SUPPORTING INFORMATION

Crystal structure, infrared spectroscopy and thermodynamic properties of a manganese member of ellenbergerite family

Larisa V. Shvanskaya,[*a] Polina V. Krikunova,[b] Tatyana M. Vasilchikova,[a] Elena Y. Borovikova,[c] Olga S. Volkova,[a] Alexander N. Vasiliev[a]

[a]Lomonosov Moscow State University, Moscow 119991, Russia.
[b]FSRC "Crystallography and Photonics" RAS, Moscow 119333, Russia.
[c]Kola Science Centre, RAS, Apatity 184209, Russia.
[*] E-mail: lshvanskaya@mail.ru

Table S1. Crystal data and details of the X-ray data collection and refinement for $Mn_{6.75}(OH)_3H_{1.20}(VO_4)_{4-2z}(V_2O_7)_z$ (z = 0.15)

M_r	880.335
Crystal system, space group	Hexagonal, $P6_3mc$
Temperature (K)	293
a, c (Å)	13.1893 (5), 5.2408 (2)
V (Å^3), Z	789.54 (7), 2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.55
Crystal size (mm)	0.251x0.043x0.036
Diffractometer	Bruker D8 Quest diffractometer with Photon III detector
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.510, 0.650
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7817, 858, 816
R_{int}	0.046
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.703
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.040, 1.08
No. of reflections/ parameters/restraints	858/68/4
ρ_{max}, ρ_{min} (e Å^{-3})	0.72, -0.53
Absolute structure	Flack x determined using 355 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.04 (2)

Computer programs: *SHELXL2018*/3 (Sheldrick, 2018).

Table S2. Bond valence data for $Mn_{6.75}(OH)_3H_{1.20}(VO_4)_{4-2z}(V_2O_7)_z$ (z = 0.15)*

Atom	Mn1	Mn2(0.749**)	V1	V2A(0.847)	V2B(0.153**)	H1	H2	H3	Σ
O1		$0.264_{3\downarrow}$	1.255						1.779
		$0.260_{3\downarrow}$							
O2	$0.429_{2\rightarrow}$		1.199						2.057
O3	0.414		$1.293_{2\downarrow}$						2.119
	0.412								
O4	$0.302_{2\rightarrow}$					0.96	0.01		2.044
	$0.235_{2\rightarrow}$								
O5	$0.400_{2\rightarrow}$			$1.095_{3\downarrow}$	$0.142_{3\downarrow}$	0.02	0.01	0.168	2.035
O6				0.944	0.089	0.02	0.696	0.01	1.759
Σ	2.192	1.572	5.040	4.229	0.515				

*The symbols $_\downarrow$ and $_\rightarrow$ show a multiplication of the corresponding contribution in the columns and rows due to symmetry

**occupation of atomic position

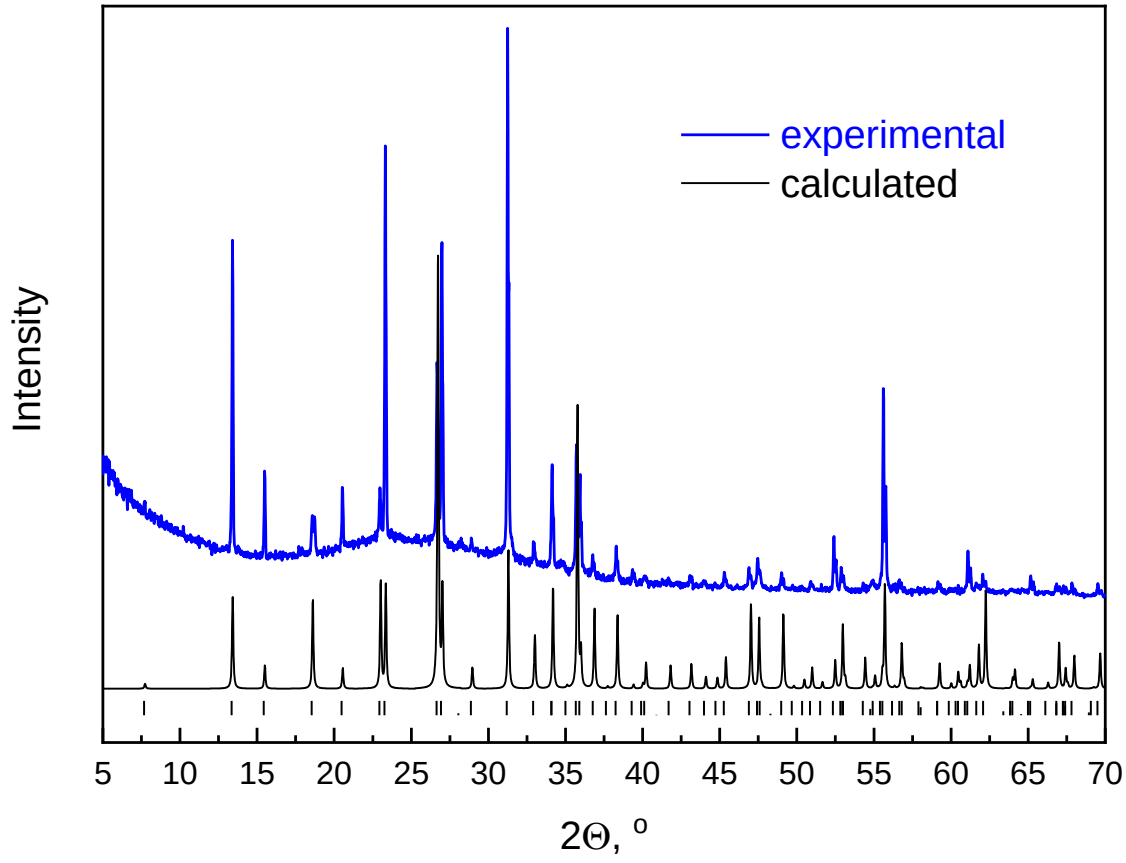

Figure S1. Experimental and calculated powder XRD patterns of $Mn_{6.75}(OH)_3H_{1.20}(VO_4)_{4-2z}(V_2O_7)_z$ ($z = 0.15$) (the vertical ticks indicate the Bragg positions).