Refinement of the Nacrite Structure

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Abstract: Nacrite crystals from a vug within a matrix of dickite at Red Mountain near Silverton, Colorado, have a = 8.906(2), b = 5.146(1), c = 15.664(3) Å, β = 113.58(3) °, V = 657.9(3) Å^3, and space group Cc. The structure was solved by direct methods to determine phase angles, followed by electron density maps to locate all atoms. Refinement by least-squares ceased at R = 4.5%. Each 7 Å layer has structural detail very similar to those of dickite and kaolinite, although nacrite stacking is based on -a/3 interlayer shifts along the 8.9 Å axis (with octahedral cations alternating between the I and II sites in successive layers), whereas dickite and kaolinite are based on shifts of -a/3 along the 5.1 Å axis (with octahedral cations in the same set of sites in each layer). The angle of tetrahedral rotation is 7.8 °, and the octahedral counter-rotations are 7.6 ° and 8.1 °. The H^+ protons were located on DED maps. The inner 0..H1 vector points exactly toward the vacant octahedron and is depressed -18.6 ° away from the level of the octahedral cations. All three surface OH groups have 0…H vectors at 50 ° to 66 ° to (001), although OH2 may not participate in interlayer hydrogen bonding. All three interlayer OH—H—O contacts are bent to angles between 132 ° and 141 ° and form contacts between 2.94 and 3.12 Å. The interlayer separation of 2.915 Å is slightly larger than in dickite, interpreted as due to a less favorable meshing of the oxygen and hydroxyl surfaces in nacrite—a direct consequence of layer shifts along the 8.9 Å axis.

Key Words: Bond lengths • Crystal structure • Hydrogen bonds • Nacrite • Refinement • Tetrahedral rotation

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