Supplementary Information

Synthesis, crystal structure, magnetic properties and electronic structure of the new ternary vanadate CuMnVO_4

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Table S1. Crystallographic and structure refinement data for CuMnVO₄

Formula	CuMnVO ₄
Crystal color	black
MW (g mol ⁻¹)	233.42
Crystal system	orthorhombic
space group	<i>Cmcm</i>
Parameters	a = 5.787(2) Å, b = 8.807(3) Å, c = 6.410(2) Å
V(Å ³)	326.69(19)
Z	4
Density calc.(g.cm ⁻³)	4.744(3)
Crystal shape	block
Temperature (K)	293
Diffractometer	Enraf-Nonius Kappa CCD
Monochromator	Oriented graphite
Radiation	MoK _α (λ = 0.71069Å)
Scan mode	CCD scan
h k l range	-10 < h < 10, -15 < k < 15, -11 < l < 11
θ _{min} , θ _{max}	4.21°, 40°
Linear absorption coeff.	12.894 mm ⁻¹
Absorption correction	Gaussian
T _{min} /T _{max}	0.612/0.785
No of reflections	6676
R _{int}	0.1017
No of independent reflections	578
Reflections used (I > 3σ(I))	433
Refinement	F ²
F(000)	436
R factors	R(F)/wR(F ²) = 0.0356/0.1091
No. of refined parameters	25
g.o.f.	1.71
Weighting scheme	w = 1/(σ ² (I) + 0.0016I ²)
Diff. Fourier residues (e ⁻ /Å ³)	[-1.77, +2.12]

Table S2. Final anisotropic displacement parameters for CuMnVO₄

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0472(6)	0.0266(5)	0.0135(4)	0	0	0
Mn	0.0098(4)	0.0114(4)	0.0069(3)	0	0	-0.0001(2)
V	0.0073(4)	0.0088(4)	0.0063(3)	0	0	0
O1	0.0098(12)	0.0155(12)	0.0091(11)	-0.0012(9)	0	0
O2	0.0143(13)	0.0138(13)	0.0112(10)	0	0	0.0005(10)