

## **Boron K-edge XANES of borate and borosilicate minerals**

**MICHAEL E. FLEET AND SWAMINATHAN MUTHUPARI**

Department of Earth Sciences, University of Western Ontario, London, Ontario N6A 5B7, Canada

### **ABSTRACT**

Synchrotron radiation B *K*-edge XANES spectra are reported for 19 borate and borosilicate minerals. The spectra are characterized by three prominent features; a sharp peak (A) at ~194 eV (the edge feature of trigonal B; <sup>III</sup>B), a broader peak (B) at 197–199 eV (the edge feature of tetrahedral B, <sup>IV</sup>B), and a broad peak (C) at 200–201 eV for tetrahedral B and 203–204 eV for trigonal B. The area of peak A is very sensitive to content of <sup>III</sup>B and its position yields information on B-O bond length and linkage of the BO<sub>3</sub> group. The area of peak B is proportional to content of <sup>IV</sup>B but quantification is limited by overlap with peak C. The width of peak B increases with increasing divergence of B-O bond lengths, responding to splitting of  $\sigma^*(t_2)$  antibonding orbitals. The tetrahedral component of peak C appears to be a  $\sigma$ -shape resonance. For trigonal B minerals, the relative intensity of peak C and its satellite peaks increases with increase in mean size and/or atomic number of next-nearest-neighbor cations, C being most intense in vonsenite (Fe<sub>2</sub>Fe<sup>3+</sup>BO<sub>5</sub>). Priceite (Ca<sub>4</sub>B<sub>10</sub>O<sub>19</sub>·7H<sub>2</sub>O), of unknown structure, has 80% <sup>IV</sup>B, and an isolated BX<sub>3</sub> group with <sup>III</sup>B-O = 1.373(5) Å. Comparison of B *K*-edge XANES spectra collected using total electron yield (sampling depth <60 Å) and fluorescence yield (sampling depth <1100 Å) shows that borates and borosilicates readily reconstruct in surface and near-surface environments. More profound structural damage involving conversion of <sup>IV</sup>B to <sup>III</sup>B occurs in minerals with high contents of <sup>IV</sup>B, and hydrous Mg borates with interstitial H<sub>2</sub>O are unstable in the high vacuum of the spectrometer.