given in Appendix 1.4.4 of *International Tables for Crystallography* Volume B (Shmueli, 2008).[3] In the past, one used to inspect the diffraction images to see which classes of reflections are symmetry equivalent within experimental and other uncertainty. Nowadays, the whole intensity data set is analyzed by software. The intensities are merged and averaged under each of the 11 Laue groups in various settings (*e.g.* $2/m$ unique axis b and unique axis c) and orientations (*e.g.* $\overline{3}m1$ and $\overline{3}1m$). For each choice of Laue group and its variant, an $R_{\rm merge}$ factor is calculated as follows:

$$R_{{\rm merge},i} = \frac{\sum_{\bf h} \sum_{s=1}^{|G|_i} |\langle |F_{\rm av}({\bf h})|^2\rangle_i - |F_{\rm av}({\bf h}{\bm W}_{si})|^2|}{|G|_i \sum_{\bf h} \langle |F_{\rm av}({\bf h})|^2\rangle_i}, \quad (1.6.2.2)$$

where ${\bm W}_{si}$ is the matrix of the sth symmetry operation of the ith Laue group, $|G_i|$ is the number of symmetry operations in that group, the average in the first term in the numerator and in the denominator ranges over the intensities of the trial Laue group and the outer summations $\sum_{\bf h}$ range over the hkl reflections. Choices with low $R_{{\rm merge},i}$ display the chosen symmetry, whereas for those with high $R_{{\rm merge},i}$ the symmetry is inappropriate. The Laue group of highest symmetry with a low $R_{{\rm merge},i}$ is considered the best indication of the Laue group. Several variants of the above procedure exist in the available software. Whichever of them is used, it is important for the discrimination of the averaging process to choose a strategy of data collection such that the intensities of the greatest possible number of Bragg reflections are measured. In practice, validation of symmetry can often be carried out with a few initial images and the data-collection strategy may be based on this assignment.

In the third stage, the intensities of the Bragg reflections are studied to identify the conditions for systematic absences. Some space groups give rise to zero intensity for certain classes of reflections. These 'zeros' occur in a systematic manner and are commonly called systematic absences (*e.g.* in the $h0l$ class of reflections, if all rows with l odd are absent, then the corresponding reflection condition is $h0l$: $l = 2n$). In practice, as implemented in software, statistics are produced on the intensity observations of all possible sets of 'reflections conditions' as given in Chapter 2.3 (*e.g.* in the example above, $h0l$ reflections are separated into sets with $l = 2n$ and those with $l = 2n + 1$). In one approach, the number of observations in each set having an intensity (I) greater than n standard uncertainties [$u(I)$] [*i.e.* $I/u(I) > n$] is displayed for various values of n. Clearly, if a trial condition for systematic absence has observations with strong or medium intensity [*i.e.* $I/u(I) > 3$], the systematic-absence condition is not fulfilled (*i.e.* the reflections are not systematically absent). If there are no such observations, the condition for systematic absence may be valid and the statistics for smaller values of n need then to be examined. These are more problematic to evaluate, as the set of reflections under examination may have many weak reflections due to structural effects of the crystal or to perturbations of the measurements by other systematic effects. An alternative approach to examining numbers of observations is to compare the mean value, $\langle I/u(I)\rangle$, taken over reflections obeying or not a trial reflection condition. For a valid reflection condition, one expects the former value to be considerably larger than the latter. In Section 3.1 of Palatinus & van der Lee (2008), real examples of marginal cases are described.

[3] The tables in Appendix 1.4.4 mentioned above actually deal with space groups in reciprocal space; however, the left part of any entry is just the indices of a reflection generated by the point-group operation corresponding to this entry.

Table 1.6.2.1

The ability of the procedures described in Sections 1.6.2.1 and 1.6.5.1 to distinguish between space groups

The columns of the table show the number of sets of space groups that are indistinguishable by the chosen technique, according to the number of space groups in the set, *e.g.* for Laue-class discrimination, 85 space groups may be uniquely identified, whereas there are 8 sets containing 5 space groups indistinguishable by this technique. The tables in Section 1.6.4 contain 416 different settings of space groups generated from the 230 space-group types.

	No. of space groups in set that are indistinguishable by procedure used					
	1	2	3	4	5	6
No. of sets for Laue-class discrimination	85	78	43	0	8	1
No. of sets for point-group discrimination	390	13	0	0	0	0

The third stage continues by noting that the systematic absences are characteristic of the space group of the crystal, although some sets of space groups have identical reflection conditions. In Chapter 2.3 one finds all the reflection conditions listed individually for the 230 space groups. For practical use in space-group determination, tables have been set up that present a list of all those space groups that are characterized by a given set of reflection conditions. The tables for all the Bravais lattices and Laue groups are given in Section 1.6.4 of this chapter. So, once the reflection conditions have been determined, all compatible space groups can be identified from the tables. Table 1.6.2.1 shows that 85 space groups may be unequivocally determined by the procedures defined in this section based on the identification of the Laue group. For other sets of reflection conditions, there are a larger number of compatible space groups, attaining the value of 6 in one case. It is appropriate at this point to anticipate the results presented in Section 1.6.5.1, which exploit the resonant-scattering contribution to the diffracted intensities and under appropriate conditions allow not only the Laue group but also the point group of the crystal to be identified. If such is the case, the last line of Table 1.6.2.1 shows that almost all space groups can be unequivocally determined. In the remaining 13 pairs of space groups, constituting 26 space groups in all, there are the 11 enantiomorphic pairs of space groups [($P4_1$–$P4_3$), ($P4_122$–$P4_322$), ($P4_12_12$–$P4_32_12$), ($P3_1$–$P3_2$), ($P3_121$–$P3_221$), ($P3_112$–$P3_212$), ($P6_1$–$P6_5$), ($P6_2$–$P6_4$), ($P6_122$–$P6_522$), ($P6_222$–$P6_422$) and ($P4_132$–$P4_332$)] and the two exceptional pairs of $I222$ & $I2_12_12_1$ and $I23$ & $I2_13$, characterized by having the same symmetry elements in a different arrangement in space. These 13 pairs of space groups cannot be distinguished by the methods described in Sections 1.6.2 and 1.6.5.1, but may be distinguished when a reliable atomic structural model of the crystal has been obtained. On the other hand, all these 13 pairs of space groups can be distinguished by the methods described in Section 1.6.6 and in detail in Saitoh *et al.* (2001). It should be pointed out in connection with this third stage that a possible weakness of the analysis of systematic absences for crystals with small unit-cell dimensions is that there may be a small number of axial reflections capable of being systematically absent.

It goes without saying that the selected space groups must be compatible with the Bravais lattice determined in stage 1, with the Laue class determined in stage 2 and with the set of space-group absences determined in stage 3.

We thank L. Palatinus (2011) for having drawn our attention to the unexploited potential of the Patterson function for the determination of the space group of the crystal. The discovery of