FOMnew in *N-TREOR09*). The first one in the list is the correct cell. It is worth mentioning that the classical M_{20} figure of merit was not able to pick up the solution. The best cell parameters, found according to FOMnew, were a = 24.0951 (50), b = 6.1697 (21), c = 12.4578 (37) Å, β = 102.724 (18)°, similar to those reported in the literature, with FOMnew = 0.61, M_{20} = 12; all the lines in the pattern were indexed. The program provided the solution thanks to its automatic check for a zero-point correction (2θ zero shift = 0.04°) and was able to correctly identify the extinction group (*I_a_*). For the second suggested cell (the wrong solution) FOMnew = 0.41, M_{20} = 15, and two lines were unindexed.

Example 4

Hexagonal turkey egg-white lysozyme (Margiolaki *et al.*, 2005). Published information: hexagonal, a = 71.0862 (3), c = 85.0276 (5) Å, $P6_122$, experimental range 0.4–12° 2θ, RES = 3.35 Å, synchrotron data. The first 94 peaks (in the range 0.4–6°, λ = 0.700667 Å) with intensities greater than a default threshold were selected. An intensity-based criterion was automatically adopted. The first 25 lines were used to find possible cells that were then refined by considering all 94 peaks. Five possible unit cells were automatically suggested by the program in the following systems: hexagonal (1), orthorhombic (1) and monoclinic (3). The highest value for WRIP20 was 0.99, and was for the correct hexagonal cell parameters: a = 71.0922 (4), c = 85.0269 (7) Å, which are similar to those reported in the literature; all the 94 selected lines in the pattern were indexed. For this cell, the program detected a geometrical ambiguity (see Section 3.4.2.2) between hexagonal and orthorhombic lattices and automatically selected the higher-symmetry one.

3.4.5. Conclusion

Indexing a powder diffraction pattern is sometimes described as a 'gateway technology', because the determination of the cell parameters is so fundamental: if no cell has been identified the execution of the subsequent steps of the structure solution process is impossible, and if a wrong cell has been used the correct solution is unreachable. Therefore extremely close attention must be paid to the indexing step of the process. From the early 1970s, the increasing interest in powder pattern indexing and the progress seen, in terms of both methods and algorithms, have strongly contributed to opening the door to modern applications of powder diffraction techniques. The availability of a quite large number of software packages, based on different indexing strategies, enables the scientist interested in solving crystal structures to switch from one program to another when the first fails, so increasing the possibility of success. In some cases indexing is still a challenging process. Good-quality data are necessary and careful inspection of each indexing step, in particular in the selection of the experimental peak positions to be used, is advisable.

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