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LETTER

Si vacancies in the 10-Å phase

M.D. WELCH,[1,2,*] A.R. PAWLEY,[3] S.E. ASHBROOK,[2] H.E. MASON,[4] AND B.L. PHILLIPS[4]

[1]Department of Mineralogy, The Natural History Museum, London SW7 5BD, U.K.
[2]Department of Earth Sciences, Cambridge University, Cambridge CB2 3EQ, U.K.
[3]School of Earth, Atmospheric and Environmental Sciences, The University of Manchester, Manchester M13 9PL, U.K.
[4]Department of Geosciences, SUNY Stony Brook, Stony Brook, New York 11794-2100, U.S.A.

ABSTRACT

^{29}Si MAS NMR spectroscopy on samples of 10-Å phase synthesized from oxides (6.0 GPa/600 °C/400 h) and from partial transformation of talc (6.5 GPa/650 °C/12.5 h) reveals that this phase contains Q^2-type Si sites in a ratio Q^3:Q^2 of 5.33:1. It is proposed that the Q^2 arise from adjacent vacancies in the tetrahedral sheets for which charge balance is most likely achieved by hydroxylation via a hydrogarnet-like substitution involving the formation of Q^2 silanol groups. Variable-contact-time ^{29}Si {^{1}H} CP/MAS NMR spectra of the talc/10-Å phase product support the assignment of Q^2 Si to the proposed $SiO_3(OH)$ groups. Electron microprobe analysis, including oxygen, gives the following empirical formula normalized to three Mg apfu and inferring a hydrogarnet component Si → 4H associated with Si vacancies: $Mg_3Si_{3.83(8)}O_{9.32}(OH)_{2.68}.1.1(4)H_2O$. The observed Mg:Si indicates a significant Si deficiency relative to talc. Comparison of the ^{29}Si MAS NMR and microprobe data indicates that Si vacancies likely occur as single isolated entities, rather than as pairs or clusters, and that between 1 in 18 and 1 in 23 Si sites is vacant. The results suggest new and intriguing possibilities for the incorporation of excess H into the 10-Å phase and, potentially, other phyllosilicates under upper-mantle conditions.

Keywords: 10-Å phase, Si vacancies, ^{29}Si NMR spectroscopy, silanol