American Mineralogist, Volume 99, pages 847–851, 2014

SPINELS RENAISSANCE: THE PAST, PRESENT, AND FUTURE OF THOSE UBIQUITOUS MINERALS AND MATERIALS

Crystal chemistry of the ulvöspinel-qandilite series†

FERDINANDO BOSI[1,2,*], ULF HÅLENIUS[2] AND HENRIK SKOGBY[2]

[1]Dipartimento di Scienze della Terra, Sapienza Università di Roma, Piazzale Aldo Moro 5, I-00185 Roma, Italy
[2]Department of Geosciences, Swedish Museum of Natural History, SE-10405 Stockholm, Sweden

ABSTRACT

Five spinel single-crystal samples within the ulvöspinel-qandilite series [$(Fe_{2-x}Mg_x)TiO_4$, $0.15 < x < 0.94$] were synthesized and structurally and chemically characterized by X-ray diffraction and electron microprobe techniques. Site populations, derived from structural and chemical analysis, show that the tetrahedrally coordinated site (T) is exclusively populated by Mg^{2+} and Fe^{2+}, while the octahedrally coordinated site (M) is populated by Ti^{4+}, Mg^{2+}, Fe^{2+}, and minor amounts of Fe^{3+}. The inverse cation distribution is characterized by parallel substitution of Mg^{2+} for Fe^{2+} at both the T and M sites along the series.

The variation in the unit-cell parameter from 8.527 to 8.495 Å is mainly related to the occurrence of Mg^{2+} at the M site rather than the T site. In fact, the substitution of Mg^{2+} for Fe^{2+} yields significant variations in M-O (from 2.045 to 2.034 Å) and only limited variation in T-O (from 2.007 to 2.002 Å). In conjunction with data from the literature, the present study provide a basis for quantitative analyses of the variation in ^{T}Mg-O bond distance from 1.966 Å for Mg-poor ulvöspinel to 1.990 Å for the qandilite end-member.

Keywords: Ulvöspinel, qandilite, electron microprobe, X-ray diffraction, cation ordering, crystal chemistry