Comment on the CIF file

The chemical composition derived from the crystallographic model does not match that obtained form electron microprobe. This is mainly due to the crystallographic model adopted for the Z site: Mg and Cr were used, instead of Mg, Cr, V and Al.

Although we tried to carry out a structural refinement considering the Z site occupied by Mg, Cr, V and Al, it was unstable (also when fixing the occupancy of Al and V to the value obtained from the chemical analysis). Such an instability is probably due to the X-ray scattering for Mg (Z = 12) and Al (Z = 13), as well as for Cr (Z = 24) and V (Z = 23), that are is too similar.

We stated this inconsistency in the "_refine_special_details" of the CIF file:

The chemical composition derived from the crystallographic model diverges from that obtained from electron microprobe because no chemical constraint was possible to apply during the refinement. The real structural formula, determined by combining structural and chemical data, is explained in detail in the manuscript subsection "Site population", and reported below in reference to the general formula XY3Z6T6B3O27V3W:

X = Na0.87 Ca0.07 vacancy0.04 K0.02

Y = Cr2.29 Mg0.71

Z = Al3.04 Mg1.54 Cr1.18 V0.22 Fe0.01

T = Si5.96 Al0.04

B = B3.00

V = OH3.00

W = O0.73 F0.25 OH0.02.