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Borate Minerals; Hilgardite, Veatchite and Volkovskite from Marine Evaporite Deposits of New Brunswick; New data and Geological Interpretation

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Chemical composition, and optical and X-ray crystallographic data were collected for borate minerals; hilgardite ($Ca_2B_2O_9Cl{\cdot}H_2O$), veatchite ($Sr_2[B_2O_8](OH)]_2B[OH]_3{\cdot}H_2O$, and volkovskite, ($KCa_4B_{22}O_{32}[OH]_{10}Cl{\cdot}4H_2O$) primarily from the Sussex mine (Penobsquis) and Millstream deposits, New Brunswick. Hilgardite and veatchite both possess polytypes, an important area of study in crystallography. Polytypism is unique to layered structured minerals and can provide information relevant to conditions of crystal growth. For hilgardite, with three polytypes (-1*A*, - 3*A*, - 4*M*), from two different locations, the Sussex mine and Millstream deposit in New Brunswick, were examined. These three polytypes show different X-ray powder diffraction (XRPD) patterns. The patterns of -1*A* and -3*A* polytypes indeed show differences in the *d* values ranging from 5.5 to 5.8 Å and from 3.1 to 3.2 Å. In the latter range, polytype -1*A* displays one single peak, whereas polytype -3*A* shows multiple peaks. The XRPD pattern of polytype -4*M* varies greatly from the -1*A* and -3*A* structures due to an increase in symmetry and cell dimensions. For veatchite, three polytypes have been identified by Grice (2012). Among three, two polytypes were examined; veatchite-2*M* from the Sussex mine, New Brunswick, veatchite-1*M* from Reyershausen, Germany and veatchite-1*A* from Emet, Turkey. These three are expected to show different XRPD patterns and our study of polytypes -1A and -2M confirmed clear differences between the two. Differences in *d*-values (Å) are observed in the ranges from 5.2 to 5.6, from 3.2 to 3.3 and from 2.7 to 2.9. The emergence of additional peak(s) in these select ranges confirms the prediction from XRPD patterns calculated from the structure determinations. Thus XRPD can be used directly to determine which polytype is present without involving crystal structure analysis. Knowing the polytype can be used as an indicator of the hosts' environment (Grice 2012). In the present study a crystal structure refinement of volkovskite confirms the basic model of Rastsvetaeva *et al*. (1992). Greatly improved data allows for a refinement of H positions that is used to elucidate H-bonding, a factor critical in better understanding of crystal structure of borate minerals and the development of efficient extraction techniques of boron. The volkovskite structure obtained in this study is applicable to many layered borates, such as biringuccite, nasinite and gowerite as previously studied by Grice et al. (1999).