

**Composition, stability, and structure of a new member of the aenigmatite group,
 $\text{Na}_2\text{Mg}_{4+x}\text{Fe}_{2-2x}^{3+}\text{Si}_{6+x}\text{O}_{20}$, synthesized at 13–14 GPa**

**TIBOR GASPARIK,^{1,*} JOHN B. PARISE,¹ RICHARD J. REEDER,¹
VICTOR G. YOUNG,² AND WENDY S. WILFORD³**

¹Center for High Pressure Research and Department of Geosciences, State University of New York at Stony Brook, Stony Brook, New York 11794, U.S.A.

²Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455, U.S.A.

³Department of Chemistry, Whitman College, Walla Walla, Washington 99362, U.S.A.

ABSTRACT

A new phase isostructural with the minerals of the aenigmatite group $\text{Na}_2\text{Mg}_{4+x}\text{Fe}_{2-2x}^{3+}\text{Si}_{6+x}\text{O}_{20}$ with $x = 0.25 - 0.5$ was synthesized at 13–14 GPa with a split-sphere anvil apparatus (USSA-2000). The structure (for $x = 0.4$) was determined from twinned-crystal X-ray diffraction data. The unit cell is triclinic, $P\bar{1}$, $a = 10.328(1)$, $b = 10.724(1)$, $c = 8.805(1)$ Å, $\alpha = 105.15(1)$, $\beta = 96.85(1)$, $\gamma = 125.47(1)^\circ$, $V = 719.67(3)$ Å³, $Z = 2$, calculated density = 3.335 g/cm³. The twin law, independently determined from electron diffraction and transmission electron microscopy and by inspection of the X-ray data collected with an area detector, relates the twin components by a 180° rotation about [110]*. Due to the coupled substitution, $2\text{Fe}^{3+} = \text{MgSi}$, which introduces octahedral Si, the stability of the phases with the aenigmatite structure apparently expands with increasing pressure. Hence, these phases could play a major role in the transition zone (410–660 km), where the more common minerals they are replacing, olivine and clinopyroxene, reach the limit of their stability. The new evidence for the stability of aenigmatite-like minerals in the deep mantle could have important implications for the origin of the parental magmas producing aenigmatite-bearing and other agpaitic rocks.