GI-MS48-01 | SOME REFLECTIONS ON SYMMETRY

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Surely nobody needs to learn any details of symmetry these days - point groups, space groups, Laue classes... After all, the decisions we once had to make are looked after now by automatic software. Diffractometer control programs choose the unit cell and probable space group, and set up an appropriate data collection strategy. The space group is more clearly decided by post-collection data processing and analysis with virtually no user intervention. Modern structure solution methods don't assume a particular space group anyway; they find it as part of solving the structure. And symmetry-imposed constraints on atom positions and displacements are worked out automatically, along with the correct asymmetric unit for Fourier map calculations. This may be true for lots of routine well-behaved structures, but major developments in radiation sources and detectors, together with research interest in more challenging materials, are increasingly presenting us with problems that are anything but routine, and a knowledge of basic symmetry concepts and their consequences is vital if we are to avoid mistakes. Particular aspects include pseudosymmetry (especially structures in which homochiral molecules are related by approximate inversion centres), structures with several chemically identical molecules in the asymmetric unit, and twinning, where the distinction between apparent and real symmetry of reciprocal and direct spaces is important. The talk will cover both principles and specific examples.