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Unraveling the dilemma of the post-spinel structure of magnetite; Mössbauer and XRD studies of $M\mathrm{Fe_2O_4}$ (M = $\mathrm{Mg^{2+}}$, $\mathrm{Fe^{2+}}$, $\mathrm{Zn^{2+}}$)

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Based on high-pressure XRD and ^{57}Fe Mössbauer studies (MS) of $M\mathrm{Fe_2O_4}$ (M = $\mathrm{Mg^{2+}}$, $\mathrm{Fe^{2+}}$, $\mathrm{Zn^{2+}}$), it was unequivocally concluded that the high-pressure, post-spinel, phases of magnetite ($\mathrm{Fe_3O_4}$), magnesio, and zinc ferrites are not of the $\mathrm{CaMn_2O_4}$ (*Pbcm*) or $\mathrm{CaTi_2O_4}$ (*Bbmm*) structure types. This conclusion is based primarily on detailed room and cryogenic temperature Mössbauer studies at P $>$ 25 GPa, the pressure region of the post-spinel (PS) phase.

The $M\mathrm{Fe_2O_4}$ (M=Fe, Zn) species, prior to the first-order phase transition at vicinity of 25 GPa, are normal spinels in which the identical ferric ions are at the six-coordinated B-sites and the M^{2+} ions at the *A-site* and $\mathrm{MgFe_2O_4}$ is an inverse spinel. Following the transition the ferric ions assume two non-equivalent sites, Fe(I) and Fe(II), characterized by their different quadrupole splitting (QS) and Isomer Shift (IS) values. Whereas QS(P) of both sotes barely changes with pressure, the IS of the I and II sites decreases with P but with different slope. Considering the fact that IS(P) $\propto$ -$\rho_s(P)$, where ρ_s is the s-density at the Fe-site, suggests that the elastic constants of the two Fe sites are different. To the highest pressure measured ($\sim$100 GPa), the ferric ions

remain at the high-spin state as manifested by the magnetic ordering observed at low temperatures.

The validity of the $CaMn_2O_4$, $CaTi_2O_4$, and $CaFe_2O_4$ structures as the characteristic HP phase of magnetite and (Mg,Zn) ferrites will be discussed.