

Phasing via full Pattern Powder Decomposition by Monte Carlo and Patterson Methods

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In a recent paper [1] a new full pattern decomposition technique has been suggested using linear ternary codes resulting from modifications of the Hamming codes. The resultant decomposition procedure consists of only 27 decomposition trials: to each of them 20 direct methods trials are applied, for a total of 540 tangent processes among which the correct solution may be found.

The above method has been combined with a technique [2] which modifies the Patterson map to obtain, by inversion, better estimates of the structure factor moduli.

The resultant procedure has been introduced in EXPO2005, and proved quite useful to solve crystal structures from powder diffraction data.

[1] Altomare A., Caliandro R., Cuocci C., da Silva I., Giacobazzo C., Moliterni A.G.G., Rizzi R., *J.Appl. Cryst.*, 2004, **37**, 204-209. [2] Altomare A., Foadi J., Giacobazzo C., Moliterni A.G.G., Burla M.C., Polidori G., *J.Appl. Cryst.*, 1998, **31**, 74-77.

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