17.5-2 SPACE GROUPS RARE FOR ORGANIC COMPOUNDS.

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Mirror planes and simple rotation axes lead to rarity of space groups for organic structures. Their inhibiting effect is mitigated by the simultaneous presence of glide planes or screw axes or both. Centred lattices tend to be less common than primitive; *P* lattices are less common than *R* in the trigonal system. The only substantial exceptions to these rules are in the cubic point groups, especially *m3m*.

Sixteen space groups (late 1986 data) have no examples (99 100 103 149 162 183 184 187 188 201 207 208 211 214 222 226), and twenty have only one example (6 28 35 38 49 101 105 112 132 151 153 156 175 193 195 196 199 202 203 230). The twenty examples are discussed individually; for some the space-group allocation is dubious; for others the structure is disordered or ionic.

17.5-3 CAUCHY DISTRIBUTION, INTENSITY STATISTICS AND PHASES OF REFLECTIONS FROM CRYSTAL PLANES.

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Recently near-Gaussian distributions have been of much interest in the field of Intensity Statistics. It has been shown (Mitra and Ghosh, 1981, Crystallographic Statistics Progress and Problems. Indian Academy of Sciences, Bangalore, p.99) that the distribution of intensities of reflections for a particular crystal can be inferred from its N(Z) curve. In the present work expressions for N(Z) for a truncated Cauchy distribution corresponding to acentric and centric cases have been derived. Expressions for P_+ the probability of sign relations for centric crystals and for P_ϕ the probability of tangent relationship for acentric crystals have been derived on the basis of the Cauchy distribution of structure factor components.
Theoretical N(Z) curves for centric and acentric Cauchy distributions have been compared with those for acentric, centric and bicentric Gaussian distributions. The N(Z) curve for the Cauchy acentric distribution follows closely that for the Gaussian acentric upto $Z = 0.5$. It then takes upward turn and surpasses the Gaussian bicentric curve at high Z-values. A similar trend is shown by N(Z) curve for the Cauchy centric distribution after being approximately intermediate between the Gaussian centric and bicentric cases upto $Z = 0.5$. The results have been compared with some known crystal structures and the agreement is quite satisfactory in the cases studied.

17.5-4 EFFECT OF INACCESSIBLE VOLUMES ACCOMPANIED BY SYMMETRY ELEMENTS ON CUMULATIVE DISTRIBUTION FUNCTIONS.

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Symmetry elements are surrounded by volumes that cannot be occupied by the centres of atoms in the unit cell. The effect of these inaccessible volumes on cumulative distribution functions of normalised intensity has been investigated in space groups belonging to crystal classes 2, m, 2/m. The modified cumulative distribution functions have been compared with the corresponding distributions based on three published structures. The examples presented clearly show that the modified cumulative distribution functions are useful in detecting a correct spacegroup when usual procedures based on Howells, Phillips and Rogers N(z) plot [Acta Cryst. (1950) 3, 210 - 214] give ambiguous results.

17.5-5 PRACTICAL RESOLUTION OF THE CENTRO-SYMMETRIC–NONCENTROSYMMETRIC AMBIGUITY WITH THE USE OF E–STATISTICS.

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While much attention has been directed to the use of statistics to resolve centrosymmetric–noncentrosymmetric ambiguity (eg. Marsh, Acta Cryst. (1981) B37, 1985–1988) we are not aware of a detailed analysis applied to a large number of structures. We have been able to plot statistics for approximately 150 data sets collected under similar operating conditions. Values of $< E^2 - 1 >$ were obtained utilizing the SHELX76 system of programs using the whole data set including weak reflections. In those cases for which the space group is unambiguous the two populations of $< E^2 - 1 >$ overlap; with non-centric values as high as 0.91 and centric values as low as 0.74 (compared with the theoretical expections of 0.736 and 0.968 respectively). However, we note that the extremes are either disordered structures or have very weak intensity sets. For the ambiguous space groups no clear cut separation is evident until the thirty–six triclinic examples are removed; the remaining twenty cases are clearly separated at a $< E^2 - 1 >$ value of 0.82. We also confirm Marsh's result that weak reflections should not be rejected from the $< E^2 - 1 >$ calculation, as this markedly increases the scatter and shifts the values to lower limits. Our analysis confirms the usefulness of $< E^2 - 1 >$ statistics to assign non–triclinic, ambiguous space groups.

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