SDPDRR-2. Indexing results samples 1 to 3

Sample 1

Monoclinic: a=8.525 Å, b=7.394 Å, c=13.230 Å, β=128.748°

FOM: 3691, rel FOM:2.93

Input peaks: 11.95, 13.30, 13.61, 17.16, 17.92, 18.15, 20.81, 23.26, 23.63, 24.04, 25.43, 26.78, 27.58, 27.72, 28.17, 29.43, 29.70, 30.13

The same solution was found if peaks 15.64 and 25.68 were also introduced in the input and the search was run on impurity level 3

Possible space groups:

AM, A2/M, A2, P2/C, PC, P21/C, PM, P2/M, P2

Sample 2

Monoclinic: a= 11.243 Å, b= 8.195 Å, c= 19.949 Å, β=106.728°

FOM: 8438, rel FOM: 21.09

Input peaks: 4.25, 4.79, 5.41, 6.07, 7.01, 7.35, 7.77, 7.80, 8.47, 8.50, 9.10, 9.30, 9.58, 9.87, 10.83, 10.90, 10.95, 11.00, 11.09, 11.17, 11.43, 11.55, 11.95, 12.16, 12.27, 12.43,12.76, 12.79, 13.23, 13.31, 13.50, 13.58, 13.90, 14.39, 14.46, 14.58, 14.63, 14.67, 14.76, 14.88, 14.92, 15.58, 15.63, 15.82, 15.90, 16.06, 16.10

Possible space groups:

P21/C, PC, P2/C, P21/M, P21, PM, P2/M, P2

Sample 3

Cubic a=18.88 Å

FOM: 9601, rel FOM: 24.00

Input peaks: 3.42, 4.84, 5.93, 7.66, 8.39, 9.06, 9.69, 10.28, 11.37, 11.88, 12.36, 13.28, 13.72, 14.15, 14.56, 14.96, 15.35, 15.73, 16.11, 16.25, 16.47, 16.83, 17.18, 17.52, 17.86, 18.19, 19.14, 19.76, 20.36, 20.65, 20.94, 21.22, 22.05, 22.59, 24.14, 24.38, 24.88, 25.36, 27.43, 27.87, 28.30, 29.57

Possible space groups:

IM-3M, I23, I-43M, IM-3, I213, I432, IA-3, I4132, PN-3N, PN-3N, PM-3N, P-43N, PN-3, PN-3M, PN-3M, PN-3, P213, P4232, P432, PM-3M, PM-3, P-43M, P23

Software

These solutions have been found using X-Cell -Neumann, M, *J. Appl. Cryst.*, **36**, submitted (2003)- implemented in Materials Studio 2.2.

The figures of merit are defined as $F_a = \dfrac{\overline{\theta}}{|\Delta\theta|} \dfrac{N_{obs}}{N_{calc}} \dfrac{4.5}{N_{par}}$ and rel. FOM= FOM/noise

Solutions were checked and refined using a modified Pawley refinement implemented in Materials Studio - Engel, G.E.; Wilke, S.; Harris, K.D.M.; Leusen, F.J.J, *J. Appl. Cryst.* **32**, 1169 (1999)-

Possible space groups were found using the space group determination tool implemented in Materials Studio, which is related to the probabilistic method published by Markvardsen - Markvardsen, A. J., David, W. I. F., Johnson, J. C. and Shankland, K., *Acta Cryst.*, **A57**, 47-54, (2000)- The groups are listed in descending order of probability and all space groups with probability equal or higher than the lowest symmetry space group in the corresponding crystal class are included.