the profile R factor (Young, 1993). B_r is a factor arbitrarily set to 6 for F and R Bravais lattices, 4 for I, 2 for A, B and C, and 1 for P. S_y is a factor equal to 6 for a cubic or a rhombohedral cell, 4 for a trigonal, hexagonal or tetragonal cell, 2 for an orthorhombic cell, and 1 for a monoclinic or triclinic cell.

(3) WRIP20 (Altomare *et al.*, 2009):

$$\mathrm{WRIP20} = \mathrm{RAT}_{Rp}^{2} \times \mathrm{RAT}_{\mathrm{Ind}} \times \mathrm{RAT}_{\mathrm{Pres}} \times w_u \times \mathrm{RAT}_{M20}^{1/2}. \quad (3.4.5)$$

Based on M_{20} (M_{20} and F_N remain the most widely used FOMs), WRIP20 has been developed for exploiting the full information contained in the diffraction profile. The factors that appear in (3.4.5) are

$$\mathrm{RAT}_{Rp} = \frac{1 - R_p}{1 - (R_p)_{\min}}, \quad \mathrm{RAT}_{\mathrm{Ind}} = \frac{\mathrm{PERC}_{\mathrm{Ind}}}{(\mathrm{PERC}_{\mathrm{Ind}})_{\max}},$$

$$\mathrm{RAT}_{\mathrm{Pres}} = \frac{(\mathrm{PERC}_{\mathrm{Pres}})_{\min}}{\mathrm{PERC}_{\mathrm{Pres}}}, \quad w_u = (N_{\mathrm{obs}} - N_u)/N_{\mathrm{obs}},$$

$$\mathrm{RAT}_{M20} = \frac{M_{20}}{(M_{20})_{\max}}, \quad \mathrm{PERC}_{\mathrm{Pres}} = \sum_{\mathrm{Pres}} \mathrm{mult} / \sum_{\mathrm{all}} \mathrm{mult}.$$

R_p is the profile-fitting agreement calculated after the Le Bail (Chapter 3.5) decomposition of the full pattern using the space group with the highest Laue symmetry compatible with the geometry of the current unit cell and no extinction conditions. $\mathrm{PERC}_{\mathrm{Ind}}$, the percentage of independent observations in the experimental profile, is estimated according to Altomare *et al.* (1995). For each extinction symbol compatible with the lattice geometry of the current unit cell, normalized intensities are calculated and subjected to statistical analysis in order to obtain a probability value associated with each extinction symbol in accordance with Altomare *et al.* (2004, 2005). For the extinction symbol with the highest probability value, the value of $\mathrm{PERC}_{\mathrm{Pres}}$ is calculated: $\sum_{\mathrm{all}}$ mult is the total number of reflections (symmetry-equivalent included) for the space group having the highest Laue symmetry and no extinction conditions. (It varies with the volume of the unit cell and the data resolution.) $\sum_{\mathrm{Pres}}$ mult, which varies according to the extinction rules of the current extinction symbol, coincides with the number of non-systematically absent reflections (with the symmetry equivalents included). The subscripts min and max mark the minimum and the maximum values of each factor respectively, calculated for the possible unit cells that are to be ranked. N_{obs} and N_u are the number of observed and unindexed lines, respectively. All the terms in (3.4.5) are between 0 and 1, so ensuring that WRIP20 also lies between 0 and 1. In addition, WRIP20 has the following properties: (*a*) it is continuous, that is, definable in any interval of the experimental pattern; (*b*) it takes into account the peak intensities, the number of generated peaks and their overlap, and the systematically absent reflections (through the extinction-symbol test); and (*c*) it is not very sensitive to the presence of impurity lines (these usually have low intensities). WRIP20 is effective in finding the correct cell among a number of possible ones and selecting the corresponding most probable extinction symbol (see Example 3 in Section 3.4.4.6.2).

(4) Two new figures of merit based on de Wolff's method, the reversed figure of merit (M_n^{Rev}) and the symmetric figure of merit (M_n^{Sym}), have recently been proposed (Oishi-Tomiyasu, 2013). As observed by Oishi-Tomiyasu, the de Wolff figure of merit M_n does not use the observed and calculated lines in a symmetrical way, consequently it is (*a*) insensitive to computed but unobserved lines (*i.e.*, extinct peaks) and (*b*) sensitive to unindexed observed lines (*e.g.*, impurity peaks). M_n^{Rev} and M_n^{Sym} aim to compensate for the disadvantages of M_n. In particular, M_n^{Rev} has characteristics opposite to those of M_n with regard to sensitivity to extinct reflections and impurity peaks, and M_n^{Sym} has intermediate properties between M_n and M_n^{Rev}. They prove useful in selecting the correct solution, particularly in case of presence of impurity peaks. (See also Section 3.4.4.3.)

3.4.2.2. *Geometrical ambiguities*

Before discussing the concept of geometrical ambiguity in indexing, it is useful to introduce the definition of a reduced cell. While a unit cell defines the lattice, a lattice can be described by an unlimited number of cells. The Niggli reduced cell (Niggli, 1928) is a special cell able to uniquely define a lattice. Methods and algorithms have been derived for identifying the reduced cell starting from an arbitrary one (Buerger, 1957, 1960; Santoro & Mighell, 1970; Mighell, 1976, 2001). The reduced cell has the advantage of introducing a definitive classification, making a rigorous comparison of two lattices possible in order to establish whether they are identical or related (Santoro *et al.*, 1980). An algorithm based on the converse-transformation theory has been developed and implemented in the Fortran program *NIST*LATTICE* for checking relationships between any two cells (Karen & Mighell, 1991).

It is very important to recognize that two lattices are derivative of each other, because many crystallographic problems (twinning, indexing of powder patterns, single-crystal diffractometry) stem from the derivative properties of the lattices. Derivative lattices are classified as super-, sub- or composite according to the transformation matrices that relate them to the lattice from which they are derived (Santoro & Mighell, 1972).

A further obstacle to the correct indexing of a powder pattern is the problem of geometrical ambiguities. It may occur when '*two or more different lattices, characterized by different reduced forms, may give calculated powder patterns with the identical number of distinct lines in identical 2θ positions*' (Mighell & Santoro, 1975). The number of planes (*hkl*) contributing to each reflection may differ, however. Such ambiguity, due to the fact that the powder diffraction pattern only contains information about the length of the reciprocal-lattice vector and not the three-dimensional vector itself, is geometrical. It mainly occurs for high-symmetry cells (from orthorhombic up). The lattices having this property are related to each other by rotational transformation matrices. In Table 3.4.2 some examples of lattices giving geometrical ambiguities and the corresponding transformation matrices are given (Altomare *et al.*, 2008). Where there are geometrical ambiguities, additional prior information (*e.g.*, a single-crystal study) may be useful in order to choose one of the two possible lattices.

A recent procedure developed by Kroll *et al.* (2011) aims to reveal numerical and geometrical relationships between different reciprocal lattices and unit cells. The procedure is based on the assumption that distinct unit cells with lines in the same 2θ positions are derivatives of each other. However, two non-derivative lattices can have identical peak positions. Very recently, Oishi-Tomiyasu (2014*a*, 2016) has developed a new algorithm able to obtain all lattices with computed lines in the same positions as a given lattice. (See also Section 3.4.4.3.)