WinPSSP: a computer program applying direct-space methods for the crystal structure solution of small molecule organic solids from X-ray powder diffraction

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Since late 1980's direct-space methods have radically changed the scope of powder diffraction, nowadays including crystal structure solution. However, the topic is young, with less than 300 structures published before 1999 [1]. To disseminate the crystal structure determination methods from powders, it has been proposed to improve the average academic training in crystallography, and to increase the user friendliness of the software [1]. Towards this end, we have made available a Windows OS version of the direct-space methods program *PSSP* (running in MS_DOS mode) [2], to solve the crystal structures of small molecule organic solids, as well as instructional videos expected to be useful for undergraduates and inexperienced users. *WinPSSP* [3] is freely downloadable at **http://users.uoi.gr/nkourkou/winpssp**. The software, which works together with the program GSAS [4] for Le Bail fits and Rietveld refinement, and this particular practical implementation of the direct-space methods will be discussed. Crystal structure determination examples will be shown, reviewing the procedure, difficulties and facilitations using *WinPSSP*.

[1]- A. Le Bail *et al., Powder Diffraction* (2009) **24:3**, 254-262. [2]- S. Pagola and P. W. Stephens, *J. Appl. Cryst.* (2010) **43**, 370-376. [3]- S. Pagola, A. Polymeros and N. Kourkoumelis, *J. Appl. Cryst.* (2017) **50**, 293-303. [4] Larson, A. C. and von Dreele, R. B. General Structure Analysis System (GSAS). Los Alamos National Laboratory Report: New Mexico, USA 2004.