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A multiple wavelength contrast variation method for envelope determination in macromolecular x-ray crystallography

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A contrast variation method using tunable x-rays and an anomalously scattering species dispersed in the solvent regions of a macromolecular crystal is presented. This method, known as MASC (multiple-wavelength anomalous solvent contrast) is similar to the MAD method (multiple-wavelength anomalous dispersion), except that the anomalous partial structure is an extended uniform density describing the solvent region of the crystal, as opposed to punctual and ordered sites. As such, MASC is applicable, in principle, to the determination of the macromolecular envelope and to the phasing of low resolution structure factors. The expected strengths of MASC signals are strongly dependent upon resolution, and the main prerequisites of a MASC experiment are similar to those for a MAD experiment with the inclusion of measurements at very low resolution. Results from experiments at LURE and the ESRF exploiting the L(III) and the K edges of ytterbium and selenate ions, respectively, show the expected anomalous signals from the solvent regions of the crystal. In certain cases, effects are also seen from anomalously scattering species bound in ordered sites at the macromolecular surface. Methods for phasing low resolution reflections using MASC data are discussed, as well as practical aspects of the experimental procedure.