

XLENS-11: A COMPUTER PROGRAM FOR SOLVING CRYSTAL STRUCTURES FROM SINGLE CRYSTAL AND POWDER DIFFRACTION DATA

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Since its discovery, the direct methods origin-free modulus sum function S , originally denoted by Z_R in [Rius (1993) *Acta Cryst.* A49, 406-409], has been used for solving some relatively complex crystal structures from single and powder X-ray diffraction data. This function was implemented in program XLENS and a complete description of this program was already published in 1999 in *Powder Diffraction* 14, 267-273. This version of XLENS refined phases of the structure factors by maximising function S with a modified tangent formula applied in sequential form. However, further progress in the powder diffraction field was hampered by the complexity of combining the tangent formula refinement (that makes explicit use of triple-phase sums) with the introduction of constraints in real space necessary to counterbalance the information loss produced by peak overlap. Recently, a considerably simpler and completely general phasing procedure (S-FFT) has been developed that maximises S by means of the FFT algorithm so that the triple-phase sums are considered implicitly. This algorithm has been adapted now to powder diffraction data and implemented in a new XLENS Windows version [Rius & Frontera (2007) *J. Appl. Cryst.*, 40, 1035-1048]. XLENS-11 is a user-friendly program that can be executed directly from the toolbar of the FULLPROF-suite of programs (<http://www.ill.fr/sites/fullprof/php/downloads.html>) (Rodriguez-Carvajal, 2008).