

TABLE S1 Parameters for the modeling of X-ray diffraction pattern of vernadite typical for nodules of this study

Atom ¹	Atomic coordinates ¹			Site occupancy ²
	x	y	z	
Mn	0.000	0	0	0.92
O	0.333	0	0.103	2
Mn	0.000	0	0.221	0.16
O	-0.333	0	0.349	0.48
K	-0.500	0	0.500	0.02
K	-0.250	0.250	0.500	0.02
K	-0.250	-0.250	0.500	0.02
O	0.160	0.000	0.500	0.02
O	-0.080	0.240	0.500	0.02
O	-0.080	-0.240	0.500	0.02

Note: symmetry operations: (x, y, z) , $(-x, -y, -z)$, $(x+1/2, y+1/2, z)$, $(-x+1/2, -y+1/2, -z)$. The structure can be drawn in the $C2/m$ space group to ease representation, but care must be taken not to generate positions from adjacent layers, as the structure is turbostratic. The refined mean coherent scattering domains are 7 nm in the **a-b** plane and 7.8 nm along **c***.

¹ Debye-Waller factors were set to 0.5 Å² for Mn1, 1 Å² for O_{Mn1} and 2 Å² for all other species.

¹ Atomic coordinates in fraction of *a*, *b* and *c* which are respectively equal to 4.940 Å, 2.852 Å and 9.750 Å. $\gamma = 90^\circ$. The structure is described using $\gamma=90^\circ$ to ease comparison with previously published structure models, but it could also be described using $\gamma=120^\circ$, as layer symmetry is hexagonal.

² Expressed per layer octahedron, and as the sum of the equivalent (x, y, z) and $(-x, -y, -z)$ sites.

Simulation of powder X-ray diffraction pattern was performed using the mathematical formalism developed by Drits and Tchoubar (1990), which allows the calculation of patterns from structures affected by various nature and density of layer crystallization defects (e.g. layer vacancies, isomorphic substitutions) and of layer stacking defects (e.g. interstratification, random stacking faults). As this method is based on a trial-and-error procedure, a correlation matrix cannot be extracted, and thus, uncertainties cannot be evaluated from a mathematic procedure. These uncertainties are retrieved from sensitivity tests, which have demonstrated that this method can accurately determine the structure of various layered structures, such as phyllomanganates, phyllosilicates and nanocrystalline calcium silicate hydrates (Manceau 1997; Villalobos et al. 2006; Lanson et al. 2008, Grangeon et al. 2010, 2013). For example, number of interlayer species sorbed in TC configuration per layer octahedron is typically ± 0.01 per layer octahedron (Manceau et al. 1997). However, because of statistical noise arising for low sample available for XRD analysis, the uncertainty is certainly higher in the present case.

Drits, V. A., and Tchoubar, C. (1990) X-ray diffraction by disordered lamellar structures: theory and applications to microdivided silicates and carbons. Springer-Verlag: Berlin, p 371.

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