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New data on the crystal-chemistry of fluoborite by means of SREF, SIMS, and EMP analysis

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ABSTRACT

The crystal structure of fluoborite [$Mg_3F_3(BO_3)$] was refined by Dal Negro and Tadini (1974) who provided a complete structural model. Previously, Takeuchi (1950) had refined an OH-dominant fluoborite (OH ~70%), but the limited quantity of data (extracted from two Weissenberg-Buerger photographs) did not permit the location of H atoms. Dal Negro and Tadini (1974) also could not locate H atoms because they used a crystal with near end-member composition. We have located the H bond in an OH-dominant fluoborite from the Betic Cordilleras (SE Spain). Excellent quality X-ray data on two crystals of fluoborite allowed discovery and refinement of the H position in this mineral. Electron microprobe (EMP) and secondary-ion mass spectrometry (SIMS) analyses of the light elements H, B, and F have resulted in the formulation of special procedures to obtain accurate, high-quality quantitative data, which are presented in this paper. EMP, SIMS, and crystal structure refinement (SREF) data are in a good agreement. Linear equations are also presented to calculate the F content directly from cell parameters.