FAST SYNTHESIS AND REFINEMENT OF THE
ATOMIC PAIR DISTRIBUTION FUNCTION

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A fast method for calculating the atomic pair distribution function is described in the context of performing refinements of structural models. Central to the speed of synthesis is the approximation of Gaussian functions of varying full width at half maximums using a narrower Gaussian with a fixed full width at half maximum. The initial Gaussians are initially laid down as delta functions which are then convoluted with the narrower Gaussian to form the final pattern. The net result is an algorithm that has been included in the Rietveld refinement computer program TOPAS that synthesises and refines structural parameters a factor of 300 to 1000 times faster than alternate algorithms/programs with speed advantages increasing as the number of atomic pairs increase.