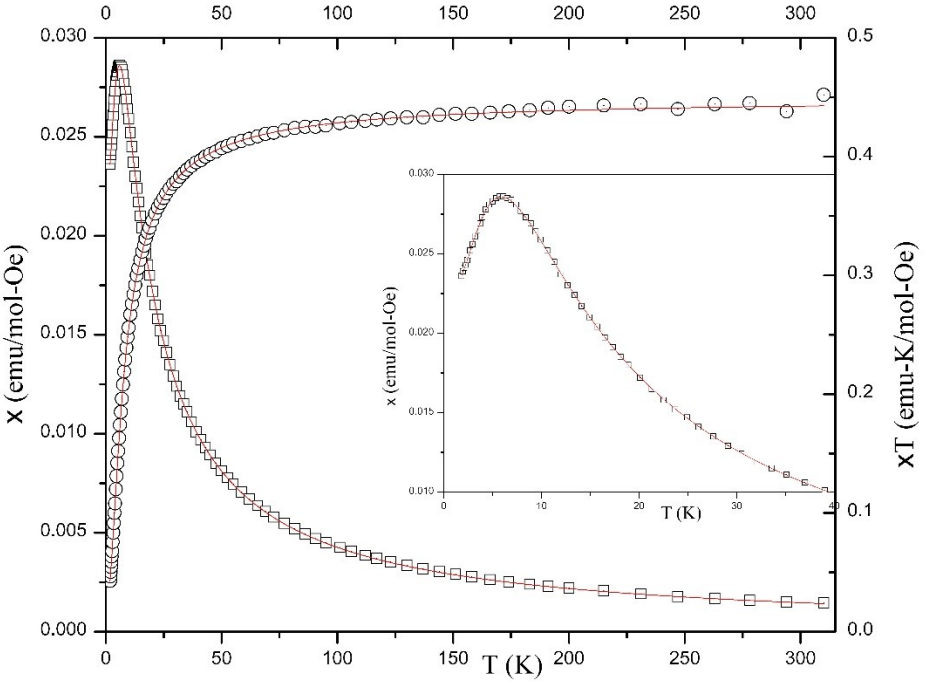


Figure S8 - χ(T) (□) and χT(T) (○) for **2**. The solids lines represent the best fit to the S = ½ Heisenberg chain model with a Curie-Weiss correction to account for interchain interactions. The inset shows an expansion of the χ(T) data in the region of the maximum.

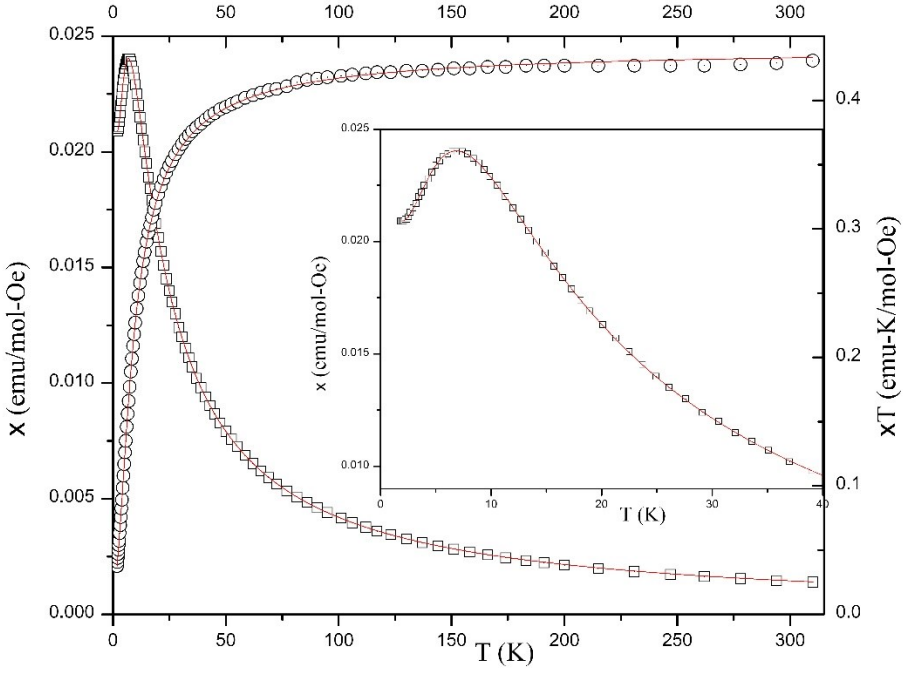


Figure S9 - χ(T) (□) and χT(T) (○) for **3**. The solids lines represent the best fit to the S = ½ Heisenberg chain model with a Curie-Weiss correction to account for interchain interactions. The inset shows an expansion of the χ(T) data in the region of the maximum.

Powder X-ray diffraction Supplementary Information

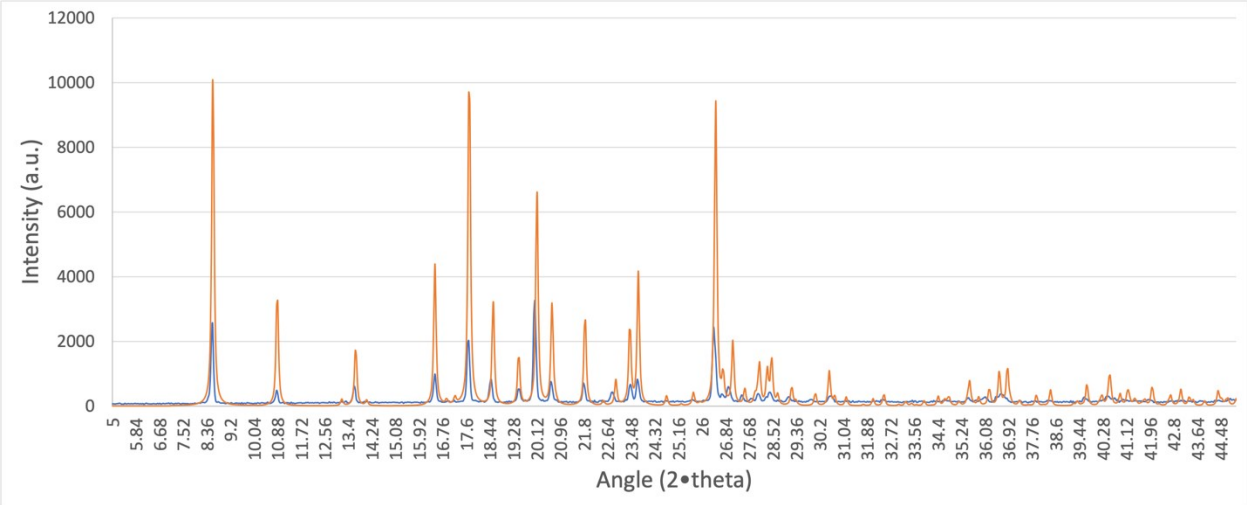


Figure S10: Comparison of the powder X-ray diffraction pattern of **1** (blue trace) with the calculated pattern based upon room temperature single crystal X-ray data (orange trace).

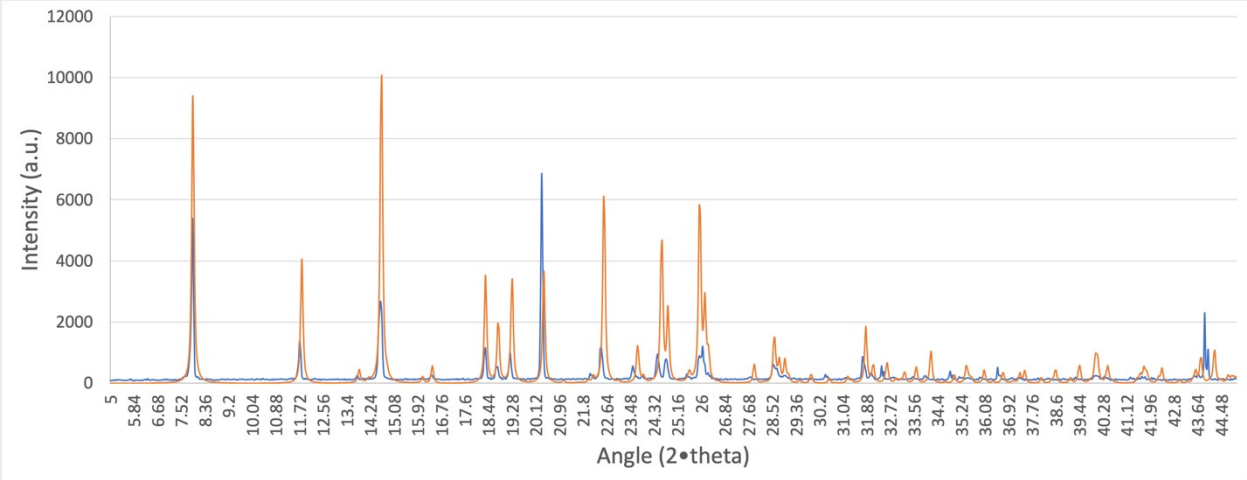


Figure S11: Comparison of the powder X-ray diffraction pattern of **2** (blue trace) with the calculated pattern based upon single crystal X-ray data at 220 K (orange trace).

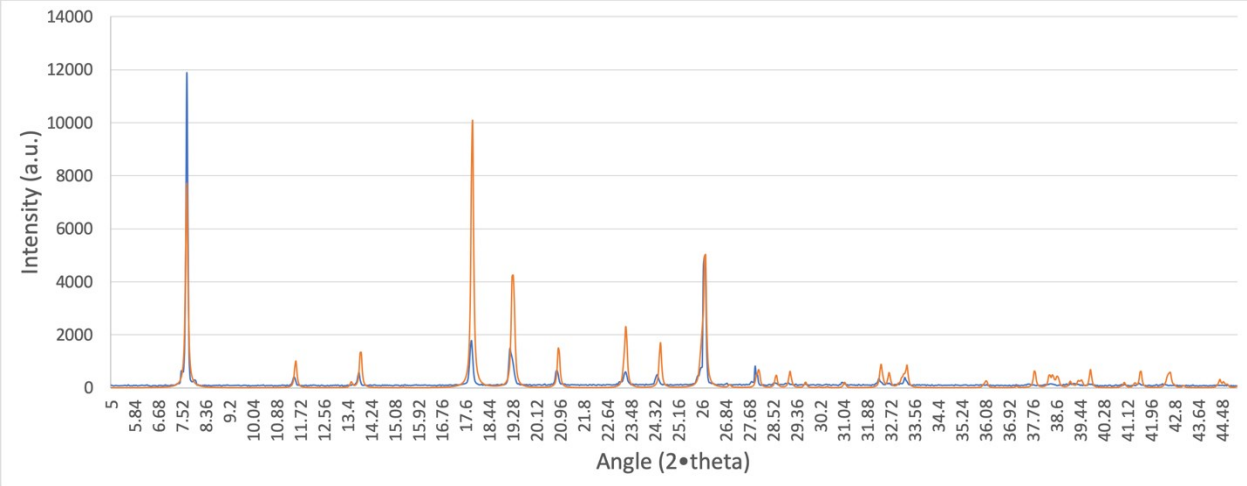


Figure S12. Comparison of the powder X-ray diffraction pattern of **3** (blue trace) with the calculated pattern based upon the single crystal X-ray data (orange trace).