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Silanol groups in minerals and inorganic compounds

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ABSTRACT

The Inorganic Crystal Structure Database (ICSD) was searched for Si-OH groups with ordered H positions leading to 31 structures with 46 Si-OH groups. The geometrical characteristics of these partly hydroxylated SiO_4 tetrahedra were analyzed. Depending on the condensation of the tetrahedra, the protonization of one tetrahedral apex allows variations in Si-O bond lengths and distorts the tetrahedron. The Si-OH distance decreases with the number of bridging O atoms (Si-O-Si) from average values of 1.668 Å for orthosilicates to 1.604 Å for tetrahedra with three bridging O atoms, whereas the ⟨Si-O⟩ distances of the non-hydroxylated Si-O bonds remain constant at 1.62 Å. This behavior was modeled by differences in bond strength sums of the tetrahedral O atoms. In the orthosilicates, the non-hydroxylated tetrahedral apices tend to be underbonded and the O of the silanol group is overbonded to satisfy the charge requirements of Si^{4+}. In contrast, an Si-OH bearing tetrahedron with three bridging O atoms is characterized by a more regular bond strength distribution consistent with minor bond length distortion.