complex technique requiring prohibitive crystal volumes and long data collection times. The technique came of age as a result of developments in many areas from sample preparation to instrumentation [5], alongside developments in complementary structural methods.

The particular case of low resolution neutron crystallography will be presented in the context of the upgrading of the monochromatic D16 neutron beamline at the Institut Laue Langevin (ILL). Similar experiments were previously carried out on the D821 beamline at the ILL, where the neutron flux and detector sensitivity were poorer. A low resolution crystallography mode is under commissioning on D16 where users will use cold neutrons to collect neutron diffraction data on crystals of 0.01mm or smaller. The role of the technique in the modern structural biology scenario will be demonstrated: typical applications and sample environment will be described, namely for membrane proteins where contrast variation is used to study areas in contact with the membrane in vivo. Obtaining suitable crystals of membrane proteins is still a challenge and information on the packing of detergent and membrane proteins in the crystal will be a significant contribution to filling an historical gap between crystallography and membrane proteins.

Keywords: neutron, contrast-variation, crystallography

MS.87.1


Handedness of two-fold helices and chiral space-groups
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We have not so far discussed about right- or left-handedness of enantiomeric assemblies with two-fold helices. In fact, a two-fold helical axis with 180 degrees rotation and translation has only a symbol P, while a distinguishable three-fold helical axis has two symbols; 3, for a right-handed helix and 3, for a left-handed helix. In daily life, one can use right- or left-handed stairs. When one walks upstairs, turns to the left on staircase landing, and further go upstairs, the stairs can be recognized to be right-handed. The reverse right-turn yields left-handed stairs.

We investigated supramolecular chirality for 1D assemblies of benzene molecules. Benzene molecules form right-handed 2, helical assembly with side-to-side contact in channels of inclusion crystals of cholic acid [1]. It was confirmed that polymorphic crystals of benzene itself have 2, helical assemblies with two and three kinds of molecular contacts for P2, c and Pbc, respectively. Moreover, we analyzed 1D hydrogen bonding networks of primary ammonium carboxylates. The networks have 2, helical connection among nitrogen and oxygen [2].

We termed such enantiomeric relation of the two-fold helices as supramolecular tilt chirality [3], [4]. This handedness definition has consistency with the helical discrimination for polymeric materials such as DNA and proteins. It is no doubt that a large amount of organic crystals consist of molecular assemblies with right- or left-handed helices, likewise biopolymers. The Cambridge Structural Database involves over 500,000 data till 2011. Among them, over seventy percent have space groups with two-fold helices. Moreover, it was found that supramolecular chirality lies in each step of hierarchical structures, such as helical molecular assemblies, bundles of the helices, complimentary helical assemblies of host and guest components.

In the crystallographic theory, the concept of both point groups and space groups in mathematics is described as assemblies of points, where materials are approximated as a single point. The theory based on one-point approximation is surely correct in the case of atoms and ions with spherical symmetry, but is not considered to be always correct in the case of molecules, particularly, organic molecules with various shapes. These molecules require multi-point approximation methods instead of the one-point method. Now we know that a two- and three- point approximation method enables us to discriminate right- or left-handedness of 2, helical assemblies.

Among 65 chiral space-groups, only eleven groups are split into the enantiomeric pairs, while the remaining 43 groups are not split into the pairs. This mainly comes from the crystallographic theory that two-fold rotations have no handedness. We checked handedness of space-groups involving 2, 4-, 6-, 2, 3-, 6-, 4-, six-rotations as well as asymmetric P1 group with multipoint approximation methods. As a result, the 43 chiral space-groups were found to be split into the enantiomeric pairs.

Keywords: organic crystal, helical structure, space groups

MS.87.2


Molecular building block approach to chiral coordination polymers and noncovalent porous materials
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Among the vast library of building blocks simple achiral bipyridines are the most commonly used linkers for constructing metal-organic frameworks (MOFs), but their chiral derivatisation have encountered difficulties. Therefore, developing versatile strategies for facile generation of chiral bipyridine-type ligands is the key challenge for

Keywords: organic crystal, helical structure, space groups