

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

### Crystal chemistry of the ulvöspinel-qandilite series†

FERDINANDO BOSI<sup>1,2,\*</sup>, ULF HÅLENIUS<sup>2</sup> AND HENRIK SKOGBY<sup>2</sup>

<sup>1</sup>Dipartimento di Scienze della Terra, Sapienza Università di Roma, Piazzale Aldo Moro 5, I-00185 Roma, Italy

<sup>2</sup>Department of Geosciences, Swedish Museum of Natural History, SE-10405 Stockholm, Sweden

#### ABSTRACT

Five spinel single-crystal samples within the ulvöspinel-qandilite series  $[(\text{Fe}_{2-x}\text{Mg}_x)\text{TiO}_4]$ ,  $0.15 < x < 0.94$ ] 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  $\text{Mg}^{2+}$  and  $\text{Fe}^{2+}$ , while the octahedrally coordinated site (M) is populated by  $\text{Ti}^{4+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Fe}^{2+}$ , and minor amounts of  $\text{Fe}^{3+}$ . The inverse cation distribution is characterized by parallel substitution of  $\text{Mg}^{2+}$  for  $\text{Fe}^{2+}$  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  $\text{Mg}^{2+}$  at the M site rather than the T site. In fact, the substitution of  $\text{Mg}^{2+}$  for  $\text{Fe}^{2+}$  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 <sup>7</sup>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