Crystal Chemistry of Hydroxyl and Water in Silicate Minerals

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Final Technical Report

Objective

This was a project to investigate the crystal chemistry of OH and H₂O substitution in silicate minerals by use of X-ray and neutron diffraction methods combined with IR spectroscopy and to interpret and generalize the results using an electrostatic model for these mineral structures.

Summary of results

The crystal structures of several hydrous silicate minerals were refined from X-ray and/or neutron diffraction data. Using these data together with published H position data electrostatic parameters for H sites were calculated from a simple electrostatic model. The data were then used to refine the model for incorporation of H into the wadsleyite structure. This has led to recent work on the synthesis and characterization of hydrous wadsleyites.

Stishovite and Rutile

The crystal structure of hydroxyl-bearing rutile (TiO₂) was refined by X-ray and neutron diffraction methods and the H position located (Swope et al. 1995). The crystal structure of a synthetic aluminous, OH bearing stishovite (SiO₂) was refined from X-ray data and Al substitution in this structure was demonstrated for the first time (Smyth et al., 1995).

Micas and Chlorites

The crystal chemistry of OH for Cl substitution in biotites was investigated by X-ray diffraction methods (Swope et al., 1995). This work is on going and further publications are in preparation. The crystal structure of an ordered triclinic clinocllore was refined from X-ray diffraction data and H positions determined. Cation ordering was deduced from X-ray and Mössbauer data. This sample shows the greatest deviation from monoclinic symmetry of any previously reported chlorite structure (Smyth et al., 1997).

Humites

The crystal structure of titano-clinohumite was refined from neutron and X-ray diffraction data. The H position has been determined. This work is on going and publication of the study is in preparation.

Wadsleyite (β -Mg₂SiO₄)

Wadsleyite is the polymorph of olivine that is stable in the upper portion of the Transition Zone of the Earth (400-525km depth). It is nominally anhydrous but has an unusual sorosilicate structure that contains both a bridging oxygen (O2) and a non-silicate oxygen (O1). Using the electrostatic model from this study, the model for incorporation of H in this structure was refined to predict the amount of H₂O that can readily substitute in the structure is about 3.3 wt %. Subsequently, this structure has been observed with up to 3.3 wt % H₂O. *This work means that if the nominally anhydrous phases commonly believed to be present in this region of the mantle were to be fully saturated, the amount of water contained in this reservoir could be up to six times the total water in the hydrosphere. This internal reservoir may then have played a significant role in maintaining or controlling ocean volume over geologic time.*

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Publications

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