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High-resolution ^{17}O MAS NMR spectroscopy of forsterite (α-Mg_2SiO_4), wadsleyite (β-Mg_2SiO_4), and ringwoodite (γ-Mg_2SiO_4)

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Abstract

The high sensitivity of the satellite-transition (ST) MAS NMR technique was exploited to obtain high-resolution ^{17}O MAS NMR spectra of the three polymorphs of Mg_2SiO_4: forsterite (α-Mg_2SiO_4), wadsleyite (β-Mg_2SiO_4), and ringwoodite (γ-Mg_2SiO_4). High NMR sensitivity was important in this application because ^{17}O-enriched, Fe-free materials are required for ^{17}O NMR and high-pressure syntheses of the dense β and γ polymorphs result in a only a few milligrams of these solids. In all, eight distinct O species were identified and assigned: three in forsterite, four in wadsleyite, and one in ringwoodite, in agreement with the number of O sites in their crystal structures. The isotropic chemical shifts extracted are in excellent agreement with a previously published correlation with Si-O bond length. However, unexpectedly large quadrupolar coupling constants were found for the non-bridging O species in the dense polymorphs wadsleyite and ringwoodite.