The points which define the anomaly bases, when connected, with the shortest spanning tree graph, will form unique base graphs. Individual points whose intensities are below the detection limit can thus provide insight into the nature of the intensities distributed throughout the two-dimensional crystallographic data image.

Data collected with the new Siemens SMART CCD diffractometer systems not only yields better quality data than conventional scintillation counter diffractometers but also leads to fewer mistakes in structure determination. The default data collection strategy used for the collection of X-ray intensity data on the SMART system involves the collection of 1.5 hemispheres of data to 0.75 resolution (at 5 cm. crystal-to-detector distance) using 10 second exposures and frame widths of 0.3 in ø. Although such a data set requires approximately six hours to complete, regardless of the size of the unit cell, the quality of data matches or exceeds that of conventional point-detector data sets collected over a much larger time periods (typically several days).

The above data collection strategy minimizes the choices which must be made by the user, thereby preventing mistakes. The determination of unit cell dimensions, reduced primitive cell, and the determination of the correct space group. Because complete frames of data are saved, twinned and incommensurate crystals are more easily identified and in some cases structures can be determined from such crystals. Since the data set contains many redundant reflections, each with direction cosines, very good empirical or face-indexed absorption corrections may also be carried out without the need for supplemental data sets (e.g., psi scans).