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In-situ high-temperature crystal-field spectroscopy of Cr(III) in oxide glasses

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The optical absorption spectra of Cr(III) have been investigated in soda-lime silicate and potassium and sodium borosilicate glasses in the UV-visible range. Measurements have been made up to 800K, using a dispersive spectrometer fitted with a furnace. The position of the various spin-allowed and spin-forbidden transitions in borosilicate glasses indicates Cr(III) crystal field parameters, which are closer to a silicate than to a borate surrounding. All spectra show a systematic modification of the position and relative intensity of the two main Cr(III) absorption bands as a function of temperature. Crystal field strength, Dq, shows a nearly linear negative dependence on temperature. As a consequence, the transmission window shifts from the green to the yellow region of the optical spectrum, giving these glasses a thermochromic character. By contrast, the antiresonances corresponding to the weak, spin forbidden electronic transitions remain at the same position, though their intensity decreases with increasing temperature. The systematic red shift of crystal field transitions is interpreted with crystal field theory, using a point charge model, in order to derive the temperature-induced variation of the Cr-O distances. The Cr-O linear thermal expansion coefficient is larger than typical bulk thermal expansion coefficient. Together with the independence of the latter on glass composition, these observations are consistent with the location of Cr(III) in cationic domains within the glass structure.