

New Strategies for the *ab-initio* Structure Solution in EXPO2005

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The full pathway in the *ab-initio* crystal structure solution from powder data has been made more straightforward by the package EXPO2004 [1] which is able to: index the diffraction pattern; identify the most plausible space group; estimate the reflection integrated intensities; solve the crystal structure by Direct Methods, in eventual combination with Monte Carlo approach; refine the structure model by Rietveld technique.

New strategies have been recently introduced in EXPO2004 in order to enhance its power, leading to EXPO2005. Among them the most relevant are: a) an improved algorithm for space group determination; b) a new definition of the background contribution; c) efficient methods for estimating the integrated intensities *via* a systematic procedure based on coding theory and/or Patterson inversion technique; d) an effective figure of merit able to identify the most plausible phases set; e) a powerful global optimization approach to be applied in case of organic structures; f) a more robust structure refinement procedure.

The EXPO2005 features and applications will be described.

[1] Altomare A., Caliendo R., Camalli M., Cuocci C., Giacobazzo C., Moliterni A.G.G., Rizzi R., *J. Appl. Cryst.*, 2004, **37**, 1025-1028.

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