Space Group Determination by EXPO2005

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The preliminary step to solve crystal structure is the determination of the space group. In case of powder diffraction data the peak overlap makes difficult the recognition of systematically absent reflections and therefore the extinction symbol identification. We have developed a new approach [1] based on the statistical analysis of the normalized intensities extracted by Le Bail method from the diffraction pattern. In order to improve the results new algorithms have been carried out regarding:

a) the removal of impurity peaks;
b) the background level determination;
c) the variance associated to integrated intensity estimated;
d) the selection of reflections relevant for the extinction group recognition;
e) the graphic interface improvement

The new approach has been implemented in EXPO2005, the evolution of EXPO2004 [2], and has been successfully tested using a large set of experimental data.

[1] Altomare A., Caliandro R., Camalli M., Cuocci C., da Silva I., Giacovazzo C., Moliterni A.G.G., Spagna R., *J. Appl. Cyst*, 2004, **37**, 957-966. [2] Altomare A., Caliandro R., Camalli M., Cuocci C., Giacovazzo C., Moliterni A.G.G., Rizzi R., *J. Appl. Cyst*, 2004, **37**, 1025-1028.

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