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Redetermination of the structure of 5*C* pyrrhotite at low temperature and at room temperature

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Abstract

The crystal structure of a 5*C* pyrrhotite from Silberberg Mine, Bodenmais, Germany, has been determined at 120 and 293 K in space group $P2_1$. The low-temperature structure refined to $R = 0.0261$ for 5727 data with $I_o > 2\sigma(I_o)$ and $R = 0.0354$ for all 7121 data. The room-temperature structure of the same crystal refined to $R = 0.0383$ for 2471 data with $I_o > 2\sigma(I_o)$ and $R = 0.0550$ for all 3419 data. In addition, the diffraction data of a 5*C* pyrrhotite crystal from Copper Cliff Mine, Sudbury, Canada, previously refined in space group *Cmce*, has been transformed and also refined in space group $P2_1$. This structure refined to $R = 0.0441$ for 2701 data with $I_o > 2\sigma(I_o)$ and $R = 0.0672$ for all 3843 data, which is a substantial improvement over the previous refinement.

The structure is characterized by iron vacancy avoidance within a layer, and with partially occupied sites projecting on top of each other in adjacent layers. Two half-occupied sites and two sites each with occupancy of 0.88 are present in the Bodenmais structure, together with one site with occupancy of 0.28. The distribution in the crystal from Sudbury is slightly different and cannot be described with the same number of partially occupied sites. Broadly, however, the two structures are similar.