

W0266

Experiences with Scaling and Absorption Corrections. George M. Sheldrick, Lehrstuhl für Strukturchemie, Univ. Göttingen, Germany.

A brief review of techniques for scaling and absorption corrections of both small-molecule and macromolecular diffraction data collected with area detectors will be followed by some examples from the author's experience with the SADABS and TWINABS programs. The ability to perform a Gaussian absorption correction within the scaling program provides a good test of empirical absorption algorithms based on spherical harmonics, and also enables the linear absorption coefficient to be determined from the agreement of equivalent reflections. This makes it possible to apply face-indexed absorption corrections even when the contents of the unit-cell are not yet known, and may also be able to compensate for other systematic effects such as absorption by the crystal support. Even if the absorption is small, this calculation is required to find the mean path length through the crystal for use in extinction corrections for charge density studies. Problems that arise in the scaling and merging of data from non-merohedrally twinned crystals will also be discussed.