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Ferromagnesian jeffbenite synthesized at 15 GPa and 1200 °C

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Abstract

Single crystals of Al-free, ferromagnesian jeffbenite up to 200 μm in size have been synthesized at 15 GPa and 1200 °C in a 1200 tonne multi-anvil press from a starting composition in the forsterite-fayalite-magnetite-water system. This phase has the approximate formula $Mg_{2.62}Fe^{2+}_{0.87}Fe^{3+}_{1.63}Si_{2.88}O_{12}$ and is observed to coexist with a Ca-free clinopyroxene plus what appears to be quenched melt. The crystal structure has been refined from single-crystal X-ray diffraction data and is similar to that determined for natural Al-bearing jeffbenite, $Mg_3Al_2Si_3O_{12}$, reported from inclusions in superdeep diamonds. The structure is a tetragonal orthosilicate in space group $I\bar{4}2d$ with a = 6.6449(4) Å, c = 18.4823(14) Å, and is structurally more closely related to zircon than to garnet. The T2 site is larger than T1, shares an edge with the M2 octahedron, and incorporates significant Fe^{3+}. Because of the tetrahedral incorporation of trivalent cations, jeffbenite appears to be compositionally distinct from garnet. Previous speculations that the phase may only occur as a retrograde decompression product from bridgmanite are not supported by its direct synthesis under transition zone conditions. The phase has a calculated density of 3.93 g/cm^3, which is indistinguishable from a garnet of comparable composition, and is a possible component in the mantle transition zone under oxidizing conditions or with Al-rich compositions.

Keywords: Jeffbenite, tetragonal almandine pyrope phase (TAPP), super deep diamonds, diamond inclusions