The results from refining the ALMET structure with different thresholds shows that for a *sufficiently extensive* data set there is little loss in precision on eliminating the weak reflections, even when the data set was reduced by almost half. This suggests that in lengthy calculations on such data sets, substantial computational economies can be achieved without loss of significant precision by use of relatively high thresholds. In fact, in the case of the ALMET refinements with different thresholds, none of the bond lengths or thermal parameters were found to differ by as much as one standard deviation.

The results reported here should not, however, give license for the indiscriminate use of high thresholds, particularly so since their use tends to eliminate a disproportionate number of the higher-angle reflections. Instead, each data set should be considered on the basis of its extent in reciprocal space, the precision of the observations, and the number of observations relative to the number of parameters to be determined. The weighting function must also be considered since use of the full data set does not necessarily lead to more reliable parameters unless the validity of the weights has been established. Finally, the results reported here shed no light on the effect of thresholds on convergence to false minima.

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