

## High-pressure crystal chemistry of Fe<sup>3+</sup>-wadsleyite, $\beta$ -Fe<sub>2.33</sub>Si<sub>0.67</sub>O<sub>4</sub>

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### ABSTRACT

The crystal structure of Fe<sup>3+</sup>-wadsleyite, (Fe<sub>1.67</sub><sup>2+</sup>Fe<sub>0.33</sub><sup>3+</sup>)(Fe<sub>0.33</sub><sup>3+</sup>Si<sub>0.67</sub>)O<sub>4</sub>, was determined by single-crystal X-ray techniques at six pressures to 8.95 GPa. The isothermal bulk modulus is  $K_{T0} = 173(3)$  GPa [ $K'_{T0} = \partial K_T / \partial P = 5.2(9)$ ], which is identical within error to bulk moduli observed for normal wadsleyites [ $\beta$ -(Mg,Fe)<sub>2</sub>SiO<sub>4</sub>]. Compression of Fe<sup>3+</sup>-wadsleyite is significantly more isotropic than for  $\beta$ -(Mg,Fe)<sub>2</sub>SiO<sub>4</sub> because Fe<sup>3+</sup> substitutes into both Si<sup>4+</sup> tetrahedral sites and (Mg,Fe<sup>2+</sup>) octahedral sites. Ferric iron thus reduces the contrast between tetrahedral and octahedral compressibilities, which in turn reduces the compressional anisotropy. Bond distance analysis and octahedral compressibilities of the three symmetrically distinct octahedral sites reveal that Fe<sup>3+</sup> orders preferentially into M1 and M3, while M2 occupancy is close to pure Fe<sup>2+</sup>.