Supplementary information for 'Orbital frustration in the $S = \frac{1}{2}$ kagome magnet vesignieite, $BaCu_3V_2O_8(OH)_2$'

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Lattice parameters							
a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
5.917849(38)	5.917849(38)	20.75995(38)	90	90	120		
Atomic information							
Site	Ox. state	Wyckoff	x	y	z	Occ	B_{iso}
Ba1	2+	3a	0.6879(19)	0	$\frac{1}{3}$	1	0.349(80)
Cu1	2+	6c	0.6857(31)	0.4924(40)	0.8344(10)	1	0.545(50)
Cu2	2+	3b	0	0.1758(24)	$\frac{1}{6}$	1	0.297(215)
O11_1	2-	6c	0.1935(97)	1.0150(73)	0.5617(10)	0.5	0.084(80)
O11_2	2-	6c	0.1417(108)	0.9661(27)	0.5558(29)	0.5	0.084(80)
O12_1	2-	6c	0.5340(46)	0.6945(115)	0.8958(7)	0.5	0.084(80)
O12_2	2-	6c	0.5390(37)	0.7167(28)	0.9174(6)	0.5	0.084(80)
O13_1	2-	6c	0.8401(41)	0.3543(91)	0.2176(7)	0.5	0.084(80)
O13_2	2-	6c	0.8064(34)	0.3536(100)	0.2382(9)	0.5	0.084(80)
O21	2-	6c	0.6747(16)	0.0234(35)	0.1268(2)	1	0.288(145)
O31	2-	6c	0.7390(12)	0.0799(9)	0.0017(5)	1	1.011(10)
V1	5+	6c	0.7154	0.0454	0.9267	1	0.2
D1	1+	6c	0.6854(17)	0.0318(17)	0.0767(2)	1	0.217(91)

Table 1: Structural information of vesignieite obtained from Rietveld refinement of powder neutron diffraction data collected at 4 K at the HRPD beamline, ISIS. The final Rietveld refined profiles are shown in Figure S1.

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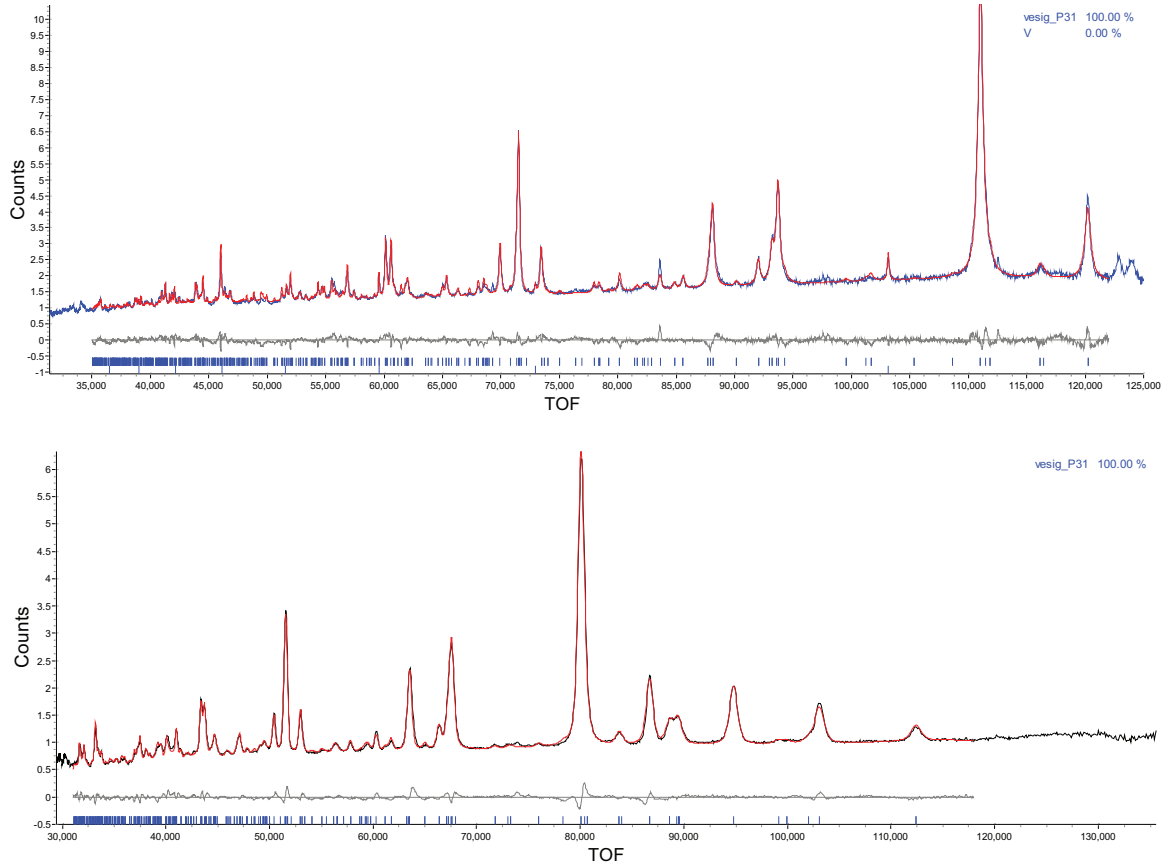

Figure 1: Final Rietveld refined profiles for the powder neutron diffraction data collected on Sample 2 at HRPD beamline, ISIS. The top figure is the fit to data collected on bank 1 ($2\Theta = 168.567°$), whilst the bottom is from bank 2 ($2\Theta = 90.248°$). The blue line is the collected data, the red line is the calculated data and the grey line is the difference. The final refined parameters are shown in Table S1.

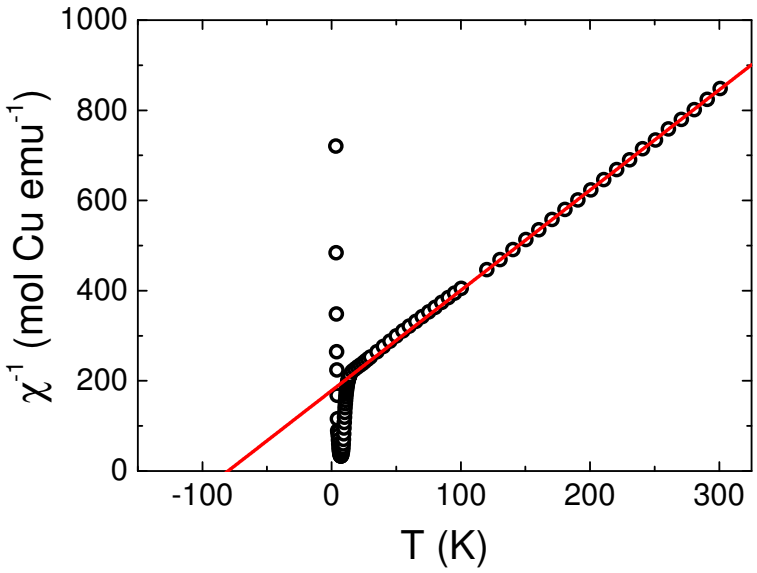

Figure 2: Fit to the Curie-Weiss law for the inverse magnetic susceptibility, $\chi^{-1}(T)$, of Sample 1. Fitting to the region $150 < T(K) < 300$ gives the Weiss temperature and Curie constant $\theta_{\mathrm{W}} = -80\,\mathrm{K}$ and $C = 0.450\,\mathrm{emu\,K\,mol^{-1}}$, respectively.

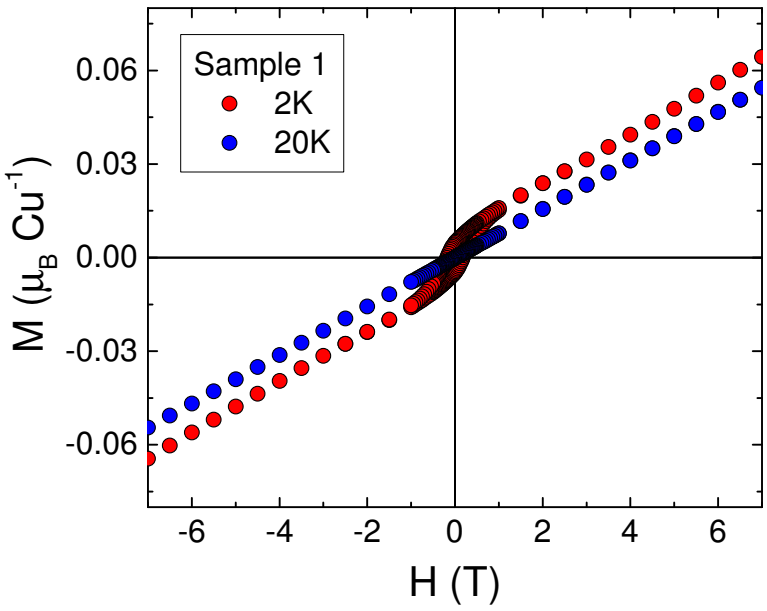

Figure 3: Isothermal magnetisation data as a function of applied magnetic field for Sample 1 taken at $T = 2$ and 20 K.

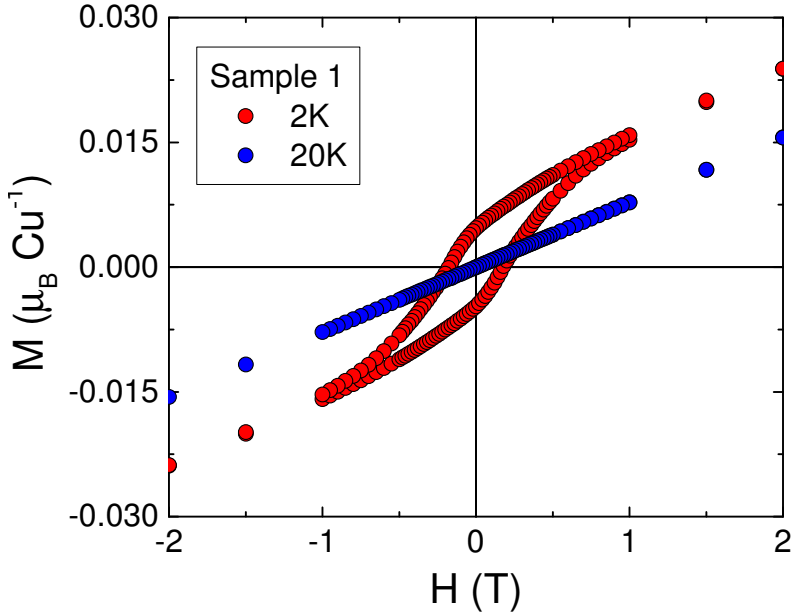

Figure 4: Isothermal magnetisation data as a function of applied magnetic field for Sample 1 at $T = 2$ and 20 K. This graph is a zoomed in region of Figure 2.