[MS19-P04] Centre of Symmetry Prediction with the Exact Probability Density Function of |E|.

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Calculation of the magnitude of the normalized structure factor, |E|, is usually performed during space group determination. Analysis of the mean of normalized structure factor magnitude $<|E|>$ and the mean $<|E^2-1|>$ can sometimes be used to predict existence of centre of symmetry. The means $<|E|>$ and $<|E^2-1|>$ can be compared with the means calculated from theoretical probability density function (PDF) for centrosymmetric and related noncentrosymmetric space groups. However, in the case of an outstandingly heavy atom in the asymmetric unit cell the distribution of |E| can differ much from that predicted by the Wilson PDF [1], i.e. the ideal one. To deal with that, the exact PDFs were developed [2-6].

In the previous work [7] the centre of symmetry prediction error, obtained with the use of ideal PDF [1] and exact PDFs [2-6], was compared within centrosymmetric and noncentrosymmetric space groups. In the current work we present a more detailed comparison.

The 41818 crystal structures with structure factors were obtained from Crystallografic Open Database [8]. The structures then were filtered out to be high quality (not causing Alert A in CheckCIF procedure) and contain at least one heavy atom in the asymmetric unit with at least 30 electrons. The 5265 crystal structures were selected that contain exactly Z heavy atoms at general positions in the unit cell, where Z is the number of asymmetric units in the unit cell. For all structures the exact PDFs were calculated with the use of CentroMK program [7]. The estimators $<|E|>$, $<|E^2-1|>$, $\%|E|>2$, $\%|E|<0.25$ and the discrepancy R function were evaluated. The comparison shows that for all estimators within the selected set of structures the prediction error with use of the exact PDFs is approximately two times lower than with use of the ideal PDFs.

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